Quantum chaos on discrete graphs

Uzy Smilansky

Department of Physics of Complex Systems, The Weizmann Institute of Science, Rehovot 76100, Israel.

and

Isaac Newton Institute for Mathematical Sciences, 20 Clarkson Road, Cambridge CB3 0EH, UK.

E-mail: uzy.smilansky@weizmann.ac.il

Abstract. Adapting a method developed for the study of quantum chaos on *quantum (metric)* graphs [1], spectral ζ functions and trace formulae for *discrete* Laplacians on graphs are derived. This is achieved by expressing the spectral secular equation in terms of the periodic orbits of the graph, and obtaining functions which belongs to the class of ζ functions proposed originally by Ihara [2], and expanded by subsequent authors [3, 4]. Finally, a model of "classical dynamics" on the discrete graph is proposed. It is analogous to the corresponding classical dynamics derived for quantum graphs [1].

1. Introduction and preliminaries

Some ten years ago quantum (metric) graphs were proposed as a convenient paradigm for the study of quantum chaos in compact [1] and scattering [5] systems. The crucial point which highlighted the close similarity between metric graphs - whose only claim to complexity is their topology - and chaotic Hamiltonian flows is the formal similarity between the trace formulae [6, 7] which express the spectral densities as sums over periodic orbits. Requiring additionally that the lengths of the bonds are rationally independent, and that the graph is well connected, render the spectrum of

the Schrödinger operator on graphs sufficiently disordered to display spectral statistics which are consistent with the predictions of Random Matrix Theory. Another important contact point was the identification of the classical dynamics on the graph, which is derived from the quantum evolution, and which describes, under certain conditions, an exponential approach to equilibrium, in analogy with mixing Hamiltonian flows. The ζ function for the Peron-Frobenius operator on the graph, can be written in terms of the same periodic orbits which are used for the quantum spectral ζ function - in close similarity with the expansion of the Ruelle ζ function as a sum over periodic orbits for chaotic Hamiltonian flows. The derivation of the trace formula for quantum graphs which was presented in [1] differs from the original method [6]. It uses another approach (called sometimes the "scattering approach"), which reveals in a natural way the underlying classical dynamics.

Discrete graphs, where only the graph *topology* and not its *metric* plays a rôle are mostly studied in number theory, combinatorics *etc.* There is abundant literature relating to various aspects of graphs. Much of the relevant material to the present discussion can be found in [8, 9]. Audrey Terras' review [10] surveys the field, and its relation to quantum chaos. The present work attempts to highlight further this quantum chaos connection, by proposing trace formulae and spectral ζ functions, and linking them with the Ihara ζ function [2] and some of its recent generalizations. To introduce these concepts, a few preliminaries and definitions are necessary, and they are provided below.

A graph $\mathcal{G}$ consists of V vertices connected by B bonds. The $V \times V$ *connectivity* (or *adjacency*) matrix C is defined such that $C_{i,j} = 1(0)$ if the vertices i, j are connected (disconnected). Graphs with parallel bonds or loops are excluded. The *valency* (some times referred to as the *degree*) of a vertex is the number of bonds which emanate from a vertex. It is denoted by $v_i = \sum_{j=1}^{V} C_{i,j}$. To any bond $b = (i, j)$ one can assign an arbitrary direction, resulting in two *directed bonds*, $d = (i, j)$ and $\hat{d} = (j, i)$. Thus, the graph can be viewed as V vertices connected by bonds $b = 1, \cdots, B$ or by $2B$

directed bonds $d = 1, \cdots, 2B$. (The notation b for bonds and d for directed bonds will be kept throughout). It is convenient to associate with each directed bond $d = (j, i)$ its *origin* $o(d) = i$ and *terminus* $t(d) = j$ so that d points from the vertex i to the vertex j. The bond d' follows d if $t(d) = o(d')$. A periodic orbit (cycle) of length n is a sequence of n successively following directed bonds $d_1, \cdots, d_n$ and d_1 follows d_n. Cyclic permutations of the bonds generate the same periodic orbit. A primitive periodic orbit is an orbit which cannot be written as a repetition of a shorter periodic orbit. The set of primitive n-periodic orbits will be denoted by $\mathcal{P}(n)$, and $\mathcal{P} = \bigcup_{n=2}^{\infty} \mathcal{P}(n)$. An important subset of $\mathcal{P}(n)$ is the set of n primitive periodic orbits without back-scatter, namely, periodic orbits where $d_{i+1} \neq \hat{d}_i$. The corresponding sets will be denoted by $\mathcal{C}(n)$ and $\mathcal{C} = \bigcup_{n=2}^{\infty} \mathcal{C}(n)$.

The Laplacian of a discrete graph is defined as

$$L \equiv -C + D, \tag{1}$$

where C is the connectivity matrix, and D is a diagonal matrix with $D_{i,i} = v_i$. It is a self-adjoint operator whose spectrum consists of V non negative real numbers. The spectrum is determined as the zeros of the secular function (characteristic polynomial)

$$Z_L(\lambda) \equiv \det(\lambda I^{(V)} - L) \ . \tag{2}$$

Here, λ is the spectral parameter and $I^{(V)}$ is the unit matrix in V dimensions. The lowest eigenvalue is 0, and it is simple if and only if the graph is connected.

It is sometimes convenient to generalize the Laplacian (1) by replacing the matrix C by a matrix $\tilde{C}$ whose zero entries coincide with those of C, but arbitrary, strictly positive weights $w_{i,j}$ $(= w_{j,i})$ replace the values 1 where $C_{i,j} = 1$. One then defines $\tilde{D}_{i,i} \equiv u_i = \sum_j \tilde{C}_{i,j}$ and the generalized Laplacian is

$$\tilde{L} \equiv -\tilde{C} + \tilde{D}. \tag{3}$$

The spectrum of $\tilde{L}$ consists of the zeros of the secular equation (characteristic polynomial) $Z_{\tilde{L}}(\lambda) \equiv \det(\lambda I^{(V)} - \tilde{L})$. The spectrum is non negative, 0 is in the spectrum and it is a simple eigenvalue if and only if the graph is connected.

The focus of the present work is on ζ functions and trace formulae for discrete graphs. This research subject was initiated by Ihara [2] who defined a ζ function for a graph as

$$\zeta(u)^{-1} \equiv \prod_n (1-u^n)^{|\mathcal{C}(n)|} \ , \tag{4}$$

where $|\mathcal{C}(n)|$ is the cardinality of the set $\mathcal{C}(n)$, and $u \in \mathbb{C}$ with $|u|$ sufficiently small to ensure the convergence of the infinite product. Following Ihara's original work, several authors (see e.g., [11] for a survey of the methods) have proved that

$$\zeta(u)^{-1} = (1-u^2)^{r-1} \det(I^{(V)} - uC + u^2 Q) \ . \tag{5}$$

Here, $r \equiv B - V + 1$ is the *rank* of the graph (the number of independent cycles on the graph or equivalently, the rank of its fundamental group). $I^{(V)}$ is the unit matrix in V dimensions, C is the connectivity matrix, and the diagonal matrix $Q \equiv D - I^{(V)}$. If the graph is v-regular, that is $v_i = v \ \ \forall i$, the non trivial poles of the Ihara ζ (the trivial poles are at $u = \pm 1$) can be easily computed from the eigenvalues of the graph Laplacian (1).

The following ζ function defined by H.M. Stark [12] will serve as an example of the more recent developments in the field. Consider a matrix Y in the space of directed bonds

$$Y_{d',d} \equiv \eta_{d',d} \ \delta_{o(d'),t(d)} \ (1 - \delta_{d',\hat{d}}). \tag{6}$$

where $\eta_{d',d}$ are arbitrary. Note that matrix elements between reversed bonds are excluded. Associate with any primitive periodic orbit $c \in \mathcal{C}$ the amplitude

$$f_c \equiv \eta_{d_n,d_{n-1}} \ \eta_{d_{n-1},d_{n-2}}, \ \cdots \ \eta_{d_2,d_1} \ \eta_{d_1,d_n} \ . \tag{7}$$

Then,

$$\zeta_E(Y)^{-1} \equiv \prod_{c \in \mathcal{C}} (1 - f_c) = \det(I^{(2B)} - Y), \tag{8}$$

where $I^{(2B)}$ is the unit matrix in $2B$ dimensions. This result will be used in the last section.

In the next section, other ζ functions are defined, discussed, and expressed as rational functions which are reminiscent of (5) and (8), but are different in many respects. Trace formulae for the spectra of the Laplacians (1,3) will also be derived. In the last section, the approach developed here will be compared with its analogues in the theory of quantum graphs, and the "classical dynamics" on the discrete graph will be proposed.

2. Secular functions, ζ functions and trace formulae

To start, an alternative form of the secular equations for the Laplacians (1,3) will be derived. It is convenient to begin with a detailed derivation for the traditional Laplacian (1). The necessary modifications for the generalized form will be indicated later. For both Laplacians, the secular function will be shown to take the form

$$Z_S(\lambda) = \frac{1}{2^B} \left(\det U(\lambda)\right)^{-\frac{1}{2}} \det\left(I^{(2B)} - U(\lambda)\right) \tag{9}$$

where $U(\lambda)$ is a unitary matrix of dimension $2B$ which depends on the spectral parameter λ. By construction, $Z_S(\lambda)$ is real for $\lambda \in \mathbb{R}$, and its zeros will be shown to coincide (with their multiplicity) with the spectrum of the Laplacian. Thus $Z_S(\lambda)$ and $Z_L(\lambda)$ can differ at most by a multiplicative function of λ which does not vanish for real λ. This construction of the secular function paraphrases the "scattering approach" introduced in [1] for quantum graphs. (Derivations which are similar in spirit were discussed in [13, 14, 15], see also [16] and references cited therein).

To compute an eigenvector $\psi = (\psi_1, \cdots, \psi_V)$ of L, corresponding to an eigenvalue λ, the following steps are taken. To each bond $b = (i, j)$ one associates a *bond wave function*

$$\psi_b(x) = a_b \, \mathrm{e}^{i\frac{\pi}{4}x} + a_{\hat{b}} \, \mathrm{e}^{-i\frac{\pi}{4}x} \quad , \quad x \in \{\pm 1\} \tag{10}$$

subject to the condition

$$\psi_b(1) = \psi_i \quad , \quad \psi_b(-1) = \psi_j \ . \tag{11}$$

Consider any vertex indexed by i, and the bonds $(b_1, b_2, ...b_{v_i})$ which emanate from i. The corresponding bond wave functions have to satisfy three requirements in order to form a proper eigenvector of L.

I. Uniqueness: The value of the eigenvector at the vertex i, ψ_i, computed in terms of the bond wave functions is the same for all the bonds emanating from i. The following $v_i - 1$ independent equalities express this requirement.

$$a_{b_1}\ \mathrm{e}^{i\frac{\pi}{4}} + a_{\hat{b}_1}\ \mathrm{e}^{-i\frac{\pi}{4}} = a_{b_2}\ \mathrm{e}^{i\frac{\pi}{4}} + a_{\hat{b}_2}\ \mathrm{e}^{-i\frac{\pi}{4}} = \ \cdots\ = a_{b_{v_i}}\ \mathrm{e}^{i\frac{\pi}{4}} + a_{\hat{b}_{v_i}}\ \mathrm{e}^{-i\frac{\pi}{4}}\ . \tag{12}$$

II. ψ is an eigenvector of L : At the vertex i, $\sum_{j=1}^{v_i} L_{i,j}\psi_j = \lambda\psi_i$. In terms of the bond wave functions this reads,

$$-\sum_{l=1}^{v_i}\left[a_{b_l}\ \mathrm{e}^{-i\frac{\pi}{4}} + a_{\hat{b}_l}\ \mathrm{e}^{+i\frac{\pi}{4}}\right] = (\lambda - v_i)\ \frac{1}{v_i}\sum_{m=1}^{v_i}\left[a_{b_m}\ \mathrm{e}^{i\frac{\pi}{4}} + a_{\hat{b}_m}\ \mathrm{e}^{-i\frac{\pi}{4}}\right]\ . \tag{13}$$

To get the equation above, ψ_i was presented as

$$\psi_i = \frac{1}{v_i}\sum_{j=1}^{v_i}\left(a_{b_j}\ \mathrm{e}^{i\frac{\pi}{4}} + a_{\hat{b}_j}\ \mathrm{e}^{-i\frac{\pi}{4}}\right)\ . \tag{14}$$

Together, (12) and (13) provide v_i homogeneous linear relations between the $2v_i$ coefficients a_d, where d stand for directed bonds which are either incoming to $(t(d) = i)$ or outgoing from $(o(d) = i)$ the vertex i. Using these equations, the outgoing coefficients are expressed in terms of the incoming ones,

$$a_d = \sum_{d'\ :\ t(d')=i} \sigma^{(i)}_{d,d'}(\lambda)\ a_{d'} \qquad \forall\ d\ :\ o(d) = i\ , \tag{15}$$

where,

$$\begin{aligned}\sigma^{(i)}_{d,d'}(\lambda)\ &= i\left(\delta_{\hat{d},d'} - \frac{2}{v_i}\frac{1}{1 - i(1 - \frac{\lambda}{v_i})}\right)\ = i\left(\delta_{\hat{d},d'} - \frac{1}{v_i}(1 + \mathrm{e}^{i\alpha_i(\lambda)})\right)\\ \mathrm{e}^{i\alpha_i(\lambda)}\ &= \frac{1 + i(1 - \frac{\lambda}{v_i})}{1 - i(1 - \frac{\lambda}{v_i})}\ .\end{aligned} \tag{16}$$

The *vertex scattering matrices* $\sigma^{(i)}(\lambda)$ are the main building blocks of the present approach. They distinguish clearly between back-scatter transitions $(\hat{d} = d')$ and the transitions to other bonds, for which the same strength is given, independently of the original and the final bonds. A straight forward computation shows that for real λ the

vertex scattering matrices are unitary matrices. They are the discrete analogues of the vertex scattering matrices derived for the Schrödinger equation on graphs [1].

III. Consistency : The linear relation between the incoming and the outgoing coefficients (15) must be satisfied simultaneously at all the vertices. However, a directed bond (i, j) when observed from the vertex j is *outgoing*, while when observed from i it is *incoming*. This consistency requirement is implemented by introducing the *Evolution Operator* $U_{d'.d}(\lambda)$ in the $2B$ dimensional space of directed bonds,

$$U_{d',d}(\lambda) = \delta_{t(d),o(d')}\ \sigma^{(t(d))}_{d',d}(\lambda)\ . \tag{17}$$

(U is also referred to in the literature as the *Bond Scattering Matrix* [1]). The evolution operator is unitary $U\ U^\dagger = I^{(2B)}$ for $\lambda \in \mathbb{R}$ due to the unitarity of its constituents $\sigma^{(i)}$. Denoting by $\mathbf{a}$ the $2B$ dimensional vector of the directed bonds coefficients a_d defined above, the consistency requirement reduces to,

$$U(\lambda)\ \mathbf{a} = \mathbf{a}\ . \tag{18}$$

This can be satisfied only for those values of λ for which

$$\xi(\lambda)\ \equiv\ \det\left(I^{(2B)} - U(\lambda)\right)\ =\ 0\ . \tag{19}$$

For real λ the spectrum of $U(\lambda)$ is restricted to the unit circle. Therefore $|\xi(\lambda)|$ is finite for all $\lambda \in \mathbb{R}$. Due to (16) the matrix elements of $U(\lambda)$ are ratios of monomials in λ. These two properties imply that $\xi(\lambda) = p(\lambda)/q(\lambda)$ where p and q are polynomials of the same degree in λ, and their degree is at most $2B$. The zeros of $q(\lambda)$ coincide with the poles of $\det U(\lambda)$. They are complex because $|\det U(\lambda)| = 1$ for $\lambda \in \mathbb{R}$. A straight forward computation yields,

$$\det U(\lambda) = \prod_{j=1}^{V} \frac{1 + i(1 - \frac{\lambda}{v_j})}{1 - i(1 - \frac{\lambda}{v_j})}\ ,\ \ \Rightarrow\ \ q(\lambda) = Const\ \prod_{j=1}^{V}\left(1 - i(1 - \frac{\lambda}{v_j})\right)\ . \tag{20}$$

Thus, $\det U$ has exactly V complex poles, implying that the degree of $p(\lambda)$ which equals the degree of $q(\lambda)$ is also V. Note finally that the zeros of $p(\lambda)$ coincide with the zeros of the secular function $Z_L(\lambda) = \det(\lambda I^{(V)} - L)$ which is also a polynomial of degree V. Hence, $p(\lambda)$ and $Z_L(\lambda)$ are identical up to a constant factor. It is convenient to

define the secular equation so that it is real on the real axis. This can be achieved by multiplying $\xi(\lambda)$ by $(\det U(\lambda))^{-\frac{1}{2}}$. A further factor of 2^{-B} normalizes the resulting function to approach 1 as $|\lambda| \to \infty$. The resulting secular equation reads

$$\begin{aligned} Z_S(\lambda) &= \frac{1}{2^B} \left(\det U(\lambda)\right)^{-\frac{1}{2}} \det\left(I^{(2B)} - U(\lambda)\right) \\ &= \frac{1}{2^B} \prod_{j=1}^{V} \left(\frac{1 + i(1-\frac{\lambda}{v_j})}{1 - i(1-\frac{\lambda}{v_j})}\right)^{\frac{1}{2}} \frac{p(\lambda)}{q(\lambda)} = \frac{\det\left(\lambda I^{(V)} - L\right)}{\prod_{j=1}^{V} (v_j^2 + (v_j - \lambda)^2)^{\frac{1}{2}}} \ . \end{aligned} \tag{21}$$

This expression for the secular equation is the basis for the further results of the present work. To begin, use is made of the fact that the spectrum of $U(\lambda)$ for $\mathcal{I}m(\lambda) < 0$ is confined to the interior of the unit circle. Thus, for for any λ with an arbitrarily small (but finite) negative imaginary part, we expand

$$\log\det(I^{(2B)} - U(\lambda)) = -\sum_{n=1}^{\infty} \frac{1}{n} \ \mathrm{tr} U^n(\lambda) \ , \tag{22}$$

and

$$\mathrm{tr} U^n(\lambda) = \sum_{m:m|n} m \sum_{p \in \mathcal{P}(m)} a_p(\lambda) \ . \tag{23}$$

The sum above is over all the primitive periodic orbits p with period m which is a divisor of n, $p = d_1, \ \cdots \ , d_m$ and

$$a_p(\lambda) = \sigma_{d_1,d_m}(\lambda) \cdots \sigma_{d_2,d_1}(\lambda) \ . \tag{24}$$

The explicit dependence of $a_p(\lambda)$ on λ is obtained from the following expressions for the vertex scattering matrix elements,

$$\sigma_{d',d} = \begin{cases} \left[\frac{4}{v_j^2 + (v_j - \lambda)^2}\right]^{\frac{1}{2}} \ \mathrm{e}^{\ i[\arctan(1-\frac{\lambda}{v_j})]/2} & \text{for} \quad d' \neq \hat{d} \ , \\ \left[1 - \frac{4(v_j - 1)}{[v_j^2 + (v_j - \lambda)^2]}\right]^{\frac{1}{2}} \mathrm{e}^{-i \arctan \frac{2(v_j - \lambda)}{(v_j - 1)^2 + (v_j - \lambda)^2 - 1}} & \text{for} \quad d' = \hat{d} \ , \end{cases} \tag{25}$$

where $j = t(d) = o(d')$. The explicit expressions above were written so that for real λ the absolute square of the a_p is a product of "transition probabilities", while the phase of a_p is a sum which plays the rôle of the "action" or "length" associated with the periodic orbit. Substituting (23) in (22), and summing over the repetition numbers $\frac{n}{m}$ one gets,

$$\det(I^{(2B)} - U(\lambda)) = \prod_{p \in \mathcal{P}} (1 - a_p(\lambda)) \ . \tag{26}$$

The ζ function which is introduced in the present work is defined as

$$\zeta_S(\lambda)^{-1} \;=\; \prod_{p\in\mathcal{P}}(1-a_p(\lambda))\;. \tag{27}$$

Combining (22) and (26) with the definition of $\zeta_S(\lambda)$ gives

$$\zeta_S(\lambda)^{-1} \;=\; \frac{\det(\lambda I^{(V)}-L)}{\prod_{j=1}^{V}\left(v_j+i(v_j-\lambda)\right)}\;. \tag{28}$$

This is one of the main results of the present work. It provides a "Ihara" - like identity which expresses an infinite product over primitive periodic orbits on the graph in terms of the characteristic polynomial of the graph discrete Laplacian. The main difference is that here, all the periodic orbits, including orbits with back-scattering, contribute to the product, and that the amplitudes a_p depend on the spectral parameter in a more complicated way. To get a closer look at the ζ_S function and its relation to the Ihara ζ function, it is instructive to write ζ_S for a general v-regular graph. For this purpose, it is convenient to define a new complex variable,

$$z=\frac{1+i(1-\frac{\lambda}{v})}{1-i(1-\frac{\lambda}{v})} \tag{29}$$

which is a $1\leftrightarrow 1$ map of $\mathbb{R}$ to the unit circle in $\mathbb{C}$. With these simplifications, $\zeta_S(z)$ (28) reduces to

$$\zeta_S(z)^{-1}=\left(\frac{2z}{z+1}\right)^{V}\;\det\left(C+iv\frac{z-1}{z+1}\;I^{(V)}\right)\;. \tag{30}$$

It is convenient to define $\gamma_S(z)=z^{\frac{V}{2}}\zeta_S(z)$, in terms of which a functional equation for ζ_S can be written as

$$\gamma_S(z^{-1})=\left(\gamma_S(z^*)\right)^*\;, \tag{31}$$

where $(\cdot)^*$ stands for complex conjugation. Functional equations of similar type are satisfied also by the Ihara ζ function (for v-regular graphs) as well as by most other functions of this genre. Typically, functional equations enable the analytical continuation of ζ functions which are defined by infinite products, beyond their radius of convergence. Here also it provides the analytic continuation of $\zeta_S(z)$ to the exterior of the unit disc.

The periodic amplitudes $a_p(z)$ simplify considerably for v-regular graphs. Denote by n_p the period of the primitive periodic orbit p, and by β_p the number of vertices in p where back-scattering occurs: $\beta_p = \sharp\left\{i \ : \ d_i = \hat{d}_{i+1},\ d_i \in p,\ d_{n_p+1} = d_1\right\}$. Then,

$$a_p(z) = \mathrm{e}^{-i\frac{\pi}{2}n_p}\left(\frac{1+z}{v}\right)^{n_p-\beta_p}\ (-1)^{\beta_p}\ \left(1-\frac{1+z}{v}\right)^{\beta_p}\ . \tag{32}$$

The results above pave the way to the derivation of trace formulae for the discrete Laplacians. Trace formulae provide a powerful tool in spectral theory. They express the spectral density (written down formally as a sum of Dirac δ functions located at the spectral set) in terms of information derived from the manifold metric. The spectral density is written as a sum of two contributions - both of which have a geometric origin. The first is a smooth function of λ whose asymptotic limit at $\lambda \to \infty$ was first studied by Weyl. The second contribution is an infinite sum over periodic geodesics on the manifold. The equality between the spectral density and its geometric representation should be understood only in the sense of distributions. An analogous trace formula will be derived now for the discrete Laplacian. Making use of Cauchy theorem and the fact that $Z_S(\lambda)$ is analytic in the vicinity of the real λ axis, and real on it, one can write,

$$d(\lambda) = \sum_{j=1}^{V}\delta(\lambda-\lambda_j) \tag{33}$$

$$= \frac{1}{\pi}\lim_{\epsilon\to 0^+}\mathcal{I}m\frac{\mathrm{d}}{\mathrm{d}\lambda}\log Z_S(\lambda-i\epsilon)\ . \tag{34}$$

Using

$$Z_S(\lambda)\ =\ \frac{1}{2^B}\left(\det U(\lambda)\right)^{-\frac{1}{2}}\det\left(I^{(2B)}-U(\lambda)\right)\ , \tag{35}$$

the explicit form of $\det U(\lambda)$ (20) and the periodic orbit expansion (23), one gets,

$$d(\lambda) = \frac{1}{\pi}\sum_{j=1}^{V}\frac{1}{v_j}\ \frac{1}{1+(1-\frac{\lambda}{v_j})^2}\ -\ \frac{1}{\pi}\mathcal{I}m\ \frac{\mathrm{d}}{\mathrm{d}\lambda}\sum_{r=1}^{\infty}\sum_{p\in\mathcal{P}}\ \frac{1}{n(p)}|a_p(\lambda)|^r\mathrm{e}^{ir\phi_p(\lambda)}\ . \tag{36}$$

The first term is the "smooth" (Weyl) contribution to the spectral density. It consists of a sum of Lorenzians with poles at $\lambda_j = v_j(1\pm i)$. The second term is an infinite sum over periodic orbits analogous in structure to the "fluctuating" contributions which appear

in any trace formula of this kind. The fluctuating part can be written down explicitly using (25). Noting that the $a_p(\lambda)$ are complex numbers with λ dependent phases $\phi_p(\lambda)$, the periodic orbit sum in the trace formula is a fluctuating function of λ. It is the term which turns the r.h.s. of (36) to a distribution when $\epsilon \to 0$.

So far, the discussion was restricted to the Laplacians (1). The extension to the generalized Laplacians, starts by modifying the definition of the bond wave functions (10) to read,

$$\psi_b = \sqrt{w}_b(a_b \mathrm{e}^{i\frac{\pi}{4}x} + a_{\hat{b}}\mathrm{e}^{-i\frac{\pi}{4}x}) \ . \tag{37}$$

Then, following the same steps as above, the vertex scattering matrices are derived, and they take the form

$$\tilde{\sigma}^{(i)}_{d,d'}(\lambda) = i\left(\delta_{\hat{d},d'} - \frac{1}{u_i}(1+\mathrm{e}^{i\alpha_i(\lambda)}\ )\sqrt{w_d w_{d'}}\right) \quad ; \quad \mathrm{e}^{i\alpha_i(\lambda)} = \frac{1+i(1-\frac{\lambda}{u_i})}{1-i(1-\frac{\lambda}{u_i})} \ , \tag{38}$$

where $u_j = \sum_j w_{i,j}$ as defined previously. The subsequent derivation follows the same steps, resulting in the generalized ζ_S function,

$$\zeta_{\tilde{S}}(\lambda)^{-1} \ \equiv \ \prod_{p\in\mathcal{P}}(1-a_p(\lambda)) \ = \ \frac{\det(\lambda I^{(V)} - \tilde{L})}{\prod_{j=1}^{V}(u_j + i(u_j-\lambda))} \ . \tag{39}$$

A trace formula is also derived in the same way,

$$\begin{aligned} d(\lambda) \quad &= \sum_{j=1}^{V}\delta(\lambda-\tilde{\lambda}_j) = \frac{1}{\pi}\lim_{\epsilon\to 0^+}\mathcal{I}m\frac{\mathrm{d}}{\mathrm{d}\lambda}\log Z_{\tilde{S}}(\lambda - i\epsilon) \\ &= \frac{1}{\pi}\sum_{j=1}^{V}\frac{1}{u_j}\ \frac{1}{1+(1-\frac{\lambda}{u_j})^2} \quad - \quad \frac{1}{\pi}\mathcal{I}m\ \frac{\mathrm{d}}{\mathrm{d}\lambda}\sum_{r=1}^{\infty}\sum_{p\in\mathcal{P}}\ \frac{1}{n(p)}|a_p|^r\ \mathrm{e}^{ir\phi_p(\lambda)} \end{aligned} \tag{40}$$

The expressions for $a_p(\lambda)$ can be derived by a simple modification of (25) and therefore they will not be written down here.

3. Classical dynamics

The present approach emerges from the alternative secular function for the spectrum of Laplacians, based on the quantum evolution operator $U(\lambda)$ in the space of directed bond amplitudes $\mathbf{a} \in l^2(\mathbf{C}^{2B})$. Consider $U(\lambda)$ as a quantum map which maps this $2B$ dimensional space onto itself. U is unitary and hence the map conserves the l^2 norm -

the quantum probability. The condition $U(\lambda)\mathbf{a} = \mathbf{a}$ can be interpreted as a requirement that λ_n is an eigenvalue if there exists a non trivial vector $\mathbf{a}$ which is stationary under the action of the quantum map [17]. The requirement of stationarity is naturally associated with the eigenvalue being in the spectrum of the underlying Hamiltonian.

The building blocks for the theory are the vertex scattering matrices. Similar matrices appear in the theory of quantum graphs. There, they emerge when the Schrödinger equation on the graph is augmented by vertex boundary conditions which render the resulting operator self adjoint. The self adjoint extension is not unique, and depends the spectral parameter k and on an arbitrary parameter κ which interpolates between the "Dirichlet" ($\kappa = 0$) and the "Neumann" ($\kappa = \infty$) boundary conditions [1, 18]. The scattering matrices for discrete graphs are obtained from their quantum graph analogues by replacing κ/k by λ.

The unitary quantum evolution operator is the starting point for the construction of a classical evolution on the discrete graph. The classical "phase space" in this case are the probability vectors $\rho \in l^2(\mathbf{R}^{2B})$ where the components of ρ are interpreted as the probabilities to find the classical system on the corresponding directed bonds. The classical transition matrix is constructed from the quantum probability to make a transition from d to d'

$$M_{d',d} = |U_{d',d}|^2 \ . \tag{41}$$

The unitarity of U implies that M is bi-stochastic, namely, $\sum_d M_{d',d} = \sum_{d'} M_{d',d} = 1$. This transition matrix induces a discrete, random walk dynamics in phase space. If n denotes the discrete "time",

$$\rho(n+1) = M\rho(n) \ . \tag{42}$$

This Markovian evolution preserves the l^1 norm - the classical probability. The spectrum of M is confined to the interior of the unit circle. 1 is always an eigenvalue corresponding to an eigenvector with equal components which describes the system in an equilibrated state. When the eigenvalue 1 is the only eigenvalue on the unit circle, the classical

dynamics drives the system to equilibrium at a rate which depends on the distance of the next highest eigenvalue to the unit circle. This classical dynamics is identical to the one which was introduced in the study of quantum graphs [1]. It plays an important rôle in the theory of spectral statistics on quantum graphs [1, 19, 20, 21]. Finally, the analogue of the Ruelle ζ function for the evolution induced by P can be easily written down starting with the secular function

$$Z_M(\mu) \equiv \det(I^{(2B)} - \mu M) \tag{43}$$

The periodic orbit sum is identical to the trace formula (36) in which the amplitudes a_p are replaced by their absolute squares.

To emphasize the intricate connections between the concepts developed here and their predecessors [2, 3, 4], consider a v-regular graph ($v > 2$), and the classical evolution operator obtain for the spectral parameter $\lambda = v + i(v-2)$, corresponding to $z = v - 1$ in (29). At this value, $\sigma_{d,\hat{d}} = 0$ and $\sigma_{d',d} = 1$ for $d' \neq \hat{d}$. The resulting classical evolution matrix $M^\sharp$ needs to be multiplied by $(v-1)^{-1}$ to make it a legitimate (probability conserving) evolution operator. The resulting evolution does not permit back-scatter, and therefore, the secular equation (43) can be computed using Stark's ζ function (8), with $Y = \frac{\mu}{v-1} M^\sharp$. The product over the set of non back-scattering primitive periodic orbits becomes identical to the one appearing in the Ihara zeta function (4). Using (5), one finally gets,

$$\begin{aligned} Z_{M^\sharp}(\mu) &= \prod_n \left(1 - (\frac{\mu}{v-1})^n\right)^{|\mathcal{C}(n)|} \\ &= \left(1 - (\frac{\mu}{v-1})^2\right)^{r-1} \det\left(I^{(V)}(1 + \frac{\mu^2}{v-1}) - \frac{\mu}{v-1} C\right) \ . \end{aligned} \tag{44}$$

Thus, the spectrum m_j of $M^\sharp$ consists of $r-1$ fold degenerate eigenvalues at $m_j^{(\pm)} = \pm\frac{1}{v-1}$, and the rest which can be computed from the spectrum of the discrete Laplacian λ_j

$$m_j^\pm = \frac{(v - \lambda_j) \pm \sqrt{(v-\lambda_j)^2 - 4(v-1)}}{2(v-1)} \ . \tag{45}$$

The eigenvalue 0 of the Laplacian corresponds to the eigenvalues 1 and $\frac{1}{v-1}$ of $M^\sharp$. The

gap in the classical evolution spectrum is determined by the first non zero eigenvalue of L.

The comment above may have interesting and novel consequences going beyond its anecdotal appearance. In quantum graphs, one can choose vertex scattering matrices from a much larger variety than offered by the vertex scattering matrices (16). Thus, it is possible to construct vertex scattering matrices which do not scatter backwards, but with equal scattering probability to the other vertices. The unitarity is maintained by a proper choice of the phases of the scattering amplitudes [23]. In such cases, and for v-regular graphs, the classical analogues are identical with $M^\sharp$ and (44) is applicable. Working with such systems is particularly interesting because in quantum chaos, the gap between the eigenvalue 1 and the rest of the spectrum determines whether the spectrum of the U matrix (and hence of the Schrödinger operator) display the statistics predicted by Random Matrix Theory, in the limit of large graphs. For non back-scattering dynamics (44) reduces the problem to the study of the spectrum of the Laplacian. The behavior of the gap in the laplacian spectrum of large graphs is an important subject in the theory of discrete graphs and number theory, related amongst others to the Ramanujan conjecture [22]. A detailed discussion of this connection will take the present manuscript far afield, and it is deferred to a future publication.

Acknowledgments

It is a pleasure to thank A Terras, M Kotani, H Stark and T Sunada for introducing me to the fascinating world of the discrete graphs, and for many discussions and suggestions. The comments and suggestions offered by P Kuchment, S Gnutzmann, I Oren and R Band are highly appreciated. J. Harrison's help in computing a few examples of vertex scattering matrices without back-scatter is also acknowledged. This work was supported by the Minerva Center for non-linear Physics, the Einstein (Minerva) Center at the Weizmann Institute and EPSRC grant 531174. I am indebted to the Isaac Newton Institute and Clare Hall for their hospitality while much of this work was carried out.

Bibliography

[1] Tsampikos Kottos and Uzy Smilansky, *Quantum Chaos on Graphs*, Phys. Rev. Lett. **79**,4794-4797, (1997). and *Periodic orbit theory and spectral statistics for quantum graphs*, Annals of Physics **274**, 76-124 (1999).

[2] Y. Ihara, *On discrete subgroups of the two by two projective linear group over a p-adic field*, J. Mat. Soc. Japan, **18** (1966), 219-235.

[3] H. M. Stark and A. A. Terras, *Zeta Functions of Finite Graphs and Coverings*, Adv. in Math. **121**, (1996) 124-165.

[4] Motoko Kotani and Toshikazu Sunada, *Zeta Functions on Finite Graphs*, J. Math. Sci. Univ. Tokyo **7** no. 1, 7-25, (2000).

[5] Tsampikos Kottos and Uzy Smilansky, *Chaotic Scattering on Graphs* , Phys. Rev. Lett., **85** 968, (2000).

[6] J. P. Roth in "Lecture notes in Mathematics: Theorie de Potential" (A. Dold and B. Eckmann, Eds.) p. 521, Springer Verlag, New-York/Berlin (1985).

[7] M.C. Gutzwiller, J. Math. Phys. **12** 343 (1971).

[8] Fan R. K. Chung, *Spectral Graph Theory*, Regional Conference Series in Mathematics **92**, American mathematical Society(1997).

[9] A. A. Terras, *Fourier Analysis on Finite Groups and Applications* London Mathematical Society Student Texts **43** Cambridge University Press, Cambridge UK (1999).

[10] A. A. Terras, *Arithmetic Quantum Chaos*, IAS/Park City Mathematical Series **12** 2002 333-375

[11] Hurt, N.E. *The prime geodesic theorem and quantum mechanics on finite volume graphs:a review.* Rev. Math. Phys. **13**, (2001), 1459-1503.

[12] H.M. Stark, *Multipath zeta functions of graphs.* preprint (2007)

[13] S. Novikov, *Schrödinger operators on graphs and symplectic geometry.* Field Inst. Communications **24** (1999), 397-413.

[14] Carla Cattaneo, *The Spectrum of the Continuous Laplacian on a Graph.* Mh. Math. **124** 215-235 (1997).

[15] P. Exner, *A duality between Schrödinger operators on graphs and certain Jacobi matrices* Ann. Inst. H. Poincare, **66** (1997) 359-371.

[16] Peter Kuchment, *Quantum Graphs: I. Some basic structures.* Waves in random Media **14** (2004), S107-S128.

[17] Sven Gnutzmann and Uzy Smilansky, *Quantum Graphs: Applications to Quantum Chaos and Universal Spectral Statistics.* Advances in Physics bf 55 (2006) 527-625.

[18] V. Kostrykin and R Schrader, *Kirchoff's Rule for quantum wires*, J. Phys. A. Math. Gen. **32**(1999)

595-630.

[19] G. Tanner, J. Phys. A **34**,8484 (2001) and *ibid* A**35**,5985 (2002).

[20] G. Berkolaiko, *Spectral gap of doubly stochastic matrices generated from equidistributed unitary matrices*, J. Phys. A **34**,(2001) 319-326.

[21] S.Gnutzmann and A. Altland, Phys. Rev. Lett. **93** 194101 (2004).

[22] A. Lubotzky, R. Phillips and P. Sarnak, *Ramanujan graphs*, Combintorica **8** (1988), 261-277.

[23] J. Harrison, private communication.