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Spectral Determinant on Quantum Graphs

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We study the spectral determinant of the Laplacian on finite graphs characterized by their number of vertices V and bonds B. We present a path integral derivation which leads to two equivalent expressions of the spectral determinant of the Laplacian in terms of either a $V \times V$ vertex matrix or a $2B \times 2B$ link matrix that couples the arcs (oriented bonds) together. This latter expression allows us to rewrite the spectral determinant as an infinite product of contributions of periodic orbits on the graph. We also present a diagrammatic method that permits us to write the spectral determinant in terms of a finite number of periodic orbit contributions. These results are generalized to the case of graphs in a magnetic field. Several examples illustrating this formalism are presented and its application to the thermodynamic and transport properties of weakly disordered and coherent mesoscopic networks is discussed. © 2000 Academic Press

1. INTRODUCTION AND MAIN RESULTS

This work is devoted to the study of the spectral properties of the Laplacian operator on finite graphs. This problem already has a long history. The properties

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of the Laplacian describing free electrons on networks made of one-dimensional wires have been investigated in the context of organic molecules [1]. Subsequently, this approach has proved useful for studying superconducting networks using linearized Ginzburg–Landau equations [2], the vibration properties of fractal structures such as the Sierpinski gasket [3], the adiabatic conductances of a network in an inhomogeneous magnetic field [4, 5], or the behavior of disordered systems in a magnetic field [6–11]. More recently, it has been shown [12–14] that the Laplacian on graphs provides an interesting framework for studying the onset of quantum manifestations of chaos. In these examples, the quantity of main interest is the spectrum of eigenenergies of the Schrödinger equation, or the diffusion equation, defined for each wire of the network with appropriate boundary conditions at the vertices. Finally we should also mention the relevance of the spectral determinant of the Laplacian on graphs in the context of statistical field theory and more precisely for the problem of the triangulation of random surfaces. There, the corresponding homology and (dual) cohomology groups provide the corresponding graphs over which the Laplacian is defined [15].

The problem of the spectrum of graphs has been also investigated thoroughly in the mathematical literature [16–20a]. The more specific question of deriving a trace formula for the heat kernel (partition function) of the Laplacian operator on a graph has been studied by Roth [21, 22].

Let us start by recalling some already known results. The partition function $Z(t)$ of the scalar Laplacian operator Δ with appropriate boundary conditions is defined as

$$Z(t) = \mathrm{Tr}\{e^{t\Delta}\}. \tag{1}$$

Evaluating the trace over a set of eigenstates of $-\Delta$ of eigenvalues E_n, we obtain

$$Z(t) = \sum_n e^{-E_n t}. \tag{2}$$

The spectral determinant $S(\gamma)$ is formally defined by $S(\gamma) = \det(-\Delta + \gamma) = \prod_n (\gamma + E_n)$ up to a regularization independent of γ. It is such that

$$\int_0^\infty dt\, Z(t)\, e^{-\gamma t} = \frac{\partial}{\partial \gamma} \ln S(\gamma). \tag{3}$$

On a graph in the presence of a magnetic field, a compact form for the determinant of the operator $\gamma - (d_x - iA(x))^2$ has recently been obtained [11],

$$S(\gamma) = \gamma^{(V-B)/2} \prod_{(\alpha\beta)} \mathrm{sh}(\sqrt{\gamma}\, l_{\alpha\beta})\, \det(M), \tag{4}$$

where V is the number of vertices, B is the number of bonds, and $l_{\alpha\beta}$ is the length of the bond $(\alpha\beta)$. M is a $V \times V$ matrix whose elements are [2, 6, 7, 11]

$$M_{\alpha\alpha} = \sum_{i=1}^{m_\alpha} \coth(\sqrt{\gamma}\, l_{\alpha\beta_i}) \tag{5}$$

$$M_{\alpha\beta} = -\frac{e^{i\theta_{\alpha\beta}}}{\mathrm{sh}(\sqrt{\gamma}\, l_{\alpha\beta})} \qquad \text{if} \quad (\alpha\beta) \text{ is a bond}$$

$$= 0 \qquad \text{otherwise,} \tag{6}$$

where the summation is taken over the m_α neighboring sites of the vertex α. $\theta_{\beta\alpha} = \int_\alpha^\beta A(x)\, \mathrm{d}x$ is a phase equal to the circulation of the vector potential $A(x)$ along the bonds $(\alpha\beta)$. This expression has been obtained by a calculation of Green's function on the graph. The derivation is recalled in Appendix A.

Although it is well known that the spectrum of the Laplacian on a graph is given by the zeros of $\det(M(\gamma = -E)) = 0$ [1, 2, 5], formula (4) is richer since it contains non-trivial multiplicative factors which depend on γ. If the relation of $S(\gamma)$ to the matrix $M(\gamma)$ allows a very simple determination of the spectrum, it cannot help to understand the structure of the spectrum in terms of periodic orbits on the graph. To do so, it is more convenient to introduce a "link matrix" E whose elements $E_{(\alpha\beta)(\mu\nu)}$ relate oriented bonds $(\alpha\beta)$ and $(\mu\nu)$. This $2B \times 2B$ matrix is defined as[1]

$$E_{(\alpha\beta)(\mu\nu)} = \frac{2}{m_\beta} e^{-\sqrt{\gamma}\, l_{\alpha\beta} + i\theta_{\alpha\beta}} \qquad \text{if} \quad \beta = \mu \tag{7}$$

$$= \left(\frac{2}{m_\beta} - 1\right) e^{-\sqrt{\gamma}\, l_{\alpha\beta} + i\theta_{\alpha\beta}} \qquad \text{if} \quad \begin{cases} \beta = \mu \\ \alpha = \nu \end{cases} \tag{8}$$

$$= 0 \qquad \text{otherwise.} \tag{9}$$

The spectrum is now given by $\det(1 - E(\gamma)) = 0$. The trace expansion of $\det(1 - E)$ leads to a description of the spectrum in terms of periodic orbits [13].

Finally, a trace formula has been obtained by Roth, which expresses the partition function as a contribution of such periodic orbits,

$$Z(t) = \frac{L}{2\sqrt{\pi t}} + \frac{V - B}{2} + \frac{1}{2\sqrt{\pi t}} \sum_C l(\tilde{C})\, \alpha(C)\, e^{-l(C)^2/4t}, \tag{10}$$

where the sum runs over closed orbits C on the graph. $\tilde{C}$ is the primitive orbit associated with C. The geometrical factor $\alpha(\tilde{C})$ will be defined in Section 6.

We now give an overview of the paper and describe rapidly our main results. In Section 2 we recall briefly how transport and thermodynamic properties of weakly disordered and coherent conductors can be related to the spectral determinant [8–10].

[1] The matrix E is the same as the matrix S_B in [13].

In particular the weak-localization correction to the conductance is a physical measure of the spectral determinant.

After having set up the notation and definitions in Section 3, we present in Section 4 a path integral formulation for the calculation of the spectral determinant of the Laplacian on a graph. It allows us to obtain an expression of the spectral determinant in terms of the vertex matrix (5) and (6). The interest of this approach relies on the fact that the path integral on each bond involves the propagator of a two-dimensional harmonic oscillator for which the role of time is played by the length along the bond. This problem corresponds to a zero-dimensional Gaussian field theory, so that the path integral is easily calculated using standard quantum mechanics. This approach has many advantages, such as allowing a simple generalization to other types of boundary conditions, or permitting very easily the elimination of vertices of coordination 2 (Appendix C).

In Section 5, we derive a dual and equivalent expression of the spectral determinant in terms of the link matrix (7) and (8):

$$S(\gamma) = \gamma^{(V-B)/2} e^{\sqrt{\gamma} L} \left(\prod_{\alpha} m_{\alpha} \right) 2^{-B} \det(1 - E(\gamma)). \tag{11}$$

By a trace expansion of the determinant $\det(1 - E)$, we find in Section 6 the result

$$S(\gamma) = \gamma^{(V-B)/2} e^{\sqrt{\gamma} L} \left(\prod_{\alpha} m_{\alpha} \right) 2^{-B} \prod_{\tilde{C}} (1 - \alpha(\tilde{C})\, e^{-\sqrt{\gamma}\, l(\tilde{C}) + i\theta(\tilde{C})}), \tag{12}$$

which allows us to recover the Roth trace formula for the partition function (10), demonstrating the equivalence between (4) and (10). The trace formula (12) for the spectral determinant involves the contribution of an infinite number of periodic orbits $\tilde{C}$ and bears some similarity to the Selberg trace formula [23] or the semiclassical trace formulae for chaotic Hamiltonian systems [24]. In Section 7 we show that the spectral determinant involves the contributions of a finite number of periodic orbits only. This provides a diagrammatic method for computing the determinant. This method is applied to a particular example.

In Section 8 the path integral formulation is shown to be a good starting point for generalizing these results to the case where a magnetic field is applied to the network. In this way we obtain a generalization of the Roth formula (10). Sections 9 and 10 discuss how to extend the previous results to the case of more general boundary conditions, and provide a discussion of the low-energy behavior of the spectrum and the existence of zero modes, respectively.

Section 11 discusses the scattering problem when the graph is connected to an infinite lead. In this case the relevant information is contained in a phase shift which is shown to be related to the ratio of two spectral determinants calculated with different boundary conditions. Finally, Section 12 gives an illustration of the formalism for the case of the complete graph K_n.

2. PHASE COHERENT PROPERTIES OF DISORDERED CONDUCTORS

In this section, we briefly recall how transport and thermodynamic properties of weakly disordered and coherent conductors can be related to the partition function $Z(t)$ or equivalently to the spectral determinant $S(\gamma)$. A more detailed derivation can be found in Refs. [8–10] and references therein. These expressions are quite general and are not specific to graphs. But their calculation on any network made of quasi-one-dimensional diffusive wires is straightforward with expression (4) [11].

The first step is to write the physical quantities in terms of the classical return probability $P(\mathbf{r}, \mathbf{r}, t)$ solution of the diffusion equation (we set $\hbar = c = 1$)

$$\left[\frac{\partial}{\partial t} - D(\nabla + 2ie\mathbf{A})^2\right] P(\mathbf{r}, \mathbf{r}', t) = \delta(\mathbf{r} - \mathbf{r}'), \tag{13}$$

where $-e$ is the electron charge and D is the diffusion coefficient. In the other sections of this paper, we have set $-2e = 1$ and $D = 1$. The return probability has actually two contributions, a purely classical P_{cl} which is the solution to Eq. (13) with $\mathbf{A} = 0$ and another one P_{int} which is the result of constructive interferences between electronic propagators associated with time-reversed trajectories. This second contribution exists only when the system is phase coherent. In the presence of a magnetic field, time-reversed trajectories accumulate opposite phases. This is why P_{int} obeys Eq. (13) with an effective charge $2e$ [25]. In this section, we use a unique notation for the two contributions.

The solution of the diffusion equation (13) has the form

$$P(\mathbf{r}, \mathbf{r}', t) = \theta_{\text{H}}(t) \sum_n \psi_n(\mathbf{r})\, \psi_n^*(\mathbf{r}')\, e^{-E_n t}, \tag{14}$$

where $\theta_{\text{H}}(t)$ is the Heaviside function. The eigenvalues E_n and the eigenfunctions ψ_n are solutions of

$$-D(\nabla + 2ie\mathbf{A})^2 \psi_n(\mathbf{r}) = E_n \psi_n(\mathbf{r}). \tag{15}$$

The integral over the whole space of the return probability is precisely the partition function of the Laplace operator $-\Delta$, or $-(\nabla + 2ie\mathbf{A})^2$ in a magnetic field, namely

$$Z(t) = \int \mathrm{d}\mathbf{r}\, P(\mathbf{r}, \mathbf{r}, t) = \sum_n e^{-E_n t}. \tag{16}$$

As recalled in the Introduction (Eq. (3)), the Laplace transform of $Z(t)$ is related to the spectral determinant $S(\gamma)$.

The electrical conductivity is a current–current correlation function and is expressed in terms of products of two electron propagators. These propagators have uncorrelated phase factors which cancel after disorder averaging. This corresponds to the classical Drude–Boltzmann conductivity $\sigma_0 = e^2 D \rho_0$, where ρ_0 is the density of states at Fermi energy. However, pairs of time-reversed trajectories have the same action

and thus the same phase. This constructive interference leads to an additional contribution to the conductivity, called the weak-localization correction [25], which is proportional to the probability of having pairs of time reversed trajectories, i.e., to the probability for a diffusive particle to return to the origin. The correction can be written as

$$\langle \Delta\sigma \rangle = \langle \sigma \rangle - \sigma_0 = -\frac{2e^2}{\pi}\frac{D}{\Omega}\int_0^\infty \mathrm{d}t\, Z(t)\, e^{-\gamma t} \tag{17}$$

with Ω being the volume of the system. The exponential damping at large time is due to the breakdown of phase coherence because of inelastic processes. This breakdown is phenomenologically described by a characteristic time $\tau_\phi = 1/\gamma$, related to the phase coherence length[2] $L_\phi = \sqrt{D\tau_\phi}$. A magnetic field or an Aharonov–Bohm flux, by breaking the time-reversal symmetry, destroys the weak-localization correction.

In a mesoscopic system, i.e., with a typical size L smaller than L_ϕ, the conductivity is known to exhibit large variations from sample to sample, with a variance which is universal in the limit $L/L_\phi \to 0$ and for a sample perfectly connected to leads. The structure of this variance results from different phase correlations between four electron propagators (two for each conductance). It can be shown that this variance can also be written in the following compact form [9],

$$\langle \delta\sigma^2 \rangle = \frac{12e^4}{\beta\pi^2}\frac{D^2}{\Omega^2}\int_0^\infty \mathrm{d}t\, t\, Z(t)\, e^{-\gamma t}, \tag{18}$$

where $\beta = 1$ if there is time-reversal symmetry and $\beta = 2$ in the absence of such symmetry.

The magnetization due to the orbital motion of the non-interacting electron gas is known as the Landau magnetization. Taking into account electron–electron interactions in the Hartree–Fock picture gives an additional contribution, known as the Aslamasov–Larkin correction [26]. The structure of this correction implies the product of four wave functions, i.e., two local density of states whose disorder-averaged product can be related to the Fourier transform of the return probability $P(\mathbf{r}, \mathbf{r}, t)$ [27]. After spatial integration, one gets

$$\langle M_{ee} \rangle = -\frac{\lambda_0}{\pi}\frac{\partial}{\partial \mathscr{B}}\int_0^\infty dt\, Z(t, \mathscr{B})\frac{e^{-\gamma t}}{t^2}, \tag{19}$$

where λ_0 is the dimensionless interaction parameter.[3] $\mathscr{B} = \nabla \times \mathbf{A}$ is the magnetic field.

[2] Integrals (17)–(20) may not converge at small time. In this case the lower bound of the integral should be the elastic time τ_e, the smallest time for diffusion.

[3] Considering higher corrections in the Cooper channel leads to a ladder summation [26, 28], so that λ_0 should be replaced by $\lambda(t) = \lambda_0/(1 + \lambda_0 \ln(\varepsilon_F t)) = 1/\ln(T_0 t)$, where T_0 is defined as $T_0 = \varepsilon_F e^{1/\lambda_0}$. The authors of Ref. [29] found $\lambda(t) = 1/\ln(\varepsilon_F t)$.

Finally the fluctuations of the magnetization $\langle \delta M^2 \rangle$, defined as $\langle \delta M^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2$, can also be written in terms of field derivatives of $Z(t)$. Neglecting electron–electron interactions, the magnetization is proportional to the density of states. Thus the fluctuations of the magnetization involve the two-point correlation function of the density of states which has been shown by Argaman *et al.* [30] to be related to the Fourier transform of $tZ(t)$. One obtains

$$\langle \delta M^2 \rangle = \frac{1}{2\pi^2} \int_0^\infty dt \, [Z''(t, \mathscr{B}) - Z''(t, 0)] \, \frac{e^{-\gamma t}}{t^3}, \tag{20}$$

where $Z''(t, \mathscr{B}) = \partial^2 Z(t, \mathscr{B})/\partial \mathscr{B}^2$.

Using standard properties of Laplace transforms, the above time integrals can be written as integrals of the logarithm of the spectral determinant, so that the physical quantities described above can be written as [11]

$$\langle \Delta\sigma \rangle = -\frac{2e^2}{\pi} \frac{D}{\Omega} \frac{\partial}{\partial \gamma} \ln S(\gamma) \tag{21}$$

$$\langle \delta\sigma^2 \rangle = -\frac{12e^4}{\beta\pi^2} \frac{D^2}{\Omega^2} \frac{\partial^2}{\partial \gamma^2} \ln S(\gamma) \tag{22}$$

$$\langle \delta M^2 \rangle = \frac{1}{2\pi^2} \int_\gamma^\infty d\gamma_1 (\gamma - \gamma_1) \frac{\partial^2}{\mathscr{B}^2} \ln S(\gamma_1)|_0^{\mathscr{B}} \tag{23}$$

$$\langle M_{ee} \rangle = \frac{\lambda_0}{\pi} \int_\gamma^\infty d\gamma_1 \frac{\partial}{\partial \mathscr{B}} \ln S(\gamma_1). \tag{24}$$

When the integrals do not converge at the upper limit, this limit should be taken as $1/\tau_e$, where τ_e is the elastic time.

3. DEFINITIONS AND NOTATION

Consider a graph $\mathscr{G}$ which consists of a set of V vertices linked by B bonds. Its adjacency matrix $a_{\alpha\beta}$ is a square matrix of size V, where $a_{\alpha\beta} = 1$ if a bond joins the vertices α and β and 0 otherwise (in particular $a_{\alpha\alpha} = 0$).[4] The coordination of vertex α is $m_\alpha = \sum_\beta a_{\alpha\beta}$. Each bond $(\alpha\beta)$ of length $l_{\alpha\beta}$ is identified with a finite interval $[0, l_{\alpha\beta}] \in \mathbb{R}$. The total length of $\mathscr{G}$ is $L = \sum_{\text{bonds}(\alpha\beta)} l_{\alpha\beta} = \frac{1}{2} \sum_{\alpha,\beta} a_{\alpha\beta} l_{\alpha\beta}$. We denote by $x_{\alpha\beta}$ the coordinate on the bond $(\alpha\beta)$, starting from vertex α (it follows that $x_{\beta\alpha} = l_{\alpha\beta} - x_{\alpha\beta}$). A scalar function on $\mathscr{G}$ is a set of B-component functions $\psi_{(\alpha\beta)}(x_{\alpha\beta})$.

[4] If a given pair of vertices is linked by $n > 1$ bonds, it is always possible to introduce additional vertices (see Fig. 9), without changing the nature of the graph, to go back to a situation where there is only one bond between two vertices. However, the formalism that is presented in this paper can be easily generalized to avoid this procedure and minimize the number of vertices by suppressing all vertices with coordination 2. It is the purpose of Appendix C to discuss this point.

When there is no possible ambiguity we will neglect to label the components. The Laplacian on $\mathcal{G}$ acts as the usual one-dimensional Laplace operator on each bond:

$$(\Delta\psi)_{(\alpha\beta)} = \frac{d^2}{dx_{\alpha\beta}^2}\psi_{(\alpha\beta)}(x_{\alpha\beta}). \tag{25}$$

Its domain is the set of functions that satisfy the following conditions at the vertices:

(i) continuity

$$\psi_{(\alpha\beta_i)}(x_{\alpha\beta_i}=0) = \psi_\alpha \qquad \text{for} \quad i=1, ..., m_\alpha; \tag{26}$$

(ii) a second condition sufficient to ensure current conservation

$$\sum_{i=1}^{m_\alpha} d_{x_{\alpha\beta_i}}\psi_{(\alpha\beta_i)}(x_{\alpha\beta_i}=0) = 0, \tag{27}$$

where $d_x \equiv d/dx$ and the β_i's label the m_α neighboring vertices of vertex α. The scalar product is defined as

$$\langle\psi\,|\,\varphi\rangle = \sum_{(\alpha\beta)}\int_0^{l_{\alpha\beta}} dx\,\psi^*_{(\alpha\beta)}(x)\,\varphi_{(\alpha\beta)}(x). \tag{28}$$

In the search for the eigenvalues of the Laplacian, one may construct the wave function of energy $E=k^2$ in such a way that condition (i) is satisfied: $\psi_{(\alpha\beta)} = (1/\sin kl_{\alpha\beta})(\psi_\alpha \sin k(l_{\alpha\beta}-x_{\alpha\beta}) + \psi_\beta \sin kx_{\alpha\beta})$. Imposing condition (ii) leads to the system of V equations $\sum_\beta M_{\alpha\beta}(\gamma=-k^2)\,\psi_\beta = 0$, where M is given by (5) and (6). The eigenvalues of the Laplacian are solutions of $\det(M(\gamma=-E))=0$ [1, 2, 5, 13].

It is useful to introduce some additional notions. An *arc*$(\alpha\beta)$ is defined as the oriented bond from α to β. Each bond is therefore associated with two arcs. A *path* on $\mathcal{G}$ is an ordered sequence of arcs such that the end of each arc coincides with the beginning of the one that immediately follows in the sequence. Closed paths will play a special role. The set of closed paths that only differ by a cyclic permutation of the arcs will be called a *circuit* (or an *orbit*). Among all possible circuits we will distinguish those that are *primitive*. A circuit is said to be primitive if it cannot be decomposed as a repetition of any smaller circuit. The length of a circuit C will be designated by $l(C)$.

As an example, let us consider the graph of Fig. 1. This graph contains six arcs: 1, 2, 3 and the reversed arcs $\bar{1}$, $\bar{2}$, $\bar{3}$. $(1, \bar{1}, 2, \bar{2})$ and $(2, \bar{2}, 1, \bar{1})$ are two different paths, two possible representations of the same circuit. $(1, \bar{1}, 1, \bar{1}, 1, \bar{1})$ is not a primitive circuit but $(1, \bar{1}, 1, \bar{1}, 1, \bar{1}, 2, \bar{2})$ is indeed primitive.

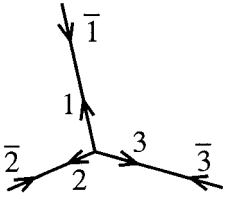


FIG. 1. A graph with four vertices, three bonds, and six arcs.

4. A PATH INTEGRAL DERIVATION OF THE SPECTRAL DETERMINANT

An expression of the spectral determinant $S(\gamma) = \det(-\Delta + \gamma)$ in terms of the determinant of a finite matrix has been derived in [11, 10] (cf. Appendix A). The purpose of this section is to provide a more direct derivation of this result using a path integral formulation. The spectral determinant may be written as

$$S(\gamma) = \det(-\Delta + \gamma) = \left(\int_{\phi \text{ on Graph}} \mathscr{D}\phi\, \mathscr{D}\bar{\phi}\, e^{-(1/2)\int_{\text{Graph}} \bar{\phi}(-\Delta+\gamma)\phi} \right)^{-1}, \tag{29}$$

where ϕ is a complex field defined on the graph $\mathscr{G}$. The path integral is performed over all fields satisfying the conditions (26) and (27) and the integral in the exponential along all branches of $\mathscr{G}$. Since the field is continuous at each vertex the path integral may be decomposed on each bond $(\alpha\beta)$ as an integration over fields that take fixed values ϕ_α and ϕ_β on the two sides of the bond

$$S(\gamma)^{-1} = \int \prod_{\text{vertices } \alpha} d\phi_\alpha\, d\bar{\phi}_\alpha \times \prod_{\substack{\text{bonds} \\ (\alpha\beta)}} \int_{\phi(0)=\phi_\alpha}^{\phi(l_{\alpha\beta})=\phi_\beta} \mathscr{D}\phi\, \mathscr{D}\bar{\phi}\, e^{-(1/2)\int_0^{l_{\alpha\beta}} dx\, \bar{\phi}(x)(-d_x^2+\gamma)\phi(x)}, \tag{30}$$

where $d\phi\, d\bar{\phi} = d\,\mathrm{Re}\,\phi\, d\,\mathrm{Im}\,\phi$. This involves, after an integration by parts, the quantity[5]

$$\prod_{(\alpha\beta)} \int_{\phi(0)=\phi_\alpha}^{\phi(l_{\alpha\beta})=\phi_\beta} \mathscr{D}\phi \mathscr{D}\bar{\phi}\, e^{(1/2)\bar{\phi} d_x\phi|_0^{l_{\alpha\beta}}} e^{-(1/2)\int_0^{l_{\alpha\beta}} dx(|d_x\phi|^2+\gamma|\phi|^2)}$$
$$= \exp\left(-\tfrac{1}{2} \sum_{\alpha=1}^{V} \bar{\phi}_\alpha \sum_{i=1}^{m_\alpha} d_{x_{\alpha\beta_i}} \phi(x_{\alpha\beta_i} = 0) \right)$$
$$\times \prod_{(\alpha\beta)} \int_{\phi(0)=\phi_\alpha}^{\phi(l_{\alpha\beta})=\phi_\beta} \mathscr{D}\phi\, \mathscr{D}\bar{\phi}\, e^{-(1/2)\int_0^{l_{\alpha\beta}} dx(|d_x\phi|^2+\gamma|\phi|^2)}. \tag{31}$$

[5] The notation $\sum_{(\alpha\beta)} \cdots$ and $\prod_{(\alpha\beta)} \cdots$ means, throughout this paper, a summation or a product over bonds (and not arcs).

For the sum of boundary terms in the exponential we have replaced the sum over the bonds by a sum over the vertices, a trick that will be frequently used throughout the rest of this paper. Equation (27) implies that the boundary terms vanish. The above path integral, involving a zero-dimensional Gaussian field theory, can easily be integrated out using standard quantum mechanical techniques. On each bond the path integral can be expressed in terms of the propagator of a two-dimensional harmonic oscillator of frequency $\omega = \sqrt{\gamma}$

$$\mathcal{N}_r^{-1} \int_{\phi(0)=\phi_\alpha}^{\phi(l_{\alpha\beta})=\phi_\beta} \mathcal{D}\phi\, \mathcal{D}\bar{\phi}\, e^{-(1/2)\int_0^{l_{\alpha\beta}} dx\, (|d_x\phi|^2 + \gamma\, |\phi|^2)}$$

$$= G_{l_{\alpha\beta}}^{\omega=\sqrt{\gamma}}(\boldsymbol{\phi}_\beta, \boldsymbol{\phi}_\alpha) = \langle \boldsymbol{\phi}_\beta |\, e^{-(l_{\alpha\beta}/2)(-\nabla_\phi^2 + \gamma \boldsymbol{\phi}^2)}\, | \boldsymbol{\phi}_\alpha \rangle, \tag{32}$$

where $\boldsymbol{\phi} = (\mathrm{Re}\,\phi, \mathrm{Im}\,\phi)$ and $\mathcal{N}_r$ is a constant independent of γ depending on the precise normalization chosen in the definition of the path integral, or in other terms on the choice of regularization made to define the determinant. In the following we will drop this inessential normalization constant. Using the expression of the propagator [31]

$$G_x^\omega(\boldsymbol{\phi}, \boldsymbol{\phi}') = \frac{\omega}{2\pi\, \mathrm{sh}(\omega x)}\, e^{-(\omega/2\, \mathrm{sh}(\omega x))(\mathrm{ch}(\omega x)(\boldsymbol{\phi}^2 + \boldsymbol{\phi}'^2) - 2\boldsymbol{\phi}\cdot\boldsymbol{\phi}')} \tag{33}$$

one may re-scale the fields ϕ_α to extract a γ-dependent factor,

$$S(\gamma)^{-1} = \gamma^{(B-V)/2} \int \prod_{\alpha=1}^{V} d\phi_\alpha\, d\bar{\phi}_\alpha \prod_{(\alpha\beta)} G_{\sqrt{\gamma}\, l_{\alpha\beta}}(\boldsymbol{\phi}_\beta, \boldsymbol{\phi}_\alpha), \tag{34}$$

where $G_x(\boldsymbol{\phi}, \boldsymbol{\phi}') \equiv G_x^{\omega=1}(\boldsymbol{\phi}, \boldsymbol{\phi}')$. This expression will be used as a starting point for the derivation of the following section. Using the $V \times V$ matrix M introduced in Section 1

$$M_{\alpha\alpha} = \sum_{i=1}^{m_\alpha} \coth(\sqrt{\gamma}\, l_{\alpha\beta_i}) \tag{35}$$

$$M_{\alpha\beta} = -\frac{1}{\mathrm{sh}(\sqrt{\gamma}\, l_{\alpha\beta})} \qquad \text{if} \quad (\alpha\beta) \text{ is a bond}$$

$$= 0 \qquad \text{otherwise,} \tag{36}$$

we may express the determinant as

$$S(\gamma)^{-1} = \gamma^{(B-V)/2} \prod_{(\alpha\beta)} \frac{1}{2\pi\, \mathrm{sh}(\sqrt{\gamma}\, l_{\alpha\beta})} \int \left(\prod_{\alpha=1}^{V} d\phi_\alpha\, d\bar{\phi}_\alpha \right) e^{-(1/2)\sum_{\alpha,\beta} \bar{\phi}_\alpha M_{\alpha\beta} \phi_\beta}. \tag{37}$$

After performing the integration over ϕ_α one finds

$$S(\gamma) = \left(\frac{\sqrt{\gamma}}{2\pi}\right)^{V-B} \prod_{(\alpha\beta)} \mathrm{sh}(\sqrt{\gamma}\, l_{\alpha\beta}) \det(M), \tag{38}$$

which is the expression given in [11] (see Appendix A) up to an inessential numerical factor $(2\pi)^{B-V}$ that will be dropped in the following.

5. THE SPECTRAL DETERMINANT IN TERMS OF THE LINK MATRIX

Equation (38) expresses the spectral determinant as the determinant of a finite $V \times V$ matrix. The matrix M describes the topology of the graph, telling us which vertices are coupled, and also contains the metric information. At this stage, the metric and topological information are inextricably mixed. The purpose of this section is to derive another expression of the spectral determinant in terms of the determinant of a $2B \times 2B$ matrix whose natural basis is the set of arcs (oriented bonds). An advantage of this formulation is that it leads to an expansion of the spectral determinant as a sum of terms that will be interpreted in the next section as the contribution of periodic orbits.

Our starting point is expression (34). Since the γ dependence of the determinant is simple, one may set $\gamma = 1$ and recover the γ dependence at the end. The first step is to find a more convenient expression of the propagator in (34). To begin let us consider the one-dimensional harmonic oscillator propagator $g_t(x, x') = \langle x|\, e^{-(t/2)(-d_x^2 + x^2)}\, |x'\rangle$. This propagator may be expanded over the eigenstates $\varphi_n(x) = (1/\pi^{1/4}\sqrt{2^n n!})\, H_n(x)\, e^{-(1/2)x^2}$ of energies $E_n = n + \frac{1}{2}$, where $H_n(x)$ are Hermite polynomials. Using the generating function of Hermite polynomials $\sum_{n=0}^{\infty} H_n(x)(\lambda^n/n!) = e^{2\lambda x - \lambda^2}$, the propagator may be rewritten as

$$g_{l_{\alpha\beta}}(x_\alpha, x_\beta) = \frac{e^{-l_{\alpha\beta}/2}}{\sqrt{\pi}}\, e^{-(1/2)(x_\alpha^2 + x_\beta^2)} \times \sum_{n=0}^{\infty} \frac{e^{-n l_{\alpha\beta}}}{2^n\, n!}\, \partial_{\lambda_{\alpha\beta}}^n e^{2x_\alpha \lambda_{\alpha\beta} - \lambda_{\alpha\beta}^2}\, \partial_{\lambda_{\alpha\beta}}^n e^{2x_\beta \lambda_{\beta\alpha} - \lambda_{\beta\alpha}^2} |_{\lambda_{\alpha\beta},\, \lambda_{\beta\alpha} = 0}\,. \tag{39}$$

A re-summation of the series gives

$$g_{l_{\alpha\beta}}(x_\alpha, x_\beta) = \frac{e^{-l_{\alpha\beta}/2}}{\sqrt{\pi}}\, e^{-(1/2)(x_\alpha^2 + x_\beta^2)} e^{(1/2)\, e^{-l_{\alpha\beta}} \partial_{\lambda_{\alpha\beta}} \partial_{\lambda_{\beta\alpha}}} e^{2x_\alpha \lambda_{\alpha\beta} + 2x_\beta \lambda_{\beta\alpha} - \lambda_{\alpha\beta}^2 - \lambda_{\beta\alpha}^2} |_{\lambda_{\alpha\beta},\, \lambda_{\beta\alpha} = 0}\,. \tag{40}$$

Writing the two-dimensional propagator as a product of one-dimensional propagators $G_{l_{\alpha\beta}}(\mathbf{r}_\alpha, \mathbf{r}_\beta) = g_{l_{\alpha\beta}}(x_\alpha, x_\beta)\, g_{l_{\alpha\beta}}(y_\alpha, y_\beta)$ one is led to an analogous expression for $G_{l_{\alpha\beta}}(\mathbf{r}_\alpha, \mathbf{r}_\beta)$. For each bond one has to introduce two couples of variables $(\lambda_{\alpha\beta}, \lambda_{\beta\alpha})$

and $(\lambda'_{\alpha\beta}, \lambda'_{\beta\alpha})$ associated to x_α, x_β and y_α, y_β respectively. Using the complex notations $z_\alpha = x_\alpha + iy_\alpha$ and $\Lambda_{\alpha\beta} = \lambda_{\alpha\beta} + i\lambda'_{\alpha\beta}$ (one recalls that $\partial_z = \frac{1}{2}(\partial_x - i\partial_y)$) one eventually finds

$$G_{l_{\alpha\beta}}(z_\alpha, z_\beta) = \frac{e^{-l_{\alpha\beta}}}{\pi} e^{-(1/2)(|z_\alpha|^2 + |z_\beta|^2)} \mathcal{O}_{\alpha\beta} e^{z_\alpha \bar{\Lambda}_{\alpha\beta} + \bar{z}_\alpha \Lambda_{\alpha\beta} + z_\beta \bar{\Lambda}_{\beta\alpha} + \bar{z}_\beta \Lambda_{\beta\alpha} - |\Lambda_{\alpha\beta}|^2 - |\Lambda_{\beta\alpha}|^2}, \tag{41}$$

where $\mathcal{O}_{\alpha\beta}$ is the operator:

$$\mathcal{O}_{\alpha\beta} = \exp(e^{-l_{\alpha\beta}}(\partial_{\Lambda_{\alpha\beta}} \partial_{\bar{\Lambda}_{\beta\alpha}} + \partial_{\bar{\Lambda}_{\alpha\beta}} \partial_{\Lambda_{\beta\alpha}}))|_{\Lambda_{\alpha\beta}, \Lambda_{\beta\alpha} = 0}. \tag{42}$$

Equation (41) shows that one has to introduce two variables $\Lambda_{\alpha\beta}$ and $\Lambda_{\beta\alpha}$ per propagator in (34); i.e., each arc$(\alpha\beta)$ is associated with a $\Lambda_{\alpha\beta}$.

From (34) and (41) it follows that

$$S(\gamma = 1)^{-1} = 2^{B-V} \frac{e^{-L}}{\pi^V} \mathcal{O} \left[\prod_{(\alpha\beta)} (e^{-|\Lambda_{\alpha\beta}|^2 - |\Lambda_{\beta\alpha}|^2}) \times \int \prod_\alpha (d\phi_\alpha \, d\bar{\phi}_\alpha \, e^{-(1/2) m_\alpha |\phi_\alpha|^2 + \sum_{i=1}^{m_\alpha} (\phi_\alpha \bar{\Lambda}_{\alpha\beta_i} + \bar{\phi}_\alpha \Lambda_{\alpha\beta_i})}) \right], \tag{43}$$

where the operator $\mathcal{O} = \prod_{(\alpha\beta)} \mathcal{O}_{\alpha\beta}$ is understood as acting on both terms that follow it (one has multiplied (34) by the numerical factor $(2\pi)^{V-B}$ to make it disappear in the final result). Again, one has replaced in (34) the product over bonds by a product over vertices. Integration over ϕ_α is then straightforward and leads to

$$S(\gamma = 1)^{-1} = \frac{2^B e^{-L}}{\prod_\alpha m_\alpha} \mathcal{O} e^{\Lambda^\dagger Q \Lambda}, \tag{44}$$

where Λ is the $2B$-component complex vector

$$\Lambda = \begin{pmatrix} \Lambda_{1\alpha_1} \\ \vdots \\ \Lambda_{1\alpha_{m_1}} \\ \hline \Lambda_{2\beta_1} \\ \vdots \\ \Lambda_{2\beta_{m_2}} \\ \hline \vdots \end{pmatrix} \tag{45}$$

and

$$\Lambda^\dagger = (\bar{\Lambda}_{1\alpha_1} \ \cdots \ \bar{\Lambda}_{1\alpha_{m_1}} \mid \bar{\Lambda}_{2\beta_1} \ \cdots \ \bar{\Lambda}_{2\beta_{m_2}} \mid \cdots), \tag{46}$$

in which the $\Lambda_{\alpha\beta}$ are grouped by vertices. The first group $(\Lambda_{1\alpha_1}, ..., \Lambda_{1\alpha_{m_1}})$ is related to the m_1 arcs $\alpha_1, \alpha_2, ..., \alpha_{m_1}$ issuing from vertex $\alpha = 1$. In this basis, Q is a $2B \times 2B$

block diagonal matrix (with V blocks); it couples only arcs that start from the same vertex

$$Q = \left(\begin{array}{c|c|c|c|c} Q_1 & 0 & 0 & \cdots & 0 \\ \hline 0 & Q_2 & 0 & \cdots & 0 \\ \hline 0 & 0 & Q_3 & \cdots & 0 \\ \hline \vdots & \vdots & \vdots & \ddots & \vdots \\ \hline 0 & 0 & 0 & \cdots & Q_V \end{array} \right), \tag{47}$$

where each $m_\alpha \times m_\alpha$ sub-matrix Q_α attached to a given vertex α has $(2/m_\alpha) - 1$ on its diagonal and $2/m_\alpha$ everywhere else. Using a tensorial notation, one may write the matrix element of Q between the two arcs $(\alpha\beta)$ and $(\mu\nu)$ as

$$Q_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\alpha\mu} \left(\frac{2}{m_\alpha} - \delta_{\beta\nu} \right), \tag{48}$$

where $\delta_{\alpha\beta}$ is the Kronecker symbol; the connectivity matrices $a_{\alpha\beta}$ and $a_{\mu\nu}$ are here to recall that $(\alpha\beta)$ and $(\mu\nu)$ are arcs.

The action of $\mathcal{O}\, e^{\Lambda^\dagger Q \Lambda}$ is complicated because the argument of the exponential is quadratic in the $\Lambda_{\alpha\beta}$'s. This action would become much more simple on the exponential of a linear form; this can be achieved by introducing an additional integration over a $2B$-component complex vector W

$$S(\gamma = 1)^{-1} = \frac{2^B e^{-L}}{(\prod_\alpha m_\alpha)\, \pi^{2B}} \det(Q^{-1}) \int dW^\dagger\, dW\, e^{-W^\dagger Q^{-1} W} \mathcal{O} e^{\Lambda^\dagger W + W^\dagger \Lambda}. \tag{49}$$

The action of $\mathcal{O}$ is now simple by noticing that $\partial_{\Lambda_{\alpha\beta}} \partial_{\bar{\Lambda}_{\beta\alpha}} e^{\Lambda^\dagger W + W^\dagger \Lambda} = \bar{w}_{\alpha\beta} w_{\beta\alpha} e^{\Lambda^\dagger W + W^\dagger \Lambda}$. To write the action of $\mathcal{O}$ on $e^{\Lambda^\dagger W + W^\dagger \Lambda}$, one has to replace $\partial_{\Lambda_{\alpha\beta}}$ by $\bar{w}_{\alpha\beta}$ and $\partial_{\bar{\Lambda}_{\alpha\beta}}$ by $w_{\alpha\beta}$. One finally ends up with

$$S(\gamma = 1)^{-1} = \frac{2^B e^{-L}}{(\prod_\alpha m_\alpha)\, \pi^{2B}} \det(Q^{-1}) \int dW^\dagger\, dW\, e^{-W^\dagger Q^{-1} W + W^\dagger R W}, \tag{50}$$

where it is clear from the expression of $\mathcal{O}$ that the matrix R couples only the arc $(\alpha\beta)$ to the time-reversed arc$(\beta\alpha)$. Thus, R may be written

$$R_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\alpha\nu} \delta_{\beta\mu} e^{-l_{\alpha\beta}}. \tag{51}$$

It is then straightforward to perform the Gaussian integration and get the final expression for the spectral determinant

$$S(\gamma) = \gamma^{(V-B)/2} e^{\sqrt{\gamma} L} \left(\prod_{\alpha} m_{\alpha} \right) 2^{-B} \det(1 - E), \tag{52}$$

where we have introduced $E = (QR)^{\mathrm{T}}$ (the transposition is defined as $(E^{\mathrm{T}})_{(\alpha\beta)(\mu\nu)} = E_{(\mu\nu)(\alpha\beta)}$).

Using this tensorial notation the product QR is particularly simple to perform

$$E_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\beta\mu} \left(\frac{2}{m_{\beta}} - \delta_{\alpha\nu} \right) e^{-\sqrt{\gamma} l_{\alpha\beta}}. \tag{53}$$

The spectral determinant is now given by the determinant of a $2B \times 2B$ matrix E whose basis consists of the set of arcs. Rewriting the matrix $E = D\varepsilon$ one may clearly separate a part ε that only depends on the topology of the graph

$$\varepsilon_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\beta\mu} \left(\frac{2}{m_{\beta}} - \delta_{\alpha\nu} \right) \tag{54}$$

and a diagonal part D depending on the metric properties

$$D_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\alpha\mu} \delta_{\beta\nu} e^{-\sqrt{\gamma} l_{\mu\nu}}. \tag{55}$$

We end this section by mentioning the physical meaning of the different matrices that appear in the derivation given above.

In order to simplify slightly our notation arcs will now be labeled by Roman letters $i, j, \ldots$ ($i \equiv (\alpha\beta)$). The matrix E is then expressed as $E_{ij} = \varepsilon_{ij} e^{-\sqrt{\gamma} l_i}$. Our ε_{ij} coincides with the one introduced in [21]: $\varepsilon_{ij} = 2/m_{\alpha}$ if the end of arc i and the beginning of arc j are the vertex α of coordinence m_{α}, $\varepsilon_{ij} = (2/m_{\alpha}) - 1$ if moreover the two arcs are time-reversed, and $\varepsilon_{ij} = 0$ otherwise.

Following Kottos and Smilansky [13], one may take a scattering point of view to construct the wave function on the graph. Let us consider first the set of arcs $i \in \{1, \ldots, m_{\alpha}\}$ starting at vertex α. On each arc i one writes the wave function as the superposition of an incoming and an outcoming plane wave (see Fig. 2):

$$\psi_i(x) = A_i e^{-ikx} + B_i e^{ikx}. \tag{56}$$

The scattering matrix s_{α} at the vertex is defined as the matrix relating incoming to outgoing amplitudes: $B_i = \sum_j (s_{\alpha})_{ij} A_j$ for $i, j \in \{1, \ldots, m_{\alpha}\}$. Conditions (26) and (27) lead to the following result: $s_{\alpha} = Q_{\alpha}$. On the graph, the $2B$ outgoing amplitudes are then coupled to the $2B$ incoming amplitudes by [13]

$$B_i = \sum_j Q_{ij} A_j \tag{57}$$

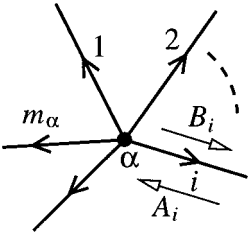


FIGURE 2

(matrix Q indeed couples arcs beginning at same vertex). The physical meaning of the matrix Q is now clear: it describes the scattering by the V vertices. As in Section 3 we use the notation $\bar{i}$ for the time-reversed arc of i. Amplitudes of two time-reversed arcs are related by the two obvious relations $B_i = A_{\bar{i}} e^{-ikl_i}$ and $A_i = B_{\bar{i}} e^{ikl_i}$ (due to the fact that $\psi_i(x) = \psi_{\bar{i}}(l_i - x)$). Then one has $B_{\bar{i}} = \sum_j Q_{ij} e^{ikl_j} B_{\bar{j}}$. Using the fact that $Q_{\bar{i}\bar{j}} = \varepsilon_{ij}$ one finds that

$$B_{\bar{i}} = \sum_j E_{ij}(\gamma = -k^2)\, B_{\bar{j}}. \tag{58}$$

Then the state (56) of energy k^2 belongs to the spectrum if $\det(1 - E(\gamma = -k^2)) = 0$ [20]. As equation $\det(M(\gamma = -k^2)) = 0$, this equation gives the spectrum of the Laplacian but not the γ-dependent pre-factor of $S(\gamma)$.

6. A TRACE FORMULA

The result (52) is particularly suitable for deriving a trace formula that expresses the determinant in terms of contributions of closed trajectories (orbits) on the graph. Again we may set $\gamma = 1$ for the sake of simplicity. We may expand the determinant

$$\ln \det(1 - E) = -\sum_{n=1}^{\infty} \frac{1}{n} \operatorname{Tr}\{E^n\} \tag{59}$$

and write the trace as a sum of terms

$$\operatorname{Tr}\{E^n\} = \sum_{i_1, \ldots, i_n} \varepsilon_{i_1 i_2} \varepsilon_{i_2 i_3} \cdots \varepsilon_{i_n i_1} e^{-(l_{i_1} + \cdots + l_{i_n})}, \tag{60}$$

each of which is associated with a sequence of arcs that forms a closed path on the graph. Following the notation of [21] one may attach the quantity

$$\alpha(C_n) = \varepsilon_{i_1 i_2} \varepsilon_{i_2 i_3} \cdots \varepsilon_{i_n i_1} \tag{61}$$

to the orbit (or circuit) $C_n = (i_1, i_2, ..., i_n)$ composed of n arcs, and denote its length by $l(C_n) = l_{i_1} + \cdots + l_{i_n}$. Each term of $\mathrm{Tr}\{E^n\}$ corresponds to a path associated with either a primitive orbit of n steps or k repetitions of a primitive orbit of p steps such as $n = k\,p$. Primitive orbits will be labeled as $\tilde{C}$. A given primitive orbit of n steps appears n times in $\mathrm{Tr}\{E^n\}$, corresponding to the n cyclic permutations of the indices that give the same orbit on the graph. On the other hand the term associated to k repetitions of a primitive orbit $\tilde{C}_p$ appears p times corresponding to the p different permutations of the indices that appear in $\mathrm{Tr}\{E^n\}$. Using these remarks, instead of summing over all paths of length n as in (60), one may sum over the k-repetition of primitive orbits of length p provided that $n = kp$:

$$\mathrm{Tr}\{E^n\} = \sum_{k,\ \tilde{C}_p \text{ with } n=kp} p\,\alpha(\tilde{C}_p)^k\, e^{-kl(\tilde{C}_p)}. \tag{62}$$

we have used the fact that if C_n is a k-repetition of $\tilde{C}_p$ then $\alpha(C_n) = \alpha(\tilde{C}_p)^k$ and $l(C_n) = kl(\tilde{C}_p)$. Introducing this expression in (59) gives

$$\ln \det(1-E) = -\sum_{\tilde{C}_p} \sum_{k=1}^{\infty} \frac{1}{kp}\, p\,\alpha(\tilde{C}_p)^k\, e^{-kl(\tilde{C}_p)}. \tag{63}$$

Instead of summing over n, k, and $\tilde{C}_p$ with the constraint $kp = n$, one may sum over all primitive orbits $\tilde{C}_p$ and their k-repetition independently. This immediately leads [32] to

$$\ln \det(1-E) = \sum_{\tilde{C}_p} \ln(1 - \alpha(\tilde{C}_p)\, e^{-l(\tilde{C}_p)}). \tag{64}$$

One thus gets an expression of the spectral determinant in terms of an infinite product over all the primitive orbits $\tilde{C}$, in infinite number,[6] that can be constructed on the graph:

$$S(\gamma) = \gamma^{(V-B)/2} e^{\sqrt{\gamma} L} \left(\prod_{\alpha} m_\alpha \right) 2^{-B} \prod_{\tilde{C}} (1 - \alpha(\tilde{C})\, e^{-\sqrt{\gamma}\, l(\tilde{C})}). \tag{65}$$

A similar trace formula for the partition function was first derived by Roth [21]. It is indeed possible to recover it by starting from (65). The log-derivative of the spectral determinant is equal to the Laplace transform of the partition function (3). From (65) one gets

$$\frac{\partial}{\partial \gamma} \ln S(\gamma) = \frac{L}{2\sqrt{\gamma}} + \frac{V-B}{2\gamma} + \frac{1}{2\sqrt{\gamma}} \sum_{\tilde{C}} l(\tilde{C}) \sum_{k=1}^{\infty} \alpha(\tilde{C})^k\, e^{-k\sqrt{\gamma}\, l(\tilde{C})}, \tag{66}$$

[6] Note, however, that there are two trivial graphs for which one can construct only one primitive orbit: the circle and the line.

where one has expanded the denominator coming from the derivative of the logarithm that appears writing $\ln S(\gamma)$. It is then possible to group the two sums in a unique sum over all orbits C, including the repetitions of the primitive orbits

$$\frac{\partial}{\partial\gamma}\ln S(\gamma)=\frac{L}{2\sqrt{\gamma}}+\frac{V-B}{2\gamma}+\frac{1}{2\sqrt{\gamma}}\sum_{C} l(\tilde{C})\,\alpha(C)\,e^{-\sqrt{\gamma}\,l(C)}. \tag{67}$$

In this summation, $\tilde{C}$ designates the primitive orbit associated with a given orbit C.

Using the identity $\frac{1}{2\sqrt{\gamma}}e^{-\sqrt{\gamma}\,l}=\frac{1}{2\sqrt{\pi}}\int_0^\infty dt\,\frac{1}{\sqrt{t}}e^{-\gamma t-(l^2/4t)}$ it is then easy to extract the inverse Laplace transform of the previous expression and recover the trace formula first obtained by Roth [21, 22]

$$Z(t)=\frac{L}{2\sqrt{\pi t}}+\frac{V-B}{2}+\frac{1}{2\sqrt{\pi t}}\sum_{C} l(\tilde{C})\,\alpha(C)\,e^{-l(C)^2/4t}. \tag{68}$$

Let us notice that if one considers a vertex α of coordination $m_\alpha=2$, the circuits that contain a reflection at this vertex have weights $\alpha(C)=0$; therefore such circuits should not be considered in the expansion. Since one can always introduce an arbitrary number of vertices on any bond without changing the properties of the graph, this remark ensures that the number of orbits will not vary doing so. Moreover this shows that a graph can always be simplified to minimize B and V by suppressing all vertices of coordination 2.

7. SIMPLIFICATION OF THE TRACE FORMULA—DIAGRAMMATIC EXPANSION OF THE SPECTRAL DETERMINANT

In the previous section one has expressed the determinant $\det(1-E)$, which can be expanded to give a finite number of terms, as an infinite product (65). The purpose of this section is to show how the infinite product eventually simplifies to give a finite number of terms. One interest of this discussion is to provide a diagrammatic method for constructing systematically the different terms of $S(\gamma)$.

We will consider the quantity that appears in (65):

$$\hat{S}=\prod_{\tilde{C}}(1-\alpha(\tilde{C})\,e^{-l(\tilde{C})}). \tag{69}$$

The generalization of the following discussion to the case with a magnetic field is straightforward (see (90)).

We will call $-\alpha(C)\,e^{-l(C)}$ the weight of the orbit. We associate to each term in the expansion of $\hat{S}$ a diagram, which represents either the contribution of an orbit or the product of such contributions; in the latter case the diagram represents the superposition of the different orbits.

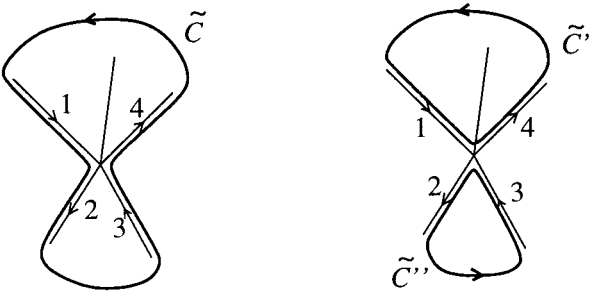


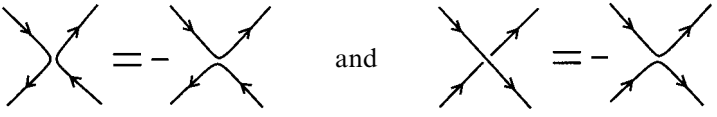
FIGURE 3

To understand how the simplifications occur let us consider a primitive orbit $\tilde{C}$ that passes twice through the same vertex without using the same arcs as in Fig. 3. Using the fact that $\varepsilon_{12}=\varepsilon_{34}=\varepsilon_{14}=\varepsilon_{32}$ it is easy to see that

$$-\alpha(\tilde{C})\, e^{-l(\tilde{C})} = -(-\alpha(\tilde{C}')\, e^{-l(\tilde{C}')})(-\alpha(\tilde{C}'')\, e^{-l(\tilde{C}'')}), \tag{70}$$

where $\tilde{C}'$ and $\tilde{C}''$ are obtained by crossing the paths at the vertex as shown in Fig. 3. The consequence is that in the expansion of $\hat{S}$, the product of the weights of orbits $\tilde{C}'$ and $\tilde{C}''$ cancels with the contribution of $\tilde{C}$.

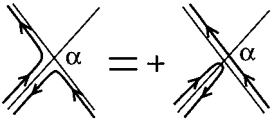
These kind of relations may be represented diagrammatically as



(71)

Using these relations one must take care of not introducing some reflection at a vertex like in Fig. 4. Indeed the diagram on the left of Fig. 4 has a weight proportional to $(2/m_\alpha)^2$ whereas the diagram on the right has a weight proportional to $-((2/m_\alpha)-1)(2/m_\alpha)$.

Note that the case of a vertex with coordination $m_\alpha=4$ is special and may bring some additional rules which simplify the expansion of $\hat{S}$. Those two additional rules are



for $m_\alpha=4$ (72)

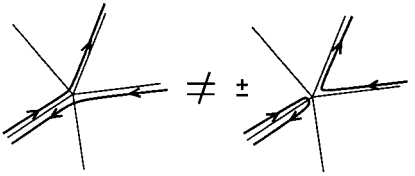
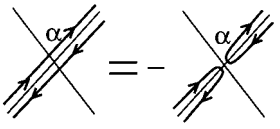


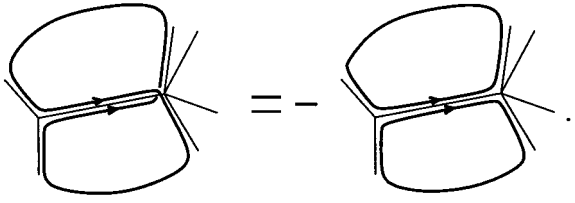
FIG. 4. Take care not to introduce some reflection at a vertex using the rules (71).

and



$$\text{for} \quad m_\alpha = 4 \tag{73}$$

What kind of consequences can be deduced from these rules (71)? Let us consider a primitive orbit that contains twice the same arc. This orbit may be factorized using the de-crossing rule (71):



(74)

This equation implies that one should not include in the expansion of $\hat{S}$ the diagrams that contain more than once a given arc. This remark implies that the number of diagrams to be considered is finite. In the diagrams that remain in the expansion, a bond appears in the orbits at most twice, corresponding to the two reversed arcs; a by-product of this remark is that the longest orbits that can be constructed satisfying this rule have lengths $2L$.

EXAMPLE OF A DIAGRAMMATIC EXPANSION. As an example, consider the diagram of Fig. 5, which consists of an arm connected to a ring pierced by a flux ϕ; this

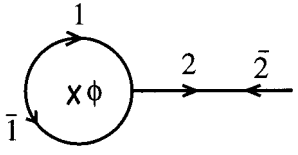
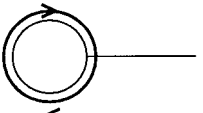
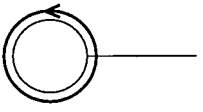
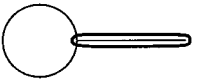
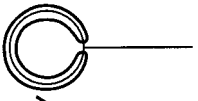
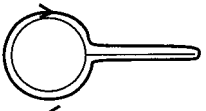
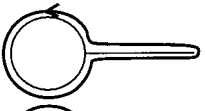
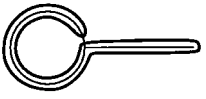
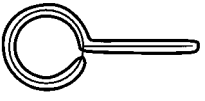


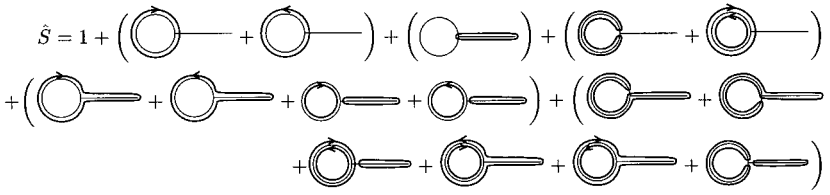
FIGURE 5

TABLE I

Primitive orbit $\tilde{C}$	Weight $-\alpha(\tilde{C})\, e^{-l(\tilde{C})+i\theta(\tilde{C})}$
	$-\frac{2}{3}\, e^{-l-i\theta}$
	$-\frac{2}{3}\, e^{-l+i\theta}$
	$\frac{1}{3}\, e^{-2b}$
	$-\frac{1}{9}\, e^{-2l}$
	$-\frac{4}{9}\, e^{-l-2b-i\theta}$
	$-\frac{4}{9}\, e^{-l-2b+i\theta}$
	$\frac{4}{27}\, e^{-2l-2b}$
	$\frac{4}{27}\, e^{-2l-2b}$

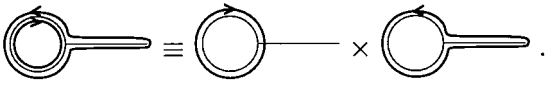
geometry was considered for the study of persistent currents in the case of a one-channel clean ring [33] and in the case of a metallic diffusive ring [11]. The first step is to construct all the periodic orbits that will be involved in the expansion (see Table I). One considers the situation in which the ring is pierced by a flux ϕ to distinguish between time-reversed orbits; $\theta = 2\pi\phi/\phi_0$, where $\phi_0 = h/e$ is the flux quantum. We call l the perimeter of the ring and b the length of the arm. As an example let us compute the $\alpha(C)$ coefficient for the last orbit of Table I $\tilde{C} = (1, 2, \bar{2}, \bar{1})$: $\alpha(\tilde{C}) = \varepsilon_{12}\varepsilon_{2\bar{2}}\varepsilon_{\bar{2}\bar{1}}\varepsilon_{\bar{1}1}$ with $\varepsilon_{\bar{1}1} = -\frac{1}{3}$, $\varepsilon_{12} = \varepsilon_{\bar{2}\bar{1}} = \frac{2}{3}$, and $\varepsilon_{2\bar{2}} = 1$.

The construction of all diagrams of the expansion requires one to combine all these orbits provided that the resulting diagrams do not contain twice the same arc. This leads to



(75)

where it is understood that a diagram with two primitive orbits is equivalent to the product of diagrams for each orbit, as said above. For example,



(76)

Using the weights of the orbits given in the table one eventually finds

$$\hat{S} = 1 - \tfrac{4}{3}\cos\theta e^{-l} + \tfrac{1}{3}e^{-2b} + \tfrac{1}{3}e^{-2l} - \tfrac{4}{3}\cos\theta e^{-l-2b} + e^{-2l-2b} \tag{77}$$

$$= \tfrac{4}{3}e^{-l-b}(\mathrm{sh}\, b\, \mathrm{sh}\, l + 2(\mathrm{ch}\, l - \cos\theta)\, \mathrm{ch}\, b). \tag{78}$$

Thus,

$$S(\gamma) = \mathrm{sh}(\sqrt{\gamma}\, b)\, \mathrm{sh}(\sqrt{\gamma}\, l) + 2[\mathrm{ch}(\sqrt{\gamma}\, l) - \cos(\theta)]\, \mathrm{ch}(\sqrt{\gamma}\, b), \tag{79}$$

a result that can also be obtained using (85) and (38) (see also Appendix C).

As one can realize looking at (77), there exists a symmetry between the coefficients of the different terms appearing in the diagrammatic expansion. It is possible to use this symmetry to reduce the number of diagrams that have to be considered, which greatly simplifies the calculation. This point is discussed in more detail in Appendix B.

To conclude this section we insist on the fact that the periodic orbit expansion of the spectral determinant involves only a finite number of contributions, despite the number of primitive orbits being infinite. In contrast, the periodic orbit expansion of the partition function (10) or the density of states involves an infinite number of contributions.

8. GRAPHS IN A MAGNETIC FIELD

In this section, we describe the appropriate modifications to the previous formalism that have to be done in the presence of a magnetic field, namely for a distribution of

Aharonov–Bohm fluxes. The operator of interest is now $-(d_x - iA)^2$. In Eq. (27) one has to replace the derivative of the function ψ by a covariant derivative $D_x = d_x - iA(x)$

$$\sum_{\beta} a_{\alpha\beta} D_{x_{\alpha\beta}} \psi_{(\alpha\beta)}(x_{\alpha\beta} = 0) = 0. \tag{80}$$

The path integral derivation of $\det(-D_x^2 + \gamma)$ follows the same lines except that all derivatives have to be replaced by covariant derivatives in (30) and (31). One is led to an expression of the determinant that involves a product of terms of the form

$$\int_{\phi(0)=\phi_\alpha}^{\phi(l_{\alpha\beta})=\phi_\beta} \mathscr{D}\phi\, \mathscr{D}\bar{\phi}\, e^{-(1/2)\int_0^{l_{\alpha\beta}} dx(|D_x\phi|^2 + \gamma|\phi|^2)}. \tag{81}$$

We may recover the Gaussian action of the harmonic oscillator by performing the following gauge transformation

$$\phi(x) = \tilde{\phi}(x)\, e^{i\int_{x_0}^{x} dx'\, A(x')}, \tag{82}$$

where the integral is performed along the bond $(\alpha\beta)$ and x_0 is an arbitrary point on this bond (a change of x_0 corresponds to adding a constant phase to the field). If we define

$$\theta_{\beta\alpha} = \int_0^{l_{\alpha\beta}} dx\, A(x) \tag{83}$$

($\theta_{\beta\alpha} = -\theta_{\alpha\beta}$), where the integral is performed along the bond $(\alpha\beta)$, and choose x_0 in such a way that $\int_{x_0}^{l_{\alpha\beta}} dx\, A(x) = \theta_{\beta\alpha}/2$ and $\int_{x_0}^{0} dx\, A(x) = \theta_{\alpha\beta}/2$, then (81) becomes

$$\int_{\tilde{\phi}(0)=\phi_\alpha e^{-i\theta_{\alpha\beta}/2}}^{\tilde{\phi}(l_{\alpha\beta})=\phi_\beta e^{-i\theta_{\beta\alpha}/2}} \mathscr{D}\tilde{\phi}\, \mathscr{D}\bar{\tilde{\phi}}\, e^{-(1/2)\int_0^{l_{\alpha\beta}} dx(|d_x\tilde{\phi}|^2 + \gamma|\tilde{\phi}|^2)}$$
$$= \sqrt{\gamma}\, G_{\sqrt{\gamma}\, l_{\alpha\beta}}(\gamma^{1/4}\phi_\beta\, e^{-i\theta_{\beta\alpha}/2}, \gamma^{1/4}\phi_\alpha e^{-i\theta_{\alpha\beta}/2}). \tag{84}$$

Introducing this expression in (34), then it is clear that (38) still holds provided that the matrix M is now defined as

$$M_{\alpha\beta} = \delta_{\alpha\beta} \sum_{\mu} a_{\alpha\mu} \coth(\sqrt{\gamma}\, l_{\alpha\mu}) - a_{\alpha\beta} \frac{e^{i\theta_{\alpha\beta}}}{\mathrm{sh}(\sqrt{\gamma}\, l_{\alpha\beta})}. \tag{85}$$

The calculations of Section 5 may also be generalized. The derivation is the same and the matrix Q now reads

$$Q_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\alpha\mu} \left(\frac{2}{m_\alpha} - \delta_{\beta\nu} \right) e^{i(\theta_{\alpha\beta} - \theta_{\alpha\nu}/2)}, \tag{86}$$

and the matrix R is unchanged. To define E it is convenient to introduce a unitary transformation $\mathscr{U}$ that makes the changes more clear. If one writes

$$QR = \mathscr{U} E^{\mathrm{T}} \mathscr{U}^{\dagger}, \tag{87}$$

where $\mathscr{U}$ is

$$\mathscr{U}_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\alpha\mu} \delta_{\beta\nu} e^{i(\theta_{\alpha\beta}/2)}, \tag{88}$$

then one has $E = D\varepsilon$, where ε is still given by (54) and all the dependence in the fluxes is now contained in the matrix D:

$$D_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\alpha\mu} \delta_{\beta\nu} e^{-\sqrt{\gamma}\, l_{\mu\nu} + i\theta_{\mu\nu}}. \tag{89}$$

Since the spectral determinant is given by the determinant of the matrix $1 - E$, the matrix $\mathscr{U}$ and its inverse disappear in the determinant and (52) still holds.

The derivation of the trace formulae only requires trivial modifications and one finally obtains for the determinant

$$S(\gamma) = \gamma^{(V-B)/2} e^{\sqrt{\gamma} L} \left(\prod_{\alpha} m_{\alpha} \right) 2^{-B} \prod_{\tilde{C}} (1 - \alpha(\tilde{C})\, e^{-\sqrt{\gamma}\, l(\tilde{C}) + i\theta(\tilde{C})}), \tag{90}$$

and the corresponding partition function,

$$Z(t) = \frac{L}{2\sqrt{\pi t}} + \frac{V-B}{2} + \frac{1}{2\sqrt{\pi t}} \sum_{C} l(\tilde{C})\, \alpha(C)\, e^{-(l(C)^2/4t) + i\theta(C)} \tag{91}$$

which generalizes Roth's formula (68). We have used the obvious notation for the flux enclosed by an orbit $C = (i_1, i_2, ..., i_n) : \theta(C) = \theta_{i_1} + \cdots + \theta_{i_n}$.

9. MORE GENERAL BOUNDARY CONDITIONS

One must sometimes consider more general boundary conditions than (80). Imposing instead of (80) the so-called mixed boundary conditions

$$\sum_{\beta} a_{\alpha\beta} D_{x_{\alpha\beta}} \psi_{(\alpha\beta)}(x_{\alpha\beta} = 0) = \lambda_{\alpha} \psi_{\alpha} \tag{92}$$

requires to generalize some of the previous results.[7] This can be easily achieved by using the path integral formalism. It is rather obvious that the boundary terms in (31) now produce additional Gaussian terms in (34) which now reads

[7] One may distinguish two cases. (i) In the Schrödinger problem, the current is $J = 2\,\mathrm{Im}(\psi^* d_x \psi)$. Conditions (92) also lead to current conservation at the vertices. (ii) For the diffusion problem, the wave function $\psi(x, t)$ has to be replaced by a probability density $P(x, t)$. The current of probability is given in this case by $J(x, t) = -\partial_x P(x, t)$. Equation (92) implies that such a current is not conserved at the vertices where $\lambda_{\alpha} \neq 0$. This condition corresponds physically to a graph connected to the external world, $\lambda_{\alpha} P(\alpha, t)$ being the current of particles exiting the graph. In the Dirichlet case ($\lambda_{\alpha} = \infty$) the graph is perfectly connected, which means that a particle exits the graph with probability 1 if it reaches the vertex α.

$$S(\gamma)^{-1} = \gamma^{(B-V)/2} \int \prod_{\alpha=1}^{V} d\phi_\alpha \, d\bar{\phi}_\alpha \, e^{-(\lambda_\alpha/2\sqrt{\gamma})\,|\phi_\alpha|^2} \times \prod_{(\alpha\beta)} G_{\sqrt{\gamma}\, l_{\alpha\beta}}(\phi_\beta e^{-i\theta_{\beta\alpha}/2}, \phi_\alpha e^{-i\theta_{\alpha\beta}/2}). \tag{93}$$

Thus only the diagonal elements of matrix M change. In (38), M is replaced by $\tilde{M}$:

$$\tilde{M}_{\alpha\beta} = M_{\alpha\beta} + \frac{\lambda_\alpha}{\sqrt{\gamma}} \delta_{\alpha\beta}. \tag{94}$$

It is also easy to see from the discussion of Section 5 how the different matrices are affected by the change of boundary conditions. Equation (43) will receive some additional Gaussian terms $e^{-(1/2)\,\lambda_\alpha |\phi_\alpha|^2/\sqrt{\gamma}}$ which implies that m_α has to be replaced by $m_\alpha + (\lambda_\alpha/\sqrt{\gamma})$. The scattering matrix Q now reads

$$Q_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\alpha\mu} \left(\frac{2}{m_\alpha + (\lambda_\alpha/\sqrt{\gamma})} - \delta_{\beta\nu} \right) e^{i(\theta_{\alpha\beta} - \theta_{\alpha\nu}/2)} \tag{95}$$

and the matrix ε is

$$\varepsilon_{(\alpha\beta)(\mu\nu)} = a_{\alpha\beta} a_{\mu\nu} \delta_{\beta\mu} \left(\frac{2}{m_\beta + (\lambda_\beta/\sqrt{\gamma})} - \delta_{\alpha\nu} \right); \tag{96}$$

the other matrices R and D remain unchanged. The factor $\alpha(C)$ of Sections 6 and 7 will be modified according to (96).

Expression (94) allows us to treat both the case of Neumann boundary conditions ($\lambda_\alpha = 0$) which has already been studied in this paper, and the case of Dirichlet boundary condition ($\lambda_\alpha = \infty$). For a diffusive conductor, these conditions correspond to a disconnected wire and a wire perfectly connected to leads at the node, respectively.

If one imposes the Dirichlet condition at all vertices of the graph, one has to consider the limit $\lambda \to \infty$ for all vertices. Then $\det(\tilde{M}) \simeq \prod_\alpha (\lambda_\alpha/\sqrt{\gamma})$. The spectral determinant is $S(\gamma) \simeq (\prod_\alpha \lambda_\alpha) \prod_{(\alpha\beta)} (\mathrm{sh}\, \sqrt{\gamma}\, l_{\alpha\beta}/\sqrt{\gamma})$. One can drop the irrelevant factor $\prod_\alpha \lambda_\alpha$ since the spectral determinant is defined up to a multiplicative numerical factor independent of γ, which depends on the regularization. One finds that the spectral determinant $S(\gamma) = \prod_{(\alpha\beta)} (\mathrm{sh}\, \sqrt{\gamma}\, l_{\alpha\beta}/\sqrt{\gamma})$ is the product of the spectral determinants associated with each bond. All bonds are then independent.

We now discuss the case where one imposes the Dirichlet boundary at only one vertex α_0 which will be useful in the next section. Taking the limit $\lambda_{\alpha_0} \to \infty$, one has

$$S(\gamma; \{\text{Dirichlet at } \alpha_0\}) = \gamma^{(V-B-1)/2} \prod_{(\alpha\beta)} \mathrm{sh}(\sqrt{\gamma}\, l_{\alpha\beta}) \det(M^{\alpha_0}), \tag{97}$$

where M^{α_0} is the $(V-1)\times(V-1)$ matrix given by the matrix M with the line α_0 and the column α_0 deleted.

As an example consider the graph pictured in Fig. 5 for which one imposes the Dirichlet boundary at the end of the arm. $S(\gamma)$ becomes

$$S_{\text{Dirich. at the end of arm}}(\gamma) = \frac{1}{\sqrt{\gamma}} \{\text{ch}(\sqrt{\gamma}\, b)\, \text{sh}(\sqrt{\gamma}\, l) + 2[\text{ch}(\sqrt{\gamma}\, l) - \cos(\theta)]\, \text{sh}(\sqrt{\gamma}\, b)\}, \tag{98}$$

to be compared with (79). It is interesting to check that the magnetization of the ring, given by (19) and (20), does not depend on the choice of the boundary conditions at the end of the arm, when its length b goes to infinity ($b \gg L_\phi = 1/\sqrt{\gamma}$).

10. ZERO-MODE AND LOW-ENERGY BEHAVIOR

The low-energy part of the spectrum can be studied by using the expansion of the spectral determinant when $\gamma \to 0$. Using this approach we prove the existence of a zero-mode state when $\mathscr{B} = 0$ and obtain the dependence of the ground state energy in the magnetic field. Using the infinite product representation $S(\gamma) = \prod_n (E_n + \gamma)$ and assuming $E_0 = 0$ imply that $S(\gamma)$ behaves linearly with γ when $\gamma \to 0$. In order to study this limit it is convenient to expand M as a power series in γ

$$M(\gamma) = \frac{1}{\sqrt{\gamma}} \hat{M}(\gamma) = \frac{1}{\sqrt{\gamma}} (\hat{M}^0 + \gamma \hat{M}^1 + \cdots), \tag{99}$$

where

$$\hat{M}^0_{\alpha\beta} = \delta_{\alpha\beta} \sum_\mu \frac{a_{\alpha\mu}}{l_{\alpha\mu}} - \frac{a_{\alpha\beta}}{l_{\alpha\beta}} \tag{100}$$

$$\hat{M}^1_{\alpha\beta} = \delta_{\alpha\beta} \frac{1}{3} \sum_\mu a_{\alpha\mu} l_{\alpha\mu} + \frac{1}{6} a_{\alpha\beta} l_{\alpha\beta}. \tag{101}$$

From these expressions, it is easy to see that $\hat{M}^0$ possesses an eigenvalue $\xi_0 = 0$ corresponding to the eigenvector v_0 whose components are $(v_0)_\alpha = 1$. Remembering that M acts on the V vector constructed with the wave function at the nodes, the vector v_0 corresponds to a wave function that takes the same value on all vertices and is constant on the graph (since $\gamma = -E = 0$). We denote by $\xi_n(\gamma)$ ($n = 0, ..., V-1$) the V eigenvalues of $\hat{M}(\gamma)$. The eigenvalue $\xi_0(\gamma)$ vanishes at $\gamma = 0$ and its behavior for small γ computed in perturbation theory is $\xi_0(\gamma) \simeq \gamma(v_0^{\mathrm{T}} \hat{M}^1 v_0 / v_0^{\mathrm{T}} v_0) = \gamma L/V$. This implies that $\det(\hat{M}(\gamma)) \simeq (\gamma L/V) \prod_{n=1}^{V-1} \xi_n(0)$. It is possible to write the product of the non-vanishing eigenvalues for $\gamma = 0$ as the determinant of the matrix $\hat{M}^0 + (v_0 v_0^{\mathrm{T}} / \| v_0 \|^2)$, where the second term is the projector on the vector v_0.

One finally obtains for the spectral determinant

$$S(\gamma) \underset{\gamma \to 0}{\simeq} \gamma \frac{L}{V} \left(\prod_{(\alpha\beta)} l_{\alpha\beta} \right) \det(K), \tag{102}$$

where the matrix K is

$$K_{\alpha\beta} = \hat{M}^0_{\alpha\beta} + \frac{1}{V}. \tag{103}$$

From the linear behavior $S(\gamma) \propto \gamma$ at small γ it follows that one has for the partition function $\lim_{t \to \infty} Z(t) = 1$.

Let us remark that if all the lengths of the bonds are equal to unity, the product $\prod_{n=1}^{V-1} \xi_n(0)$ is equal to $\mathscr{T}(\mathscr{G})$, the number of trees that cover the graph (Tutte theorem) [16, 17].

It is also interesting to see how the spectral determinant behaves at non-vanishing magnetic field. For the sake of simplicity we denote the ensemble of fluxes $\{\theta_{\alpha\beta}\}$ by $\mathscr{B}$. The matrix $\hat{M}$ now depends on the fluxes. The spectral determinant may be expressed in terms of the eigenvalues of $\hat{M}(\gamma, \mathscr{B})$:

$$S(\gamma, \mathscr{B}) = \prod_{(\alpha\beta)} \frac{\mathrm{sh}\sqrt{\gamma}\, l_{\alpha\beta}}{\sqrt{\gamma}} \prod_{n=0}^{V-1} \xi_n(\gamma, \mathscr{B}). \tag{104}$$

At zero magnetic field and small γ, one has shown above how $S(\gamma)$ behaves (102) by a perturbative expansion of $\xi_0(\gamma, 0)$. Similarly, at a small magnetic field, one may compute the eigenvalue $\xi_0(0, \mathscr{B})$ in perturbation theory. Starting from

$$\hat{M}_{\alpha\beta}(0, \mathscr{B}) = \delta_{\alpha\beta} \sum_{\mu} \frac{a_{\alpha\mu}}{l_{\alpha\mu}} - a_{\alpha\beta} \frac{e^{i\theta_{\alpha\beta}}}{l_{\alpha\beta}} \tag{105}$$

and expanding this expression at small fluxes, it is easy to show that $\xi_0(0, \mathscr{B}) \simeq (1/2V) \sum_{\alpha,\beta} a_{\alpha\beta}(\theta^2_{\alpha\beta}/l_{\alpha\beta})$. Since $\prod_{n=1}^{V-1} \xi_n(0, 0) = \det(K)$ the spectral determinant behaves like

$$S(0, \{\theta_{\alpha\beta}\}) \underset{\{\theta_{\alpha\beta}\} \to 0}{\simeq} \frac{1}{V} \sum_{(\alpha\beta)} \frac{\theta^2_{\alpha\beta}}{l_{\alpha\beta}} \left(\prod_{(\alpha\beta)} l_{\alpha\beta} \right) \det(K). \tag{106}$$

One may extract from these expressions the ground state energy at a small magnetic field. At small γ one has $S(\gamma, 0) \simeq \gamma \prod_{n>0} E_n(0)$. On the other hand, when the magnetic field goes to zero, the ground state energy is the only energy to vanish, and then $S(0, \mathscr{B}) \simeq E_0(\mathscr{B}) \prod_{n>0} E_n(0)$. The ratio $S(0, \mathscr{B})/S(\gamma, 0) \simeq E_0(\mathscr{B})/\gamma$ gives the expression of the ground state energy

$$E_0(\{\theta_{\alpha\beta}\}) \simeq \frac{1}{L} \sum_{(\alpha\beta)} \frac{\theta^2_{\alpha\beta}}{l_{\alpha\beta}}. \tag{107}$$

Let us notice that the expression (107) of the ground state energy at a small magnetic field may be recovered in a simpler way by perturbation theory. The eigenfunction of the ground state at zero field is $\psi_0(x \in \mathscr{G}) = 1/\sqrt{L}$. Thus the correction to the energy at small field is $E_0(\{\theta_{\alpha\beta}\}) \simeq \langle \psi_0 |\, A(x)^2 \,| \psi_0 \rangle = (1/L) \sum_{(\alpha\beta)} \int_0^{l_{\alpha\beta}} dx\, A(x)^2$.

By choosing a gauge such that $A(x) = A_{\beta\alpha}$ is constant on the bond $(\alpha\beta)$, one recovers (107) since $\theta_{\beta\alpha} = A_{\beta\alpha} l_{\alpha\beta}$.

So far we have not described the effect of a change of boundary conditions on the low-energy behavior of the spectral determinant. The matrix M at zero magnetic field now becomes

$$\hat{\tilde{M}}_{\alpha\beta}(0, \{\lambda_\alpha\}) = \hat{M}^0_{\alpha\beta} + \lambda_\alpha \delta_{\alpha\beta}. \tag{108}$$

As in the presence of a small magnetic field one may compute the lowest eigenvalue $\xi_0(0, \{\lambda_\alpha\})$ of the matrix $\hat{\tilde{M}}(0, \{\lambda_\alpha\})$ by perturbation theory. This gives

$$S(0, \{\lambda_\alpha\}) \underset{\{\lambda_\alpha\} \to 0}{\simeq} \frac{1}{V} \sum_\alpha \lambda_\alpha \left(\prod_{(\alpha\beta)} l_{\alpha\beta} \right) \det(K). \tag{109}$$

One may also deduce from this result the behavior of the ground state energy:

$$E_0(\{\lambda_\alpha\}) \simeq \frac{1}{L} \sum_\alpha \lambda_\alpha. \tag{110}$$

Let us notice that in a particular case, one may recover this result by another way. Consider a ring with V vertices with mixed boundary conditions. This problem is equivalent to a ring with a potential made of δ scatterers: $W(x) = \sum_\alpha \lambda_\alpha \delta(x - x_\alpha)$, where the x_α's are the positions of the vertices on the ring. In this case it is possible to compute perturbatively the energy of the ground state: $E_0(\{\lambda_\alpha\}) \simeq \langle \psi_0 | W(x) | \psi_0 \rangle$ which indeed leads to (110).

The result (110) has a physical interpretation in the context of diffusion. The zero-mode $E_0 = 0$ is associated with the uniform stationary distribution at long time. As soon as the graph is connected to the external world, which may be described by taking mixed boundary conditions, the probability of remaining on the graph decreases at long time $\int_{\text{Graph}} dx\, P(x, x', t) \sim e^{-E_0 t}$ which means the absence of a zero mode. In this case, E_0 is the inverse escape time of the graph.

11. THE GRAPH CONNECTED TO AN INFINITE LEAD

In this section, we consider the case of a graph connected to an infinite lead attached to the vertex α (see Fig. 6). In that case, we are dealing with a quantum scattering problem where the relevant information like the spectrum, the Wigner time delays, or thermodynamic quantities like the persistent currents is encoded in the (unitary) scattering matrix [34]. To the purpose of calculating the scattering phase shifts, let us suppose that along the lead an incoming plane wave e^{-ikx} enters the graph at the vertex α and is reflected with a phase shift $\delta_\alpha(E)$. Below we derive a formula expressing the phase shift in terms of $\det(M)$. Although such a formula is in fact a special case of the one given in [13, 14], it is nevertheless interesting to

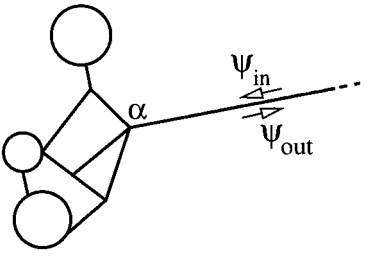


FIGURE 6

present an independent derivation of it and show the relation with spectral determinants. m_α is the coordinence of vertex α in the absence of the external lead. We first write the wave function of energy $E=k^2$ on the bond $(\mu\beta)$ in a form that ensures continuity,

$$\psi_{(\mu\beta)}(x_{\mu\beta}) = \frac{e^{iA_{\beta\mu}x_{\mu\beta}}}{\sin kl_{\mu\beta}} (\psi_\mu \sin k(l_{\mu\beta}-x_{\mu\beta}) + \psi_\beta e^{-iA_{\beta\mu}l_{\mu\beta}} \sin kx_{\mu\beta}), \tag{111}$$

where $A_{\beta\mu}l_{\mu\beta}=\theta_{\beta\mu}$. On the incoming lead, the wave function is written in terms of stationary scattering states

$$\psi_{\text{lead}}(x) = \frac{\psi_\alpha}{\cos(\delta_\alpha/2)} \cos(kx+\delta_\alpha/2) \propto e^{-ikx} + e^{ikx+i\delta_\alpha}, \tag{112}$$

where $x \in [0, \infty[$ is a current point on the lead. Continuity of the wave function at vertex α is already ensured with the previous expression. Current conservation at the vertex α gives

$$\sum_\beta a_{\alpha\beta} \left(-\psi_\alpha \operatorname{cotg} kl_{\alpha\beta} + \psi_\beta \frac{e^{i\theta_{\alpha\beta}}}{\sin kl_{\alpha\beta}} \right) - \psi_\alpha \tan(\delta_\alpha/2) = 0. \tag{113}$$

Since the boundary conditions on the other vertices are obviously unchanged we are left with the linear system of V equations

$$-i \sum_\beta M_{\mu\beta}(\gamma=-k^2)\, \psi_\beta = \delta_{\mu\alpha}\psi_\alpha \tan(\delta_\alpha/2), \tag{114}$$

where $\mu = 1, ..., V$. Cramer's formula then gives

$$\psi_\alpha = i \tan(\delta_\alpha/2) \frac{\det(M^\alpha(-k^2))}{\det(M(-k^2))} \psi_\alpha, \tag{115}$$

where $M^{\alpha}(\gamma)$ is the matrix introduced in Section 9. Then the phase shift is obviously given by

$$\operatorname{cotg}(\delta_{\alpha}(E)/2) = i \frac{\det(M^{\alpha}(-E))}{\det(M(-E))}. \tag{116}$$

This result, together with (97), shows that the phase shift is related to the ratio of two spectral determinants: one calculated with a Dirichlet boundary at the vertex connected to the lead and a Neumann boundary at all other vertices (97), and the other calculated with a Neumann boundary at all vertices (4):

$$\operatorname{cotg}(\delta_{\alpha}(k^2)/2) = -k \frac{S(-k^2; \{\text{Dirichlet at } \alpha\})}{S(-k^2)}. \tag{117}$$

This expression shows that $\delta_{\alpha} = 0 \bmod 2\pi$ if k^2 coincides with an energy of the graph with the Neumann boundary, and $\delta_{\alpha} = \pi \bmod 2\pi$ if k^2 is an energy of the graph with Dirichlet at vertex α.

As an example the phase shift of the graph of Fig. 5 is given by the ratio of (98) and (79) if the lead is connected to the end of the arm

$$\operatorname{cotg}(\delta/2) = \frac{\cos kb \sin kl + 2(\cos kl - \cos\theta) \sin kb}{\sin kb \sin kl - 2(\cos kl - \cos\theta) \cos kb}. \tag{118}$$

As a second example the phase shift in the case of the complete graph K_n that will be studied in the next section reads

$$\operatorname{cotg}(\delta/2) = \cos(\varphi) \frac{\cos(k\ell) + \cos(\varphi) - 1}{\cos(k\ell) + \cos(\varphi)} \operatorname{cotg}(k\ell/2), \tag{119}$$

where $\cos(\varphi) = 1/(n-1)$. As expected the scattering length $d\delta/dk|_{k=0} = 2(n(n-1)/2)\,\ell = 2L$ is a measure of the total length of the graph.

12. APPLICATION TO THE CASE OF THE COMPLETE GRAPH K_n

As an illustration of the previous formalism it is interesting to consider the particular case where the graph $\mathcal{G}$ is the complete graph K_n whose $V = n$ vertices are all connected (see Fig. 7). Then the number of bonds is $B = n(n-1)/2$.

In the case where all the bonds of a graph have the same length ℓ one obtains

$$\det(M) = \left(\frac{1}{\sinh\sqrt{\gamma}\,\ell}\right)^{n} P((n-1)\operatorname{ch}(\sqrt{\gamma}\,\ell)), \tag{120}$$

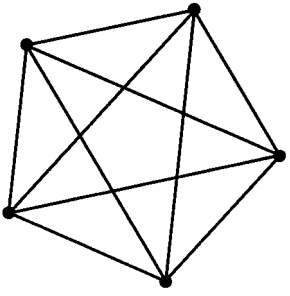


FIG. 7. The complete graph K_5.

where $P(X) = \det(X\delta_{\alpha\beta} - a_{\alpha\beta})$ is the characteristic polynomial of the graph. The characteristic polynomial of K_n can be found in classical textbooks. For the complete graphs $a_{\alpha\beta} = 1 - \delta_{\alpha\beta}$; thus the determinant involved in $P(X)$ is of the same form as the determinant of matrix F given in Appendix D. This gives the following expression for the spectral determinant

$$S(\gamma) = (\sqrt{\gamma})^{(3n/2)-(n^2/2)} (\operatorname{sh} \sqrt{\gamma}\,\ell)^{(n^2/2)-(3n/2)} (n-1)(\operatorname{ch} \sqrt{\gamma}\,\ell - 1) \times [(n-1) \operatorname{ch} \sqrt{\gamma}\,\ell + 1]^{n-1}. \tag{121}$$

By calculating the inverse Laplace transform of $(\partial/\partial\gamma) \ln S(\gamma)$ one obtains the partition function

$$Z(t) = \frac{n(n-1)\ell}{4\sqrt{\pi t}} + \frac{n(3-n)}{4} + \frac{\ell}{2\sqrt{\pi t}} \left\{ \left[\theta\left(\frac{\ell^2}{4\pi t}\right) - 1 \right] + \frac{n(n-3)}{2} \left[\theta\left(\frac{\ell^2}{\pi t}\right) - 1 \right] + 2(n-1) \sum_{k=1}^{\infty} (-1)^k T_k\left(\frac{1}{n-1}\right) e^{-k^2\ell^2/4t} \right\}, \tag{122}$$

where $\theta(x) = \sum_{k=-\infty}^{+\infty} \exp(-\pi k^2 x)$ is the Jacobi θ function, and $T_k(x)$ are Tchebychev polynomials.

(a) *Short Time Limit*

Equation (122) is written in the form of the Roth formula, appropriate for short times. The first contributions coming from the expansion of (122) in the limit $t \to 0$ give

$$Z(t) = \frac{L}{2\sqrt{\pi t}} + \frac{V-B}{2} + \frac{1}{2\sqrt{\pi t}} \left\{ \frac{n(n-1)}{2} 2\ell \left(\frac{2}{n-1} - 1\right)^2 e^{-\ell^2/t} + 2\frac{n(n-1)(n-2)}{3!} 3\ell \left(\frac{2}{n-1}\right)^3 e^{-9\ell^2/4t} + \cdots \right\}. \tag{123}$$

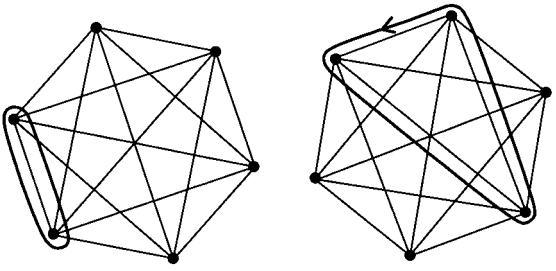


FIG. 8. Some orbits associated with the first terms in the brackets of (124) for the complete graph K_6.

The first two terms coincide with the first terms of the Roth formula. For the two following terms we recognize the contributions of the shortest orbits represented in Fig. 8. For the orbits of length 2ℓ, the factor $((2/n-1)-1)^2$ is the weight $\alpha(C)$ of those orbits and $n(n-1)/2$ their number. The next term corresponds to orbits of length 3ℓ with weight $\alpha(C)=(2/(n-1))^3$. Their number is $2(n(n-1)(n-2)/3!)$ where the additional factor 2 comes from time-reversed orbits.

(b) *Long Time Limit*

For the graph K_n it is also possible to study the limit $t\to\infty$. Introducing φ, defined by $\cos\varphi=1/(n-1)$, one may use the identity $T_k(\cos\varphi)=\cos k\varphi$ and the Poisson summation formula to find

$$Z(t)=\theta\left(\frac{4\pi t}{\ell^2}\right)+\frac{n(n-3)}{4}\left[\theta\left(\frac{\pi t}{\ell^2}\right)-1\right]+(n-1)\sum_{k=-\infty}^{+\infty} e^{-4\pi^2/\ell^2)[k-(1/2\pi)(\varphi+\pi)]^2 t}. \tag{124}$$

It is easy to see that

$$Z(t)=1+O(e^{-\kappa t}), \tag{125}$$

where the contribution of the first term comes from the constant zero mode $\psi_0(x\in\mathcal{G})=1/\sqrt{L}$.

(c) *The Eigenvalue Spectrum*

Equation (124) provides the whole spectrum of K_n. The first two terms describe a series of states $E_{12,k}=k^2(\pi^2/\ell^2)$, $k\in\mathbb{N}$, with degeneracies $d_{12,k=0}=1$, $d_{12,k}=n(n-3)/2$ if k is odd and $d_{12,k}=2+(n(n-3)/2)$ if k is even. The third term generates energies $E_{3,k}=(\pi^2/\ell^2)(2k-1-\frac{\varphi}{\pi})^2$, $k\in\mathbb{Z}$, with degeneracies $d_{3,k}=n-1$. These states are similar to those of a ring pierced by a flux, where the parameter φ related to the coordination plays the role of the flux.

For $n \geqslant 3$, $\frac{\varphi}{\pi} \in [\frac{1}{3}, \frac{1}{2}[$ and one may reorganize the energy levels:

Energy	Degeneracy
$E_0 = E_{12,0} = 0$	$d_0 = 1$
$E_1 = E_{3,1} = \frac{\pi^2}{\ell^2}\left(1 - \frac{\varphi}{\pi}\right)^2$	$d_1 = n - 1$
$E_2 = E_{12,1} = \frac{\pi^2}{\ell^2}$	$d_2 = \frac{n(n-3)}{2}$
$E_3 = E_{3,0} = \frac{\pi^2}{\ell^2}\left(1 + \frac{\varphi}{\pi}\right)^2$	$d_3 = n - 1$
$E_4 = E_{12,2} = \frac{\pi^2}{\ell^2} 2^2$	$d_4 = 2 + \frac{n(n-3)}{2}$
$E_5 = E_{3,2} = \frac{\pi^2}{\ell^2}\left(3 - \frac{\varphi}{\pi}\right)^2$	$d_5 = n - 1$
$\vdots$	$\vdots$

The case $n = 3$ corresponds to the ring of length 3ℓ. In this case $\varphi/\pi = 1/3$ and one recovers the well-known spectrum.

It is interesting to note that despite the particle exploring a volume $L \simeq \frac{1}{2} n^2 \ell$ at large n, the energy of the first excited state $E_1 \simeq \pi^2/4\ell^2$ is not of order $1/L^2$, as one could have naively guessed, but instead of order $1/\ell^2$.

13. CONCLUSION

We have investigated spectral properties of the Laplacian on graphs by providing several equivalent representations of the corresponding spectral determinant. This has been achieved thanks to a path integral formulation and to the fact that the spectral determinant can be written in terms of the propagator of a 2D harmonic oscillator thus leading to a set of straightforward Gaussian integrals. We have thus obtained an expression of the spectral determinant as a trace formula involving the contribution of an infinite number of periodic orbits. Using a systematic diagrammatic method, we expressed the finite number of terms of the determinant as contributions of a finite number of orbits. Although it has been already clear in the literature that such a reduction is possible, the present formalism allows us to implement it directly for any given graph.

The flexibility and the relative simplicity of this formalism are a hint for using it in a broader range of problems. For networks of mesoscopic and coherent conductors, it may help to compute both thermodynamic and transport properties in some non-trivial situations such as the local distribution of persistent currents in a network driven by a far remote Aharonov–Bohm flux. Along the same lines, it could be

possible to address the problem of topological properties of fractal networks like the Sierpinski gasket subject to a distribution of Aharonov–Bohm fluxes.

APPENDIX A

The Spectral Determinant Obtained by Constructing Green's Function on the Graph

We want to solve the diffusion equation

$$(\gamma - d_x^2)\, G(x, y) = \delta(x - y) \tag{126}$$

on a graph made of V vertices (or nodes) linked by B bonds. y is the source for the diffusion. The solution of (126) is of the form

$$G(x, y) = \sum_n \frac{\psi_n(x)\, \psi_n^*(y)}{\gamma + E_n}, \tag{127}$$

where ψ_n are the eigenfunctions of the operator $-d_x^2$. The spectral determinant is obtained by spatial integration of the diagonal Green's function $G(y, y)$:

$$\int dy\, G(y, y) = \sum_n \frac{1}{\gamma + E_n} = \frac{\partial}{\partial \gamma} \ln S(\gamma). \tag{128}$$

For a given source located in y, the diffusion equation is solved on each bond $(\alpha\beta)$ in terms of the values $G(\alpha, y)$ and $G(\beta, y)$ at the nodes

$$G(x, y) = G(\alpha, y)\, \mathrm{ch}\, \sqrt{\gamma}\, x + (G(\beta, y) - G(\alpha, y)\, \mathrm{ch}\, \sqrt{\gamma}\, l_{\alpha\beta}) \frac{\mathrm{sh}\, \sqrt{\gamma}\, x}{\mathrm{sh}\, \sqrt{\gamma}\, l_{\alpha\beta}}, \tag{129}$$

where x is the linear coordinate on the bond $(\alpha\beta)$ of length $l_{\alpha\beta}$.

Current conservation at the vertex α

$$-\sum_\beta d_{x_{\alpha\beta}} G(x_{\alpha\beta} = 0, y) = \delta_{\alpha, y}, \tag{130}$$

where the sum stands over the nearest vertices of α, leads to the equations

$$G(\alpha, y) \sum_\beta \coth \eta_{\alpha\beta} - \sum_\beta \frac{G(\beta, y)}{\mathrm{sh}\, \eta_{\alpha\beta}} = \frac{\delta_{\alpha, y}}{\sqrt{\gamma}}, \tag{131}$$

where $\eta_{\alpha\beta} = \sqrt{\gamma}\, l_{\alpha\beta}$. We have thus obtained a system of $(V+1)$ linear equations for the $(V+1)$ variables $G(\alpha, y)$, where α can be either a node of the graph or the source point y,

$$M_y \begin{pmatrix} G(\alpha_1, y) \\ \vdots \\ G(y, y) \\ \vdots \\ G(\alpha_V, y) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 1/\sqrt{\gamma} \\ \vdots \\ 0 \end{pmatrix}, \tag{132}$$

where the $(V+1)\times(V+1)$ matrix M_y is defined by Eqs. (35) and (36). Here, α and β are either vertices of the graph or the source point located in y. One now wants to calculate $G(y, y)$. First, using (131), it is written in terms of $G(a, y)$ and $G(b, y)$, where a and b are the vertices ending the bond to which y belongs,

$$G(y, y)(\coth \eta_{ay} + \coth \eta_{yb}) - \frac{G(a, y)}{\operatorname{sh} \eta_{ay}} - \frac{G(b, y)}{\operatorname{sh} \eta_{by}} = \frac{1}{\sqrt{\gamma}}, \tag{133}$$

so that

$$G(y, y) = \frac{1}{\operatorname{sh} \eta_{ab}} \left(\frac{\operatorname{sh} \eta_{ay} \operatorname{sh} \eta_{by}}{\sqrt{\gamma}} + G(a, y) \operatorname{sh} \eta_{by} + G(b, y) \operatorname{sh} \eta_{ay} \right). \tag{134}$$

The variable $G(y, y)$ can then be eliminated in the previous system. The two equations for $G(a, y)$ and $G(b, y)$ are modified as

$$G(a, y) \sum_{\beta} \coth \eta_{a\beta} - \sum_{\beta} G(\beta, y) \frac{1}{\operatorname{sh} \eta_{a\beta}} = \frac{1}{\sqrt{\gamma}} \frac{\operatorname{sh} \eta_{yb}}{\operatorname{sh} \eta_{ab}} \tag{135}$$

and the $(V-2)$ other equations are unchanged. We obtain now a system for the V variables $G(\alpha, y)$,

$$M \begin{pmatrix} G(\alpha_1, y) \\ \vdots \\ G(a, y) \\ \vdots \\ G(b, y) \\ \vdots \\ G(\alpha_{V-2}, y) \end{pmatrix} = \frac{1}{\sqrt{\gamma} \operatorname{sh} \eta_{ab}} \begin{pmatrix} 0 \\ \vdots \\ \operatorname{sh} \eta_{yb} \\ \vdots \\ \operatorname{sh} \eta_{ay} \\ \vdots \\ 0 \end{pmatrix}, \tag{136}$$

where M is defined in (35) and (36). a and b are now two of the V vertices and the source point y is now excluded.

By inversion of the matrix M, one obtains $G(a, y)$ and $G(b, y)$,

$$G(a, y) = \frac{1}{\sqrt{\gamma}\,\mathrm{sh}\,\eta_{ab}} (T_{aa}\,\mathrm{sh}\,\eta_{yb} + T_{ab}\,\mathrm{sh}\,\eta_{ay}), \tag{137}$$

where $T = M^{-1}$. From (134), one finally obtains $G(y, y)$:

$$G(y, y) = \frac{1}{\sqrt{\gamma}} \left\{ \frac{\mathrm{sh}\,\eta_{ay}\,\mathrm{sh}\,\eta_{yb}}{\mathrm{sh}\,\eta_{ab}} + \frac{1}{\mathrm{sh}^2\,\eta_{ab}} [\, T_{aa}\,\mathrm{sh}^2\,\eta_{by} + T_{bb}\,\mathrm{sh}^2\,\eta_{ay} + 2T_{ba}\,\mathrm{sh}\,\eta_{ay}\,\mathrm{sh}\,\eta_{yb}\,] \right\}. \tag{138}$$

The spatial integral of $G(y, y)$ on the bond (ab) can be written as

$$\int_a^b dy\, G(y, y) = \frac{1}{2\gamma} \left\{ \eta_{ab} \coth \eta_{ab} - 1 + (T_{aa} + T_{bb}) \left(1 + 2\gamma \frac{\partial}{\partial \gamma} \right) \coth \eta_{ab} - 2T_{ba} \left(1 + 2\gamma \frac{\partial}{\partial \gamma} \right) \frac{1}{\mathrm{sh}\,\eta_{ab}} \right\}, \tag{139}$$

where we have used the equalities

$$\frac{-\eta}{\mathrm{sh}^2\,\eta} = 2\gamma \frac{\partial}{\partial \gamma} \coth \eta \tag{140}$$

$$-\eta \frac{\cosh \eta}{\mathrm{sh}^2\,\eta} = 2\gamma \frac{\partial}{\partial \gamma} \frac{1}{\mathrm{sh}\,\eta}. \tag{141}$$

Summing over all the bonds of the graph and using the following identities:

$$\sum_{(ab)} \left((T_{aa} + T_{bb}) \coth \eta_{ab} - 2 \frac{T_{ba}}{\mathrm{sh}\,\eta_{ab}} \right) = \mathrm{Tr}\,\{TM\} = V, \tag{142}$$

$$\sum_{(ab)} \left((T_{aa} + T_{bb}) \frac{\partial}{\partial \gamma} \coth \eta_{ab} - 2T_{ba} \frac{\partial}{\partial \gamma} \frac{1}{\mathrm{sh}\,\eta_{ab}} \right) = \mathrm{Tr} \left\{ T \frac{\partial}{\partial \gamma} M \right\}, \tag{143}$$

$$\eta \coth \eta = 2\gamma \frac{\partial}{\partial \gamma} \ln \mathrm{sh}\,\eta, \tag{144}$$

we find that the sum $P = \int_{\mathrm{Graph}} dy\, G(y, y,)$ simplifies considerably into

$$P = \frac{\partial}{\partial \gamma} \sum_{(ab)} \ln \mathrm{sh}\,\eta_{ab} + \frac{V - B}{2\gamma} + \mathrm{Tr} \left\{ M^{-1} \frac{\partial}{\partial \gamma} M \right\}. \tag{145}$$

Using the following property $\mathrm{Tr}\{M^{-1}(\partial/\partial\gamma)M = (\partial/\partial\gamma)\ln\det(M)$ one finally obtains

$$P = \frac{\partial}{\partial\gamma}\ln S(\gamma), \tag{146}$$

where

$$S(\gamma) = \gamma^{(V-B)/2}\prod_{(ab)}\mathrm{sh}\,\eta_{ab}\det(M). \tag{147}$$

APPENDIX B

The Symmetry of the Coefficients of the Diagrammatic Expansion

The purpose of this appendix is to discuss the symmetry properties between the coefficients appearing in the expansion of the determinant discussed in Section 7. This symmetry, a consequence of properties of the matrix E, considerably symplifies the calculation of the spectral determinant by the diagrammatic method. Since the presence of a magnetic field does not affect any point of the following discussion, one will forget it. We shall start by considering first the case of Neumann boundary conditions and we will indicate at the end of the appendix how to extend the result to the more general case.

Let us write $\det(1-E) = \det(E)\det(1-E^{-1})$. The inverse of E is easily calculated since $\varepsilon^{-1} = \varepsilon^{\mathrm{T}}$ and D is diagonal: $D_{ij}^{-1} = \delta_{ij}e^{\sqrt{\gamma}\,l_i}$. Then one has

$$\det(1-E) = \det(1-\varepsilon D) = (-1)^{V-B}e^{-2\sqrt{\gamma}L}\det(1-\varepsilon D^{-1}) \tag{148}$$

(for the calculation of $\det(E)$, see Appendix D). The matrix εD^{-1} is equal to the matrix E in which one has replaced $\sqrt{\gamma}$ by $-\sqrt{\gamma}$. This implies that $\det(1-\varepsilon D)$ and $\det(1-\varepsilon D^{-1})$ exhibit similar expansions (with the same numerical factors).

To use this relation it is convenient to organize the expansion of $\det(1-E)$ in terms associated with diagrams or product of diagrams involving the same set of arcs. Let us call $g_n = \{i_1, ..., i_n\}$ a set of n arcs of $\mathcal{G}$ (in particular $g_0 = \phi$ and $g_{2B} = \mathcal{G}$). One may write

$$\det(1-E) = \sum_{n=0}^{2B}\sum_{g_n}\kappa[g_n]\,e^{-\sqrt{\gamma}\,l[g_n]}, \tag{149}$$

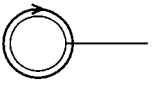
where $l[g_n] = l_{i_1} + \cdots + l_{i_n}$. The coefficient $\kappa[g_n]$ is a sum of coefficients $\alpha(\tilde{C})$ or a sum of the product of such coefficients. Equation (148) implies that there is a relation between the terms involving diagrams with a large number of arcs and a small number of arcs. More precisely, as a consequence of the obvious relation $l[\mathcal{G}-g_n] = 2L - l[g_n]$, we obtain

$$\kappa[\mathcal{G}-g_n] = (-1)^{V-B}\kappa[g_n], \tag{150}$$

where $\mathscr{G} - g_n = \{i / i \notin g_n\}$ is the set of all arcs of $\mathscr{G}$ except those of g_n. As a simple consequence, the term $\det(1-E)$ related to the diagrams of length $2L$ is precisely $(-1)^{V-B} e^{-2\sqrt{\gamma} L}$ since $\kappa[\mathscr{G}] = (-1)^{V-B} \kappa[\phi]$

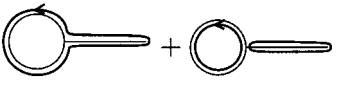
The use of relation (150) is particularly powerful since it allows one to consider only half of the expansion (149). Moreover the terms $\kappa[g_n] e^{-\sqrt{\gamma} l[g_n]}$ for small n involve not only a small number of diagrams but also the simplest diagrams, constructed with less than B arcs. Taking into account only the B first terms in (149) considerably reduces the number of diagrams to be considered.

As an example, one may apply this relation for the graph of Fig. 5. For the term $n=1$ in (149), the sum over g_1 brings four ensembles $\{1\}$, $\{\bar{1}\}$, $\{2\}$, and $\{\bar{2}\}$. Only the first two give some contributions since $\{2\}$ and $\{\bar{2}\}$ are not associated with any orbit. Consider the case where $g_1 = \{1\}$. Then the term $\kappa[\{1\}] e^{-\sqrt{\gamma} l[\{1\}]}$, given by the diagram



(151)

has the same numerical factor as $\kappa[\{\bar{1}, 2, \bar{2}\}] e^{-\sqrt{\gamma} l[\{\bar{1}, 2, \bar{2}\}]}$ associated with the two following diagrams:



(152)

In (75) only the first 3 diagrams, among the 15, have to be considered and all other terms are given by relation (150). It is also possible to check the symmetry (150) on Eq. (77).

To end this appendix let us explain how relation (150) is generalized for mixed boundary conditions. In this case the inverse of ε is given by ε^{T} in which one has replaced $\sqrt{\gamma}$ by $-\sqrt{\gamma}$ (the coefficients $\alpha(C)$ and $\kappa[g_n]$ now depend on $\sqrt{\gamma}$). One has $\det(1-E) = \det(E)[\det(1-\varepsilon D)|_{\sqrt{\gamma} \to -\sqrt{\gamma}}]$. Then Eq. (150) reads in the more general case

$$\kappa[\mathscr{G} - g_n] = \det(\varepsilon)\, \kappa[g_n]|_{\sqrt{\gamma} \to -\sqrt{\gamma}}, \tag{153}$$

$\det(\varepsilon)$ being given by (170).

APPENDIX C

Precisions on Loops and Multiple Bonds between Vertices

In Section 3 we have assumed that a bond links always two different vertices and that there is only one bond between two different vertices. Formule (35) and (36)

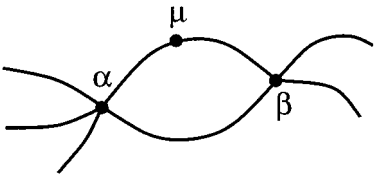


FIGURE 9

apply to those kinds of graph. As we remarked in a footnote, if two vertices are linked by two bonds, one can introduce a vertex in one of those bonds to fall back to the situation of Section 3 (see Fig. 9). Similarly if a bond starts and finishes at the same vertex to form a loop it is possible to separate it into two bonds by introducing an additional vertex (see Fig. 10). Of course, these operations do not change the spectral properties of the graph. Any graph can be described as in Section 3 but the price to pay is to add some vertices with coordination 2, which increases V and B. In Sections 6 and 7 one has already noticed that vertices of coordination 2 play no role in the construction of orbits. On the other hand, since the sizes of the matrices that we have introduced are related to B and V, the calculations would become easier if it were possible to minimize those numbers. It is the purpose of this section to explain how to generalize (35) and (36) to the more general case where a loop can be present at a vertex and several bonds link two vertices. A discussion is also given in [10] using a different method. We set $\gamma = 1$.

(i) Expression (34) is again a good starting point. One considers the determinant of a graph, one part of which is represented in Fig. 9. In (34), the terms that involve vertex μ are

$$S(\gamma)^{-1} = \int \cdots \int d\phi_\mu \, d\bar{\phi}_\mu G_{l_{\beta\mu}}(\phi_\beta, \phi_\mu) \, G_{l_{\mu\alpha}}(\phi_\mu, \phi_\alpha) \cdots . \tag{154}$$

Since ϕ_μ does not appear anywhere else one can integrate over ϕ_μ, using the completeness relation for the propagator. One finds

$$S(\gamma)^{-1} = \int \cdots G_{l_{\beta\mu} + l_{\mu\alpha}}(\phi_\beta, \phi_\alpha) \cdots . \tag{155}$$

In (155), the integral contains two propagators that propagate the field from vertex α to vertex β: $G_{l_{\beta\mu} + l_{\mu\alpha}}(\phi_\beta, \phi_\alpha)$ and $G_{l_{\alpha\beta}}(\phi_\beta, \phi_\alpha)$. It is now easy to see what is the natural generalization of (35) and (36) if $B_{\alpha\beta}$ bonds of lengths $l^j_{\alpha\beta}$ link the two vertices:

$$M_{\alpha\alpha} = \sum_{j=1}^{B_{\alpha\beta}} \coth(\sqrt{\gamma}\, l^j_{\alpha\beta}) + \cdots \tag{156}$$

$$M_{\alpha\beta} = -\sum_{j=1}^{B_{\alpha\beta}} \frac{e^{i\theta^j_{\alpha\beta}}}{\operatorname{sh}(\sqrt{\gamma}\, l^j_{\alpha\beta})} . \tag{157}$$

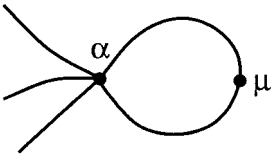


FIGURE 10

Let us stress that the elimination of a vertex of coordination $m_\mu = 2$ is particularly straightforward with expression (34), since it is a consequence of the completeness relation for the propagtor of the two-dimensional harmonic oscillator.

(ii) If one now considers a graph as in Fig. 10, one can use the same trick as before. It is then easy to see that the contribution of the loop is

$$S(\gamma)^{-1} = \int \cdots G_{l^1_{\alpha\mu}+l^2_{\alpha\mu}}(\phi_\alpha \mathrm{e}^{-i\theta^1_{\alpha\mu}}, \phi_\alpha e^{-i\theta^2_{\alpha\mu}}) \cdots, \tag{158}$$

where $l^1_{\alpha\mu}$ and $l^2_{\alpha\mu}$ are the lengths of the two bonds. Writing $l_{\alpha\alpha} = l^1_{\alpha\mu} + l^2_{\alpha\mu}$ for the length of the loop and $\theta_{\alpha\alpha} = \theta^1_{\alpha\mu} + \theta^2_{\mu\alpha}$ for the flux that pierces it, it is easy to see that the loop gives only a contribution to $M_{\alpha\alpha}$:

$$M_{\alpha\alpha} = 2\coth(\sqrt{\gamma}\, l_{\alpha\alpha}) - 2\frac{\cos\theta_{\alpha\alpha}}{\mathrm{sh}(\sqrt{\gamma}\, l_{\alpha\alpha})} + \cdots. \tag{159}$$

To conclude, gathering points (i) and (ii) together one gives the general expression for M,

$$M_{\alpha\beta} = \delta_{\alpha\beta}\left[\sum_\mu a_{\alpha\mu} \sum_{j=1}^{B_{\alpha\mu}} \coth(\sqrt{\gamma}\, l^j_{\alpha\mu}) + 2\sum_{j=1}^{L_\alpha}\left(\coth(\sqrt{\gamma}\, l^j_{\alpha\alpha}) - \frac{\cos(\theta^j_{\alpha\alpha})}{\mathrm{sh}(\sqrt{\gamma}\, l^j_{\alpha\alpha})}\right)\right] - a_{\alpha\beta}\sum_{j=1}^{B_{\alpha\beta}} \frac{e^{i\theta^j_{\alpha\beta}}}{\mathrm{sh}(\sqrt{\gamma}\, l^j_{\alpha\beta})}, \tag{160}$$

where L_α is the number of loops at vertex α (we did not change[8] the definition of $a_{\alpha\beta}$ which is still 0 or 1 depending on whether or not the vertices are connected; $a_{\alpha\alpha} = 0$). Let us remark that $M_{\alpha\beta}$ may be expressed in the more condensed form [6, 10]

$$M_{\alpha\beta} = \delta_{\alpha\beta}\left[\sum_{\substack{\text{arcs } b \text{ starting} \\ \text{from vertex } \alpha}} \coth(\sqrt{\gamma}\, l_b) - 2\sum_{j=1}^{L_\alpha} \frac{\cos(\theta^j_{\alpha\alpha})}{\mathrm{sh}(\sqrt{\gamma}\, l^j_{\alpha\alpha})}\right] - a_{\alpha\beta}\sum_{\substack{\text{arcs } b \text{ linking} \\ \text{vertices } \alpha \text{ and } \beta}} \frac{e^{i\theta_b}}{\mathrm{sh}(\sqrt{\gamma}\, l_b)}, \tag{161}$$

[8] This implies that $\sum_\beta a_{\alpha\beta}$ is no more the coordination of vertex α. One has $m_\alpha = \sum_\beta a_{\alpha\beta} B_{\alpha\beta} + 2L_\alpha$.

where in the first sum over all arcs starting from vertex α, the case of a loop brings twice the same contribution, as in (159), since it is associated with two arcs starting from the vertex.

As an example let us consider the graph of Fig. 5. The number of vertices can be reduced to 2 and the spectral determinant is given by a determinant of a 2×2 matrix,

$$S(\gamma)=\operatorname{sh} l \operatorname{sh} b \begin{vmatrix} \coth b+2\coth l-2\dfrac{\cos\theta}{\operatorname{sh} l} & -\dfrac{1}{\operatorname{sh} b} \\ -\dfrac{1}{\operatorname{sh} b} & \coth b \end{vmatrix}, \tag{162}$$

which gives (79).

APPENDIX D

Some Properties of the Matrices Q, R, D, ε, and E

In the more general case, in the presence of a magnetic field and with mixed boundary conditions, the four matrices that we have introduced in Section 5 read

$$Q_{(\alpha\beta)(\mu\nu)}=a_{\alpha\beta}a_{\mu\nu}\delta_{\alpha\mu}\left(\frac{2}{m_\alpha+\dfrac{\lambda_\alpha}{\sqrt{\gamma}}}-\delta_{\beta\nu}\right)e^{i(\theta_{\alpha\beta}-\theta_{\alpha\nu}/2)}, \tag{163}$$

$$R_{(\alpha\beta)(\mu\nu)}=a_{\alpha\beta}a_{\mu\nu}\delta_{\alpha\nu}\delta_{\beta\mu}e^{-\sqrt{\gamma}\,l_{\alpha\beta}}, \tag{164}$$

$$\varepsilon_{(\alpha\beta)(\mu\nu)}=a_{\alpha\beta}a_{\mu\nu}\delta_{\beta\mu}\left(\frac{2}{m_\beta+\dfrac{\lambda_\beta}{\sqrt{\gamma}}}-\delta_{\alpha\nu}\right), \tag{165}$$

and

$$D_{(\alpha\beta)(\mu\nu)}=a_{\alpha\beta}a_{\mu\nu}\delta_{\alpha\mu}\delta_{\beta\nu}e^{-\sqrt{\gamma}\,l_{\mu\nu}+i\theta_{\mu\nu}}. \tag{166}$$

The inverses of those matrices are easily calculated. They are given by their hermitic conjugates in which one replaces $\sqrt{\gamma}$ by $-\sqrt{\gamma}$: $Q^{-1}=Q^{\dagger}|_{\sqrt{\gamma}\to-\sqrt{\gamma}}$, *etc.* (let us recall that the transposition is defined as $Q^{\mathrm{T}}_{(\alpha\beta)(\mu\nu)}=Q_{(\mu\nu)(\alpha\beta)}$). For example,

$$\varepsilon^{-1}_{(\alpha\beta)(\mu\nu)}=a_{\alpha\beta}a_{\mu\nu}\delta_{\alpha\nu}\left(\frac{2}{m_\alpha-\dfrac{\lambda_\alpha}{\sqrt{\gamma}}}-\delta_{\beta\mu}\right). \tag{167}$$

This shows that in the positive part of the spectrum, when $\gamma = -k^2$, the five matrices Q, R, D, ε, and E are unitary matrices. Let us notice that for Neumann boundary conditions $\lambda_\alpha = 0$, then $Q^{-1} = Q$ and $\varepsilon^{-1} = \varepsilon^{\mathrm{T}}$.

We now compute the determinants of those matrices. To start with, one considers the sub-matrices Q_α defined in (47). We write the matrix element

$$(Q_\alpha)_{\beta\nu} = \left(\frac{2}{m_\alpha + \lambda_\alpha/\sqrt{\gamma}} - \delta_{\beta\nu} \right) e^{i(\theta_{\alpha\beta} - \theta_{\alpha\nu}/2)},$$

where it is understood that β and ν belong to the set of m_α neighbors of α.

To compute the determinant of the matrix, the first step is to eliminate all the phases with a unitary transformation. Then one has to consider an $n \times n$ matrix of the form $F_{\alpha\beta} = a - \delta_{\alpha\beta}$. It is possible to compute the determinant of such a matrix using a recursive method; one finds $\det(F) = (-1)^n (1 - n\,a)$. Coming back to Q_α one has $\det(Q_\alpha) = (-1)^{m_\alpha + 1} ((m_\alpha - \lambda_\alpha/\sqrt{\gamma})/(m_\alpha + \lambda_\alpha/\sqrt{\gamma}))$. It follows that

$$\det(Q) = (-1)^V \prod_{\alpha=1}^{V} \frac{m_\alpha - \lambda_\alpha/\sqrt{\gamma}}{m_\alpha + \lambda_\alpha/\sqrt{\gamma}}. \tag{168}$$

If $\gamma = -k^2$, this is indeed a complex number of unit modulus.

Next one would like to compute $\det(R)$. The matrix R which couples time-reversed arcs has $2B$ non-vanishing elements. The determinant of R is then given by the product of all elements of R times the sign of the permutation $\mathscr{P}(1, \bar{1}, ..., B, \bar{B}) = (\bar{1}, 1, ..., \bar{B}, B)$ that exchanges each arc with its time-reversed arc; it follows that

$$\det(R) = (-1)^B e^{-2\sqrt{\gamma} L}. \tag{169}$$

Since $\varepsilon = (\mathscr{U}^\dagger Q(\gamma)\, R(\gamma = 0)\, \mathscr{U})^{\mathrm{T}}$, it is easy to deduce its determinant,

$$\det(\varepsilon) = (-1)^{V-B} \prod_{\alpha=1}^{V} \frac{m_\alpha - \lambda_\alpha/\sqrt{\gamma}}{m_\alpha + \lambda_\alpha/\sqrt{\gamma}}, \tag{170}$$

which involves the topological invariant $V - B$.

The determinant of E is given by $\det(E) = \det(\varepsilon)\, e^{-2\sqrt{\gamma} L}$. For Neumann boundary conditions $\det(E) = (-1)^{V-B} e^{-2\sqrt{\gamma} L}$.

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