Trace formulae and spectral statistics for discrete Laplacians on regular graphs (*I*)

2009 J. Phys. A: Math. Theor. 42 415101

(http://iopscience.iop.org/1751-8121/42/41/415101)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 415101 (20pp) doi:10.1088/1751-8113/42/41/415101

Trace formulae and spectral statistics for discrete Laplacians on regular graphs (I)

Idan Oren[1], **Amit Godel**[1] **and Uzy Smilansky**[1,2]

[1] Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel
[2] School of Mathematics, Cardiff University, Cardiff, Wales, UK

E-mail: idan.oren@weizmann.ac.il, amit.godel@weizmann.ac.il and uzy.smilansky@weizmann.ac.il

Received 2 June 2009, in final form 17 August 2009
Published 29 September 2009
Online at stacks.iop.org/JPhysA/42/415101

Abstract
Trace formulae for d-regular graphs are derived and used to express the spectral density in terms of the periodic walks on the graphs under consideration. The trace formulae depend on a parameter w which can be tuned continuously to assign different weights to different periodic orbit contributions. At the special value $w = 1$, the only periodic orbits which contribute are the non-back-scattering orbits, and the smooth part in the trace formula coincides with the Kesten–McKay expression. As w deviates from unity, non-vanishing weights are assigned to the periodic walks with backscatter, and the smooth part is modified in a consistent way. The trace formulae presented here are the tools to be used in the second paper in this sequence, for showing the connection between the spectral properties of d-regular graphs and the theory of random matrices.

PACS numbers: 05.45.Mt, 02.10.Ox

(Some figures in this article are in colour only in the electronic version)

1. Introduction and preliminaries

Discrete graphs stand at the confluence of several research directions in physics, mathematics and computer science. Notable physical applications are, e.g., the tight-binding models, which are used to investigate transport and spectral properties of mesoscopic systems [1], and numerous applications in statistical physics (e.g., percolation [2]). The mathematical literature is abundant with studies of spectral, probability and number theory, in relation to discrete graphs [3, 32, 33]. Models of communication networks or the theory of error correcting codes in computer science use graph theory as a prime tool.

In the present series of papers, we would like to add yet another link to the list above, namely, to study graphs as a paradigm for quantum chaos. In making this contact, we hope to enrich quantum chaos by the enormous amount of knowledge accumulated in the study of graphs and offer the language of quantum chaos as a useful tool in graph research.

The first hints of a possible connection between quantum chaos and discrete graphs emerged a few years ago when Jakobson *et al* [4] studied numerically the spectral fluctuations for simple d-regular graphs (graphs where the number of neighbors of each vertex is d and no parallel or self-connections are allowed). In particular, they sampled randomly the ensemble of d-regular graphs, computed the spectra of the adjacency matrices and deduced the mean nearest-neighbor distributions (for $d = 3, 4, 5$). They found that within the statistical uncertainty, the computed distributions match the prediction of random matrix theory. The work of Terras [34] should also be consulted in this context. The purpose of the present work is to adopt the techniques developed in quantum chaos to investigate the connection between the spectral statistics of d-regular graphs and random matrix theory. The main tools which we shall use to this end are trace formulae, which, in the present case, relate spectral statistics to the counting statistics of periodic walks on the graphs. In this paper, the first in this series, we shall develop the tool kit—namely—we will derive trace formulae for regular graphs. We shall show that a large variety of trace formulae exist, all of them provide expression for the *same* spectral density but using *differently weighted* periodic walks. We shall also show that there exists an *optimal* trace formula, in the sense that the *smooth* density coincides with the *mean* density (with respect to the $\mathcal{G}_{V,d}$ ensemble). For this optimal trace formula, the oscillatory part stems only from a subset of periodic orbits. These are periodic orbits in which there are no back-scattering (reflections). In the second paper in the series, we shall use the optimal trace formula to obtain some results which support the conjecture that spectral statistics for regular graphs follow the predictions of random matrix theory. In many respects, the present study follows the development of the research in quantum chaos where it was conjectured [5] that the quantum spectra of systems whose classical analogs are chaotic behave statistically as predicted by random matrix theory. This conjecture, which was originally based on a few numerical studies, brought about a surge of research, and using the relevant (semi-classical) trace formula [6], the connection with random matrix theory was theoretically established [7–9].

To provide a proper background for the ensuing discussion, we have to start with a short section of definitions and a summary of known facts.

1.1. Definitions

A graph $\mathcal{G}$ is a set $\mathcal{V}$ of vertices connected by a set $\mathcal{E}$ of edges. The number of vertices is denoted by $V = |\mathcal{V}|$ and the number of edges is $E = |\mathcal{E}|$. The $V \times V$ *adjacency* (*connectivity*) matrix A is defined such that $A_{i,j} = s$ if the vertices i, j are connected by s edges. In particular, $A_{i,i} = 2s$ if there are s loops connecting the vertex i to itself. A graph in which there are loops or parallel edges is called a *multigraph*.

In the present work, we mainly deal with connected *simple graphs* where there are no parallel edges ($A_{i,j} \in \{0, 1\}$) or loops ($A_{i,i} = 0$). The *degree* d_i (*valency*) is the number of edges emanating from the vertex, $d_i = \sum_{j=1}^{V} A_{i,j}$. A d-regular graph satisfies $d_i = d \ \forall i : 1 \leqslant i \leqslant V$, and for such graphs dV must be even. The ensemble of all d-regular graphs with V vertices will be denoted by $\mathcal{G}_{V,d}$. Averaging over this ensemble will be carried out with uniform probability and will be denoted by $\langle \cdots \rangle$.

To any edge $b = (i, j)$ one can assign an arbitrary direction, resulting in two *directed edges*, $e = [i, j]$ and $\hat{e} = [j, i]$. Thus, the graph can be viewed as V vertices connected by edges $b = 1, \ldots, E$ or by $2E$ directed edges $e = 1, \ldots, 2E$ (the notation b for edges and e for directed edges will be kept throughout). It is convenient to associate with each directed edge $e = [j, i]$ its *origin* $o(e) = i$ and *terminus* $t(e) = j$ so that e points from the vertex i to the vertex j. The edge e' follows e if $t(e) = o(e')$.

A *walk* of length t from the vertex x to the vertex y on the graph is a sequence of successively connected vertices $x = v_1, v_2, \ldots, v_t = y$. Alternatively, it is a sequence of $t-1$ directed edges $e_1, \ldots, e_{t-1}$ with $o(e_i) = v_i, t(e_i) = v_{i+1}, o(e_1) = x, t(e_{v-1}) = y$. A *closed walk* is a walk with $x = y$. The number of walks of length t between x and y equals $(A^t)_{y,x}$. The graph is *connected* if for any pair of vertices there exists t such that $(A^t)_{y,x} \neq 0$.

We have to distinguish between several kinds of walks. There seems to be no universal nomenclature, and we shall consistently use the following.

A walk where $e_{i+1} \neq \hat{e}_i$, $1 \leqslant i \leqslant t-2$ will be called a *walk with no back-scatter* or an *nb-walk* for short.

A walk without repeated indices will be called a *path*. Clearly, a path is a non-self-intersecting nb-walk.

A *t-periodic walk* is a closed walk with t vertices (and t edges). Any cyclic shift of the vertices on the walk produces another t-periodic walk (which is not necessarily different from the original one). All the t-periodic walks which are identical up to a cyclic shift form a *t-periodic orbit*. A primitive periodic orbit is an orbit which cannot be written as a repetition of a shorter periodic orbit.

Among the t-periodic orbits, we shall distinguish those which do not have back-scattered edges and refer to them as periodic nb-orbits. The frequently used term *cycles* stands for periodic paths (non-self-intersecting nb-orbits).

In order to count periodic walks, it is convenient to introduce the $2E \times 2E$ matrix B which describes the connectivity of the graph in terms of its directed edges:

$$B_{e,e'} = \delta_{t(e),o(e')}. \tag{1}$$

The matrix which singles out edges connected by backscatter is

$$J_{e,e'} = \delta_{\hat{e},e'}. \tag{2}$$

The Hashimoto connectivity matrix [10],

$$Y = B - J, \tag{3}$$

enables us to express the number of t periodic nb-walks as $\mathrm{tr}\, Y^t$. A slightly more general form

$$Y(w) = B - wJ, \qquad w \in \mathbb{C} \tag{4}$$

gives a weight 1 to transmission and weight $1 - w$ to back-scatter. Now, $\mathrm{tr}\, Y^t(w) = \sum_g N(t; g)(1-w)^g$, where $N(t; g)$ is the number of t periodic walks with exactly g back-scatters. Clearly, $\mathrm{tr}\, Y^t(w)$ can be considered as a generating function for counting periodic walks with specific t and g:

$$N(t; g) = \frac{(-1)^g}{g!} \frac{\partial^g \mathrm{tr}\, Y^t(w)}{\partial w^g}\bigg|_{w=1}. \tag{5}$$

The discrete Laplacian on a graph is defined in general as

$$L \equiv -A + D, \tag{6}$$

where A is the connectivity matrix and D is a diagonal matrix with $D_{i,i} \equiv d_i$. It is a self-adjoint operator whose spectrum consists of V non-negative real numbers. For d-regular graphs, D is proportional to the unit matrix and therefore it is sufficient to study the spectrum of the adjacency matrix A. This will be the subject of this paper.

The spectrum $\sigma(A)$ is determined as the zeros of the secular function (characteristic polynomial)

$$Z_A(\mu) \equiv \det(\mu I^{(V)} - A). \tag{7}$$

Here, μ is the spectral parameter and $I^{(V)}$ is the unit matrix in V dimensions. The largest eigenvalue is d, and it is simple if and only if the graph is connected. If the graph is bipartite, $-d$ is also in the spectrum.

The *spectral measure* (spectral density) is defined as

$$\rho(\mu) \equiv \frac{1}{V} \sum_{\mu_a \in \sigma(A)} \delta(\mu - \mu_a). \tag{8}$$

The 'magnetic' Laplacian [11] is defined by

$$L^{(M)}_{i,j} = -A_{i,j} \mathrm{e}^{\mathrm{i}\phi_{i,j}} + d_i \delta_{i,j}, \qquad \phi_{i,j} = -\phi_{j,i}. \tag{9}$$

The phases $\phi_{i,j}$ attached to the edges (i, j) play the role of 'magnetic fluxes' (to be precise, the phases are the analog of gauge fields, and a sum of gauge fields over a cycle is a magnetic flux). The Laplacian is complex Hermitian, and therefore the evolution it induces breaks time reversal symmetry. Again, for d-regular graphs it suffices to study the *magnetic adjacency matrix*

$$A^{(M)}_{i,j} = A_{i,j}\, \mathrm{e}^{\mathrm{i}\phi_{i,j}}. \tag{10}$$

The *ensemble of random magnetic graphs* consists of the random graph ensemble $\mathcal{G}_{V,d}$ with independently and uniformly distributed magnetic phases $\phi_{i,j}$.

A weighted Laplacian is defined by

$$L^{(W)}_{i,j} = -A_{i,j} W_{i,j} + W_{i,i}\delta_{i,j}, \qquad W_{i,j} = W_{j,i} \quad W_{i,j} \in \mathbb{R}, \tag{11}$$

where $W_{i,j}$ are weights defined on the edges of the graph. We shall restrict our attention to the weighted adjacency matrix: $A^{(W)}_{i,j} = A_{i,j} W_{i,j}$. The *ensemble of random weighted graphs* consists of the random graph ensemble $\mathcal{G}_{V,d}$ with independently and uniformly distributed weights $W_{i,j}$ in the interval $|W_{i,j}| \leqslant 1$.

1.2. Background

Adjacency matrices of random d-regular graphs have some remarkable spectral properties. An important discovery which marked the starting point of the study of spectral statistics for d-regular graphs was the derivation of the mean spectral density by Kesten [12] and McKay [13]:

$$\rho_{\mathrm{KM}}(\mu) = \lim_{V\to\infty} \langle \rho(\mu) \rangle = \begin{cases} \dfrac{d}{2\pi} \dfrac{\sqrt{4(d-1) - \mu^2}}{d^2 - \mu^2} & \text{for} \quad |\mu| \leqslant 2\sqrt{d-1} \\ 0 & \text{for} \quad |\mu| > 2\sqrt{d-1}. \end{cases} \tag{12}$$

The proof of this result relies on the very important property of random d-regular graphs, namely, that almost surely every subgraph of diameter less than $\log_{d-1} V$ is a tree. Counting periodic orbits on the tree can be done explicitly, and using the close relations between these numbers and the spectrum, one obtains (12).

If the entire spectrum of A (except from the largest eigenvalue) lies within the support $[-2\sqrt{d-1}, 2\sqrt{d-1}]$, the graph is called Ramanujan (for a review, see, e.g., [23] and references cited therein).

Trace formulae for regular graphs were discussed in the literature in various contexts. The late Robert Brooks [14] studied the connection between the number of closed paths on a graph and its spectrum, and proposed a Selberg-like trace formula. Some of the ideas developed in the present work are related to Brook's results. In this paper, we derive two families of trace formulae which depend on a continuous (complex) parameter w. The optimal trace formula alluded to in the introduction is obtained when $w = 1$. In this case, the trace formula uses the subset of nb-walks which have some advantages (see, for example, [15, 16]). We shall see that with this choice of w, we get the Kesten–McKay measure as a limiting distribution, and an oscillatory part which vanishes under an ensemble average. We will make use of this part in the following paper in this series of papers. The trace formula for this choice of w coincides with a trace formula derived by Mnëv [41] in an entirely different way.

A different, more physical approach, in which a scattering formalism was used, resulted in a trace formula [17] (see also [24]), which is formally similar to the trace formula for the spectrum of the Laplacian on metric graphs [18, 19]. For d-regular graph it reads

$$\rho(\mu) = \frac{1}{\pi}\frac{d}{\mu^2+d^2} + \frac{1}{V\pi}\lim_{\epsilon\to 0^+}\mathcal{I}m\frac{\mathrm{d}}{\mathrm{d}\mu}\sum_{t=1}^{\infty}\frac{1}{t}\,\mathrm{tr}(U(\mu+i\epsilon)^t), \tag{13}$$

where $U(\mu)$, the graph evolution operator, is a $2E \times 2E$ unitary matrix defined as

$$U(\mu) = i\left[-\frac{2}{d-i\mu}Y + \left(1-\frac{2}{d-i\mu}\right)J\right] = i\left[-\frac{2}{d-i\mu}B + J\right]. \tag{14}$$

Y, J and B were introduced before. The infinite sum in (13) can be written as a sum over t-periodic walks. Denoting by g the number of back-scattering along the walk,

$$\mathrm{tr}\,U^t = \frac{2^t}{(d^2+\mu^2)^{\frac{t}{2}}}\,\mathrm{e}^{\mathrm{i}t(\arctan\frac{\mu}{d}-\frac{\pi}{2})}\sum_g N(t;g)\frac{((d-2)^2+\mu^2)^{\frac{g}{2}}}{2^g}\,\mathrm{e}^{-\mathrm{i}g\arctan\frac{\mu}{d-2}}. \tag{15}$$

The first term in the trace formula (as usual, an algebraic function of the spectral parameter) is referred to as the 'smooth' spectral density. It consists here of a Lorentzian of width d centered at 0. The sum over the periodic walks is formal and it diverges at the spectrum of the adjacency matrix. We shall show below that there exists another continuum of trace formula and that (13) is obtained as a special case.

It has already been observed in [17] that the trace formula above is not satisfactory in the sense that the leading Lorentzian is very different from the asymptotic *mean* spectral density (12). It was suggested that a re-summation of the infinite sum would extract the difference between the Lorentzian and the Kesten–McKay expression. Indeed, summing up the contribution of the shortest, $t = 2$ periodic orbits, one obtained a correction term which exactly canceled the $\frac{1}{\mu^2}$ tails of the Lorentzian. However, a systematic re-summation of (13) to extract $\rho_{\mathrm{KM}}(\mu)$ requires a new approach which will be presented in section 2. The discussion of this problem leads naturally to a more general question: Can one distinguish among the periodic orbits on the graph distinct subsets, each responsible to a different feature in the spectral density? The Kesten–McKay theory seems to favor an affirmative answer since the asymptotic density is derived from tree-like periodic orbits. But what about the rest? Does one really need all the legitimate periodic orbits on the graph, or can one do with a subset? Is this distinction unique? These, and other questions, will be further discussed in the following sections.

The paper is organized as follows. The Bartholdi identity is the cornerstone of the theory presented in this paper. However, since the derivation is strictly technical, we leave it to an appendix. The appendix reviews shortly the Bartholdi identity and its proof, which is generalized here to include the cases of magnetic adjacency matrices, multigraphs and weighted graphs as well.

In section 2, we derive the family of trace formulae, which depend on real w. Then, we specialize to the choice $w = 1$ in both the magnetic and non-magnetic cases.

The different forms of the trace formula will help to elucidate the question posed in the previous paragraph regarding the different roles played by periodic orbits of different topologies. Furthermore, the dependence on w can be exploited to unravel combinatorial information about the graph at hand. Finally, the trace formula (13) will be shown to be one of a (continuous) family of trace formulae which have one feature in common, namely that they are based on traces of unitary operators of the type (14). This is achieved by allowing w to assume complex values.

2. A continuous family of trace formulae

In this section, we shall derive a continuous family of trace formulae which depend on a real parameter w. The parameter w controls the weights which are given to periodic walks with different numbers of back-scatters. Consider the matrix $Y(w)$ (4). For d-regular graphs, the Bartholdi identity reads (see the appendix)

$$\det\left(I^{(2E)} - s(B - wJ)\right) = (1 - w^2 s^2)^{E-V} \det\left(I^{(V)}(1 + w(d-w)s^2) - sA\right). \tag{16}$$

Its importance in the present context comes from the fact that it connects the spectrum of the adjacency matrix A with that of the matrices $Y(w) = B - wJ$, which can be used to count various types of cycles and walks on the corresponding graph. It implies that the spectrum of $Y(w) = B - wJ$ is

$$\begin{aligned}\sigma(Y(w)) = \{&(d-w), w, +w \times (E-V), -w \times (E-V),\\ &(\sqrt{w(d-w)}\mathrm{e}^{\mathrm{i}\phi_k}, \sqrt{w(d-w)}\,\mathrm{e}^{-\mathrm{i}\phi_k}, k = 1, \ldots, (V-1))\}\\ \text{where} \qquad &\phi_k = \arccos\frac{\mu_k}{2\sqrt{w(d-w)}} \qquad \text{for all} \quad k = 1, \ldots, V-1.\end{aligned} \tag{17}$$

μ_k's with $k = 1, \ldots, (V-1)$ are the non-trivial eigenvalues of the adjacency matrix, whose spectrum is ordered as a non-increasing sequence

$$d = \mu_0 > \mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_{V-1} \geqslant -d. \tag{18}$$

(μ_{V-1} assumes the value $-d$ if and only if the graph is bipartite. The bipartite graphs are rare in $\mathcal{G}_{V,d}$ and are excluded from the discussion from now on.) If w is in the interval $\left[1, \frac{d-1}{2}\right]$, we have $2\sqrt{d-1} \leqslant 2\sqrt{w(d-w)} \leqslant \sqrt{d^2-1}$. This ensures that for generic graphs one can always find a value of $w \in \left[1, \frac{d-1}{2}\right]$ so that for all k, $|\mu_k| \leqslant 2\sqrt{w(d-w)}$, and all ϕ_k's are real. The freedom to choose w allows us to use the trace formula for almost all d-regular graphs and in particular for non-Ramanujan graphs.

It is convenient to introduce the quantities $y_t(w)$,

$$y_t(w) = \frac{1}{V}\frac{\operatorname{tr} Y^t(w) - (d-w)^t}{(\sqrt{w(d-w)})^t}, \tag{19}$$

which (unlike $\operatorname{tr} Y^t(w)$) are bounded as $t \to \infty$. The explicit expressions for the eigenvalues of $Y(w)$ are now used to write,

$$y_t(w) = \frac{1}{V}\left(\frac{w}{d-w}\right)^{\frac{t}{2}} + \frac{d-2}{2}\left(\frac{w}{d-w}\right)^{\frac{t}{2}}(1 + (-1)^t) + \frac{2}{V}\sum_{k=1}^{V-1} T_t\left(\frac{\mu_k}{2\sqrt{w(d-w)}}\right), \tag{20}$$

where $T_t(x) \equiv \cos(t \arccos x)$ are the Chebyshev polynomials of the first kind of order t. The fact that $y_t(w)$ are bounded is guaranteed since $\frac{w}{d-w} < 1$ whenever $w \in \left[1, \frac{d-1}{2}\right]$, and $d \geqslant 3$, and since the Chebyshev polynomials are bounded.

Multiplying both sides of (20) by $\frac{1}{\pi(1+\delta_{t,0})}T_t\big(\frac{\mu}{2\sqrt{w(d-w)}}\big)$ and summing over t, we get

$$\frac{1}{\pi}\sum_{t=0}^{\infty}\frac{1}{(1+\delta_{t,0})}T_t\left(\frac{\mu}{2\sqrt{w(d-w)}}\right)y_t(w)$$
$$=\frac{1}{\pi V}\sum_{t=0}^{\infty}\frac{1}{(1+\delta_{t,0})}\left(\sqrt{\frac{w}{d-w}}\right)^t T_t\left(\frac{\mu}{2\sqrt{w(d-w)}}\right)$$
$$+\frac{(d-2)}{2\pi}\sum_{t=0}^{\infty}\frac{1}{(1+\delta_{t,0})}\left[\left(\sqrt{\frac{w}{d-w}}\right)^t+\left(-\sqrt{\frac{w}{d-w}}\right)^t\right]T_t\left(\frac{\mu}{2\sqrt{w(d-w)}}\right)$$
$$+\frac{1}{V}\sum_{k=1}^{V-1}\delta_T\left(\frac{\mu}{2\sqrt{w(d-w)}},\frac{\mu_k}{2\sqrt{w(d-w)}}\right), \tag{21}$$

where $\delta_T(x,y)$ is defined by

$$\delta_T(x,y)\equiv\frac{2}{\pi}\sum_{t=0}^{\infty}\frac{1}{1+\delta_{t,0}}T_t(x)T_t(y). \tag{22}$$

Here, $\delta_T(x,y)$ is the unit operator in the $L^2[-1,1]$ space where the scalar product is defined with a weight $\frac{1}{\sqrt{1-x^2}}$. Indeed,

$$\int_{-1}^{1}\frac{\mathrm{d}x}{\sqrt{1-x^2}}\delta_T(x,y)f(x)=f(y). \tag{23}$$

For $t=0,1,2$ one can easily show that

$$y_0=d-\frac{1}{V};\qquad y_1=\frac{-1}{V}\sqrt{\frac{d-w}{w}};\qquad y_2=\frac{d(1-w)^2}{w(d-w)}-\frac{1}{V}\frac{d-w}{w}.$$

Writing $\sqrt{1-x^2}\cdot\delta(x-y)=\delta_T(x,y)$ and using elementary identities involving the Chebyshev polynomials, we get an expression for the density of states which is supported in the interval $|\mu|\leqslant 2\sqrt{w(d-w)}$:

$$\rho(\mu)=\rho^{\text{smooth}}(\mu;w)+\rho^{\text{osc}}(\mu;w)+\frac{1}{V}\rho^{\text{corr}}(\mu;w), \tag{24}$$

where

$$\rho^{\text{smooth}}(\mu;w)=\frac{d/(2\pi)}{\sqrt{4w(d-w)-\mu^2}}\left(1-\frac{(d-2w)(d-2)}{d^2-\mu^2}+\frac{(w-1)^2(\mu^2-2w(d-w))}{w^2(d-w)^2}\right)$$
$$\rho^{\text{osc}}(\mu;w)=\frac{1}{\pi}\sum_{t=3}^{\infty}\frac{y_t(w)}{\sqrt{4w(d-w)-\mu^2}}T_t\left(\frac{\mu}{2\sqrt{w(d-w)}}\right)$$
$$=\frac{1}{\pi}\mathcal{R}e\left(\sum_{t=3}^{\infty}\frac{y_t(w)}{\sqrt{4w(d-w)-\mu^2}}\exp^{(\mathrm{i}t\arccos\frac{\mu}{2\sqrt{w(d-w)}})}\right)$$
$$\rho^{\text{corr}}(\mu;w)=\frac{-1}{2\pi\sqrt{4w(d-w)-\mu^2}}\left(1+\frac{\mu}{w}+\frac{\mu^2-2w(d-w)}{w^2}+\frac{d-2w}{d-\mu}\right). \tag{25}$$

Equations (24) and (25) are the main result of this section. In form, they are very similar to well-known trace formulae from other branches of mathematical physics. They are composed of a smooth part $\rho^{\text{smooth}}(\mu;w)$ which is an algebraic expression in μ as shown in figure 1, and an oscillatory part, computed from information about the periodic walks. The amplitudes are obtained from the (properly regularized) count of t-periodic walks, and the phase factors

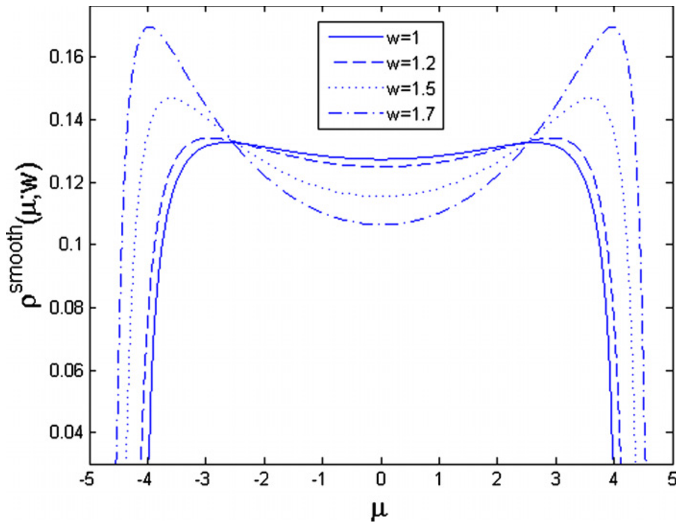

Figure 1. $\rho^{\text{smooth}}(\mu; w)$ for five regular graphs for various values of w: solid: $w = 1$; dashed: $w = 1.2$; dotted: $w = 1.5$; dash-dot: $w = 1.7$.

explicitly given in the second line are the analogs of the 'classical actions' accumulated along the walks. (24) is a generalization of (13), as will be shown in 4.

It is important to note that the left-hand side of (24) does not depend on w, because the density of states of the adjacency operator depends only on the graph and not on the choice of w. Therefore, the right-hand side must also be w-independent. In other words, the w dependence of the smooth part is offset by a partial sum of the oscillatory part. This is reminiscent of the partition of the trace formula (13), where the smooth part is a Lorentzian, and it was shown that the sum over 2-periodic orbits gives a contribution which exactly cancels the leading $1/\mu^2$ behavior for large $|\mu|$.

Having the freedom to choose w, it is natural to look for the most appropriate or convenient partition of the spectral density into smooth and oscillatory parts. We shall show in the following that this is obtained when $w = 1$, because the smooth density coincides with the *mean* density (with respect to the $\mathcal{G}_{V,d}$ ensemble) (12).

Finally, we also mention that a trace formula for multigraphs can be derived in an analogous fashion. The smooth part remains unaltered, and in the oscillatory part, the sum starts from $t = 1$ since loops are allowed.

2.1. Trace formula in terms of periodic nb-walks ($w = 1$)

The case $w = 1$ plays a special role in the present theory and its applications. The fact that the smooth part of the trace formula is identical to the Kesten–McKay expression was mentioned above, and will be discussed further in the following. As will be shown, this is a direct consequence of the fact that the counting statistics of t-periodic nb-walks in $\mathcal{G}_{V,d}$ is Poissonian for $t < \log_{d-1} V$ with $\langle \operatorname{tr} Y^t \rangle = (d-1)^t$ [31].

The trace formula can be obtained by substituting $w = 1$ in (25). Alternatively, one can start from the Bass formula for d-regular graphs [21]:

$$\det(I^{(2E)} - sY) = (1 - s^2)^{E-V} \det(I^{(V)}(1 + (d-1)s^2) - sA), \qquad (26)$$

where Y is the Hashimoto matrix defined in section (1), and $\mathrm{tr}\, Y^t$ counts the number of t-periodic nb-walks. One can now follow the same steps as in the previous section. However, this requires restricting the discussion to Ramanujan graphs only. Under this condition, $|\mu_k| \leqslant 2\sqrt{d-1}, k = 1, \ldots, (V-1)$, and the spectrum of Y is

$$\sigma(Y) = \{(d-1), 1, +1 \times (E-V), -1 \times (E-V),\\ (\sqrt{d-1}\,\mathrm{e}^{\mathrm{i}\phi_k}, \sqrt{d-1}\,\mathrm{e}^{-\mathrm{i}\phi_k}, k = 1, \ldots, (V-1))\}\\ \text{where} \qquad \phi_k = \arccos \frac{\mu_k}{2\sqrt{d-1}}, \qquad 0 \leqslant \phi_k \leqslant \pi. \tag{27}$$

For large t, the number of t-periodic walks is dominated by the largest eigenvalue, so that asymptotically $\mathrm{tr}\, Y^t \sim (d-1)^t$. Shortening the notation by using $y_t = y_t(w=1)$ we have

$$y_t = \frac{1}{V} \frac{\mathrm{tr}\, Y^t - (d-1)^t}{(\sqrt{d-1})^t}, \tag{28}$$

which is the properly regularized number of t-periodic nb-walks. Going through exactly the same steps as in section (2), we get

$$\rho(\mu) = \frac{d}{2\pi} \cdot \frac{\sqrt{4(d-1)-\mu^2}}{d^2-\mu^2} + \frac{1}{\pi} \mathrm{Re} \sum_{t=3}^{\infty} \frac{y_t}{\sqrt{4(d-1)-\mu^2}} \mathrm{e}^{\mathrm{i}t \arccos(\frac{\mu}{2\sqrt{(d-1)}})} + \frac{1}{V} \rho^{\mathrm{corr}}(\mu). \tag{29}$$

The first term is the smooth part and can be identified as the Kesten–McKay density. For large t, since $\mathrm{tr}\, Y^t$ is dominated by $(d-1)^t$, it is clear that in the limit of large V, y_t tends to zero. The counting statistics of t-periodic nb-walks with $t < \log_{d-1} V$ is Poissonian, with $\langle \mathrm{tr}\, Y^t \rangle = (d-1)^t$. Thus, the mean value of y_t vanishes as $\mathcal{O}\left(\frac{1}{V}\right)$. Hence,

$$\lim_{V\to\infty} \langle \rho(\mu) \rangle = \rho_{\mathrm{KM}}(\mu). \tag{30}$$

The above can be considered as an independent proof of the Kesten–McKay formula (12). The original derivation relied on the fact that d-regular graphs look locally like trees, for which the spectral density is of the form (12). Here, it emerged without directly invoking the tree approximation, rather, it appears as a result of an algebraic manipulation.

The last term, $\frac{1}{V}\rho^{\mathrm{corr}}(\mu)$, is the correction to the smooth part, for finite V, which results from y_0, y_1, y_2. It is given explicitly by

$$\rho^{\mathrm{corr}}(\mu) = \frac{-1}{2\pi\sqrt{4(d-1)-\mu^2}} \left(1 + \mu + \mu^2 - 2(d-1) + \frac{d-2}{d-\mu}\right). \tag{31}$$

Equation (29) is identical to a trace formula derived by Mnëv [41]. Our derivation, however, follows an entirely different path which allows us to place the trace formula as a special case in a more general setting, and provides the leading-order correction, $\frac{1}{V}\rho^{\mathrm{corr}}(\mu)$.

If the graph at hand is non-Ramanujan, the theory should be modified since some of the phases ϕ_k in (27) become complex. Consequently, y_t diverge exponentially with t and the resulting trace formula (29) is ill defined. There are two ways to circumvent this problem. Either to use the trace formula with $w > 1$, at the cost of using periodic walks with back-scatter, or to remain with nb-walks but reformulate the trace formula so that it describes a coarse-grained version of the spectral density. We shall discuss below the latter option.

Consider a non-Ramanujan graph $\mathcal{G}$ and denote by $\gamma(\mathcal{G})$ the set of eigenvalues which lie outside the Kesten–McKay support $[-2\sqrt{d-1}, 2\sqrt{d-1}]$. The rigorous and numerical information available to date on the set of eigenvalues $\gamma(\mathcal{G})$ suggests that generic (V, d) regular graphs have the following properties [42, 43].

- The distance between $\gamma(\mathcal{G})$ and the Kesten–McKay support is smaller than $aV^{-\alpha}$, with $\alpha > 0$ and a positive constant a. Numerical simulations show that $\alpha \approx 2/3$.
- The cardinality of the set $\gamma(\mathcal{G})$ is bounded, and $\langle|\gamma(\mathcal{G})|\rangle = \mathcal{O}(1)$.

The derivation of the trace formula for Ramanujan graphs (29) used (22) which expresses the identity operator in terms of the orthonormal set of Chebyshev polynomials. Truncating the infinite sum in (22) at $t = t_{\max}$, one obtains the identity operator in the finite space spanned by the first $t_{\max}$ Chebyshev polynomials. The resulting sum

$$\tilde{\delta}(x, x') = \frac{2}{\pi\sqrt{1-x^2}} \sum_{t=0}^{t_{\max}} \frac{1}{1+\delta_{t,0}} T_t(x) T_t(x') \tag{32}$$

displays a peak centered at $x = x'$ of width $\approx \frac{1}{t_{\max}}$. The coarse-grained spectral density for μ in the Kesten–McKay interval is defined as

$$\tilde{\rho}(\mu) = \frac{2\sqrt{d-1}}{V - |\gamma(\mathcal{G})|} \cdot \sum_{\mu_k \in \mathcal{G}\setminus\gamma(\mathcal{G})} \tilde{\delta}\left(\frac{\mu}{2\sqrt{d-1}}, \frac{\mu_k}{2\sqrt{d-1}}\right). \tag{33}$$

We now return to (20) with $w = 1$ and separate the sum on the spectrum to its Ramanujan and non-Ramanujan components:

$$\begin{aligned} y_t = &\frac{1}{V}(d-1)^{-\frac{t}{2}} + \frac{d-2}{2}(d-1)^{-\frac{t}{2}}(1+(-1)^t) \\ &+ \frac{2}{V} \sum_{\mu_k \in \mathcal{G}\setminus\gamma(\mathcal{G})} T_t\left(\frac{\mu_k}{2\sqrt{d-1}}\right) + \frac{2}{V} \sum_{\mu_k \in \gamma(\mathcal{G})} T_t\left(\frac{\mu_k}{2\sqrt{d-1}}\right). \end{aligned} \tag{34}$$

Upon multiplying both sides by $\frac{1}{\pi(1+\delta_{t,0})} T_t\left(\frac{\mu}{2\sqrt{d-1}}\right)$ and performing the sum over $t = 0, \ldots, t_{\max}$ we have to consider in particular the last term since it involves the exponentially increasing contributions from the non-Ramanujan spectral values. Consider $\mu_k \in \gamma(\mathcal{G})$. It is bounded by $|\mu_k| \leqslant 2\sqrt{d-1}(1 + aV^{-\alpha})$, and therefore the contribution of the sum of the last terms in (34) is bounded by

$$\frac{2|\gamma(\mathcal{G})|}{V} \frac{\exp(t_{\max} a V^{-\alpha/2})}{\sqrt{a} V^{-\alpha/2}}.$$

Choosing $t_{\max} < \frac{V^{\alpha/2}}{a} \log V^{1-\alpha/2}$ ensures that the sum converges to zero as V increases. Summing the other terms in (34) results in the finite $t_{\max}$ analog of the Kesten–McKay density, which converges exponentially quickly to the limit expression (the correction goes to zero as $z^{t_{\max}}$, $z < 1$). The truncated oscillatory contribution arises from the truncated sum over the left-hand side of equation (34). Truncating the t sum at $t_{\max}$ implies that the trace formula cannot resolve spectral intervals of order $\frac{1}{t_{\max}}$, which are larger than the mean spectral spacing which is of order $\frac{1}{V}$. In many applications, this does not pose a severe problem.

2.2. *The magnetic case* ($w = 1$)

The magnetic spectrum differs from the corresponding non-magnetic one in one important aspect, namely, there is no analog to the phenomenon that the maximal eigenvalue μ_0 is identically d. Rather, when averaged over the magnetic ensemble, it falls right on the boundary of the Kesten–McKay support. This can be shown by the following heuristic argument (a rigorous proof can be found in [43]). Consider the magnetic edge-connectivity matrix which excludes back-scatter: $Y^{(M)} = B^{(M)} - J$. The ensemble mean of its maximal eigenvalue can be estimated by studying the behavior of $\langle \mathrm{tr}\,[(Y^{(M)})^t]\rangle_\Phi$ for large t, where

$\langle\cdots\rangle_\Phi$ denotes the average over the magnetic ensemble. The only non-vanishing contributions to $\langle \mathrm{tr}\,[(Y^{(M)})^t]\rangle_\Phi$ come from *self-tracing* periodic nb-walks where each edge is traversed an equal number of times in both directions. The periodic walks which asymptotically dominate $\langle \mathrm{tr}\,[(Y^{(M)})^t]\rangle_\Phi$ consist of two cycles which share a single vertex, and each cycle is traversed twice in opposite directions. The common vertex enables the inversion of the traversal direction without back-scatter. On average, the number of such periodic walks is of order $t(d-1)^{\frac{t}{2}}$ hence, $\langle|\eta_0|\rangle_\Phi \simeq \sqrt{d-1}$, where η_0 is the largest eigenvalue of $Y^{(M)}$ in absolute magnitude. Using the connection between the spectra of $Y^{(M)}$ and $A^{(M)}$ which is implied by the Bartholdi identity, we deduce $\langle|\mu_0|\rangle_\Phi \simeq 2\sqrt{d-1}$.

Starting from equation (A.7), we continue by assuming that the graph is Ramanujan in the sense that all eigenvalues of $A^{(M)}$ including the largest one satisfy $|\mu| < 2\sqrt{d-1}$. The spectrum of $Y^{(M)}$ consists of

$$\begin{aligned}\sigma(Y^{(M)}) = \{&+1\times(E-V), -1\times(E-V),\\ &(\sqrt{d-1}\,\mathrm{e}^{\mathrm{i}\phi_k}, \sqrt{d-1}\,\mathrm{e}^{-\mathrm{i}\phi_k}, k=1,\ldots,V)\}\\ \text{where} \qquad &\phi_k = \arccos\frac{\mu_k}{2\sqrt{(d-1)}}, \qquad 0\leqslant\phi_k\leqslant\pi.\end{aligned} \tag{35}$$

The scaled traces y_t are defined as

$$y_t = \frac{1}{V}\frac{\mathrm{tr}\,(Y^{(M)})^t}{(\sqrt{(d-1)})^t} \tag{36}$$

and we end up with a trace formula, similar to equation (29). The smooth part is again the Kesten–McKay density. The oscillatory part is different, because the terms in y_t contributed by t-periodic walks are now decorated by magnetic phases which are accumulated along the walks. We have shown previously that $\langle \mathrm{tr}\,[(Y^{(M)})^t]\rangle_\Phi \sim t(d-1)^{\frac{t}{2}}$. Thus, $\langle y_t\rangle_\Phi \to 0$ if the limits $t\to\infty$ and $V\to\infty$ are taken such that $\frac{t}{V}\to 0$. Therefore the *mean* spectral density is again the Kesten–McKay measure, as in the non-magnetic $w=1$ case.

3. Applications of the w-trace formula

The w-trace formula offers a bridge between the spectral and the combinatorial aspects of graph theory. This connection can be exploited in order to compute combinatorial quantities, as will be shown in this section.

Throughout this section we shall assume the large V limit of the spectral density (24) and neglect the term $\frac{1}{V}\rho^{\mathrm{corr}}(\mu; w)$:

$$\rho(\mu) = \rho^{\mathrm{smooth}}(\mu; w) + \rho^{\mathrm{osc}}(\mu; w).$$

The explicit expressions for $\rho^{\mathrm{smooth}}(\mu; w)$ and $\rho^{\mathrm{osc}}(\mu; w)$ are given in (25).

In section 1, we have shown that $\mathrm{tr}\,Y^t(w)$ can be considered as a generating function for the number $N(t; g)$ of t periodic walks which scatter back exactly g times:

$$N(t; g) = \frac{(-1)^g}{g!}\frac{\partial^g\,\mathrm{tr}\,Y^t(w)}{\partial w^g}\bigg|_{w=1}. \tag{37}$$

Here, we shall use the w-trace formula to compute $N(t, g=1)$ explicitly and show how expressions for higher g can be obtained. To start, we take the first derivative of (24) with respect to w. The left-hand side vanishes, since $\rho(\mu)$ does not depend on w. Moreover, it can easily be checked that $\frac{d\rho^{\mathrm{smooth}}(\mu;w)}{dw}\big|_{w=1} = 0$. Thus, the first derivative of $\rho^{\mathrm{osc}}(\mu; w)$ computed at $w=1$ must vanish identically for any μ. We shall show that the first derivative can be written in the form $\sum_l a_l T_l\big(\frac{\mu}{2\sqrt{d-1}}\big)$, and therefore the coefficients a_l must vanish. This requirement provides a recurrence relation from which $N(t, g = 1)$ can be computed for any t.

From now on we shall denote $\frac{d}{dw}$ by $()'$. Taking the derivative is quite tedious, since w appears in (25) both in the coefficients of the Chebyshev polynomials and in their argument. However, using elementary relations between the Chebyshev polynomials and their derivatives, and after some lengthy but straightforward computations, one gets

$$a_l = (d-2)\left(\tfrac{1}{4}(l-2)y_{l-2}(1) - \tfrac{1}{4}(l+2)y_{l+2}(1) - y_l(1)\right) + (d-1)\left(y_l'(1) - \tfrac{1}{2}y_{l-2}'(1) - \tfrac{1}{2}y_{l+2}'(1)\right). \tag{38}$$

We now recall that

$$y_l(w) = \frac{1}{V}\frac{\operatorname{tr} Y^l(w) - (d-w)^l}{(w(d-w))^{\frac{l}{2}}} \tag{39}$$

and we write (38) in terms of $\operatorname{tr} Y^l$:

$$a_l = \frac{1}{2}\left((d-2)(l-2)\frac{\operatorname{tr} Y^{l-2}(1)}{(d-1)^{\frac{l-2}{2}}} - (d-2)(l+2)\frac{\operatorname{tr} Y^l(1)}{(d-1)^{\frac{l}{2}}}\right) + \frac{1}{2}\left(-\frac{(\operatorname{tr} Y^{l-2})'(1)}{(d-1)^{\frac{l-4}{2}}} + 2\frac{(\operatorname{tr} Y^l)'(1)}{(d-1)^{\frac{l-2}{2}}} - \frac{(\operatorname{tr} Y^{l+2})'(1)}{(d-1)^{\frac{l}{2}}}\right). \tag{40}$$

The requirement that $a_l = 0$ results in an expression for $(\operatorname{tr} Y^l)'$ in terms of $(\operatorname{tr} Y^k)$, where $k < l$. It is convenient to define

$$\begin{aligned} p_l &\equiv \frac{(\operatorname{tr} Y^l)'(1)}{(d-1)^{\frac{l-2}{2}}} \\ q_l &\equiv \left((d-2)(l-2)\frac{\operatorname{tr} Y^{l-2}(1)}{(d-1)^{\frac{l-2}{2}}} - (d-2)(l+2)\frac{\operatorname{tr} Y^l(1)}{(d-1)^{\frac{l}{2}}}\right) \end{aligned} \tag{41}$$

and after some further computations, the following inhomogeneous recursion relation emerges:

$$p_{l+2} - p_l = \begin{cases} \displaystyle\sum_{k=1}^{l/2} q_{2k}, & \text{if } l \text{ is even} \\ \displaystyle\sum_{k=0}^{\lfloor l/2 \rfloor} q_{2k+1}, & \text{if } l \text{ is odd.} \end{cases} \tag{42}$$

Substituting q_l from(41), we get that

$$p_{l+2} - p_l = \begin{cases} -2(d-2)\left[\displaystyle\sum_{k=1}^{l/2}\frac{\operatorname{tr} Y^{2k}(1)}{(d-1)^k} + \frac{l}{2}\frac{\operatorname{tr} Y^l(1)}{(d-1)^{\frac{l}{2}}}\right], & \text{if } l \text{ is even} \\ -2(d-2)\left[\displaystyle\sum_{k=1}^{\lfloor l/2 \rfloor}\frac{\operatorname{tr} Y^{2k+1}(1)}{(d-1)^{k+\frac{1}{2}}} + \frac{l}{2}\frac{\operatorname{tr} Y^l(1)}{(d-1)^{\frac{l}{2}}}\right], & \text{if } l \text{ is odd.} \end{cases} \tag{43}$$

It can be verified by substitution that the solution of the recursion relation is

$$p_l = \begin{cases} -l(d-2)\displaystyle\sum_{k=1}^{l/2-1}\frac{\operatorname{tr} Y^{2k}(1)}{(d-1)^k}, & \text{if } l \text{ is even} \\ -l(d-2)\displaystyle\sum_{k=1}^{\lfloor l/2 \rfloor - 1}\frac{\operatorname{tr} Y^{2k+1}(1)}{(d-1)^{k+\frac{1}{2}}}, & \text{if } l \text{ is odd} \end{cases} \tag{44}$$

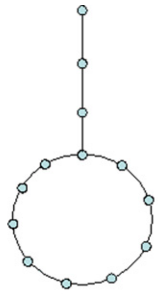

Figure 2. A periodic walk of length 16 composed of a cycle of length 10 and a tail of length 6.

or, equivalently:

$$(\operatorname{tr} Y^l)'(1) = \begin{cases} -l(d-2)\displaystyle\sum_{k=1}^{l/2-1} \operatorname{tr} Y^{2k}(1)(d-1)^{\frac{l-2k-2}{2}}, & \text{if } l \text{ is even} \\ -l(d-2)\displaystyle\sum_{k=1}^{\lfloor l/2\rfloor-1} \operatorname{tr} Y^{2k+1}(1)(d-1)^{\frac{l-2k-3}{2}}, & \text{if } l \text{ is odd.} \end{cases} \tag{45}$$

Finally, $N(t; g = 1) = -(\operatorname{tr} Y^l)'(1)$ is the number of periodic walks of length l with one back-scatter. This result can be derived directly by the following argument. For simplicity, let us consider the case where l is even. A periodic walk of length l with one back-scatter must consist of a periodic walk of length $2k$ with no back-scatter, and a 'tail' of length $l-2k$. A tail is a periodic walk which goes over some path and then comes back in the opposite direction. Clearly, it has one back-scatter, as demonstrated in figure 2. The number of periodic walks of length $2k$ with no back-scatter is just $\operatorname{tr} Y^{2k}(1)$. The first edge in the tail can be chosen in $d-2$ ways. Any other edge, until we reach the end of the tail, can be chosen in $d-1$ ways. There are $\frac{l-2k-2}{2}$ such choices to make. The way back along the tail can be made in only one way. We now need to sum over k. Since both l and the length of the tail are even, the shortest periodic walk with no back-scatter is of length 4, so the sum must start at $k = 2$, and it must end at $k = \frac{l}{2} - 1$, since the shortest tail is of length 2.

We have thus seen that using the w-trace formula, we were able to extract combinatorial information about the graph. The computation above was the simplest case, but it is clear that $N(t; g > 1)$ can be derived by further differentiations, and the use of known recursion relations involving the Chebyshev polynomials and their derivatives.

4. Unitary evolution

The trace formula (13) which was discussed in section (1) was originally derived by constructing the graph evolution operator $U(\mu)$ (14). The zeros of the secular function $z(\mu) \doteq \det(I - U(\mu))$ provide the spectrum of the graph, and using standard methods, the trace formula followed. In view of the results derived in the previous sections, it is natural to expect that together with $U(\mu)$ there exists a one-parameter family of *unitary* operators, by which other secular equations can be written down, and corresponding trace formula can be derived. This is indeed the case, and to prove it, we go back to the Bartholdi identity for regular graphs (16). It is convenient to slightly modify the free parameters w, s and use $\alpha = s, \beta = ws$. Bartholdi's formula now reads

$$\det(I^{(2E)} - (\alpha B - \beta J)) = (1 - \beta^2)^{E-V} \det((1 + d\alpha\beta - \beta^2)I^{(V)} - \alpha A) \tag{46}$$

for any complex $\alpha \neq 0, \beta$.

Defining the $2E \times 2E$ matrix $U = \alpha B - \beta J$ and using the properties of B, J it is straightforward to show that

$$U \text{ is unitary} \iff \text{both} \begin{cases} |\beta|^2 = 1 \\ |\alpha|^2 d = \alpha\beta^* + \alpha^*\beta. \end{cases} \tag{47}$$

The above implies that $\beta = \mathrm{e}^{\mathrm{i}\phi}$ where ϕ is an arbitrary real parameter. If we impose further the relation

$$\alpha\mu = 1 + d\alpha\beta - \beta^2 \tag{48}$$

between α, β and the spectral parameter μ, Bartholdi's formula may be written as

$$\det(I^{(2E)} - U(\mu, \phi)) = (1 - \mathrm{e}^{2\mathrm{i}\phi})^E (\mu - d\,\mathrm{e}^{\mathrm{i}\phi})^{-V} \det(\mu I^{(V)} - A), \tag{49}$$

where

$$U(\mu, \phi) = \frac{1 - \mathrm{e}^{2\mathrm{i}\phi}}{\mu - d\,\mathrm{e}^{\mathrm{i}\phi}} B - \mathrm{e}^{\mathrm{i}\phi} J$$

is a unitary evolution operator depending parametrically on the real and independent parameters μ and ϕ in the domain $\mathcal{D} = \{\mu \in (-d, d), \phi \in \mathbb{R}\backslash\{\pi\mathbb{Z}\}\}$. ϕ is restricted away from zero and any integer multiples of π since for these values $\alpha = 0$ and (49) does not provide a relationship between the spectrum of A and $U(\mu, 0) = -J$.

For $\mu, \phi \in \mathcal{D}$ the secular equation

$$Z_A(\mu) \doteq \det(\mu I - A) = (1 - \mathrm{e}^{2\mathrm{i}\phi})^{-E} (\mu - d\,\mathrm{e}^{\mathrm{i}\phi})^V \det(I^{(2E)} - U(\mu, \phi))$$

is the characteristic polynomial of A which is real on the real axis and its zeros coincide with the spectrum of A. The spectral density function, $\rho(\mu) \equiv \frac{1}{V}\sum_{j=1}^{V} \delta(\mu - \mu_j)$, which can be written as

$$\rho(\mu) = -\frac{1}{V\pi} \lim_{\epsilon\to 0^+} \mathcal{I}m \frac{\mathrm{d}}{\mathrm{d}\mu} \log Z_A(\mu + i\epsilon), \tag{50}$$

will now be a sum of a 'smooth' contribution from the phase of the $(1 - \mathrm{e}^{2\mathrm{i}\phi})^{-E}(\mu - d\,\mathrm{e}^{\mathrm{i}\phi})^V$ term and a fluctuating contribution from the sum over periodic orbits on the graph, with amplitudes which are determined by the forward and backward scattering defined by the evolution operator $U(\mu, \phi)$:

$$\rho(\mu) = -\frac{1}{V\pi} \frac{\mathrm{d}}{\mathrm{d}\mu} \log ((1 - \mathrm{e}^{2\mathrm{i}\phi})^{-E} (\mu - d\,\mathrm{e}^{\mathrm{i}\phi})^V) + \frac{1}{V\pi} \lim_{\epsilon\to 0^+} \mathcal{I}m \frac{\mathrm{d}}{\mathrm{d}\mu} \sum_{t=1}^{\infty} \frac{1}{t} \operatorname{tr}(U(\mu + i\epsilon)^t). \tag{51}$$

Various real functions $\phi = \phi(\mu)$ can be defined, which yield various smooth and fluctuating parts. One interesting case is choosing $\phi = \text{const}$. For this choice, the spectral density function takes the form

$$\rho(\mu) = -\frac{1}{\pi d} \frac{\sin\phi}{\left(\frac{\mu}{d}\right)^2 + 1 - 2\frac{\mu}{d}\cos\phi} + \frac{1}{V\pi} \lim_{\epsilon\to 0^+} \mathcal{I}m \frac{\mathrm{d}}{\mathrm{d}\mu} \sum_{t=1}^{\infty} \frac{1}{t} \operatorname{tr}(U(\mu + i\epsilon)^t), \tag{52}$$

where

$$\operatorname{tr} U(\mu)^t = \frac{(2\sin\phi)^t}{(\mu^2+d^2-2\mu d\cos\phi)^{\frac{t}{2}}}\,\mathrm{e}^{\mathrm{i}t\left(\phi-\arctan\frac{d\cos\phi-\mu}{d\sin\phi}\right)}\cdot \sum_g N(g;t)\tilde{a}^g\,\mathrm{e}^{\mathrm{i}g\left(\frac{\pi}{2}-\phi+\arctan\frac{d\sin 2\phi-\sin 2\phi-\mu\sin\phi}{1-\cos 2\phi-\mu\cos\phi+d\cos 2\phi}\right)} \tag{53}$$

and

$$\tilde{a}=\tilde{a}(\mu)=\frac{\sqrt{2+d(d-2)+\mu^2-2\mu d\cos\phi+2(d-1)\cos 2\phi}}{2\sin\phi}.$$

Specifically, the case of $\phi=-\frac{\pi}{2}$ corresponds to the evolution operator chosen in (13). Another interesting choice would be that for which the smooth part is the Kesten–McKay measure (12). This will be achieved for $\phi(\mu)$ which satisfies

$$\frac{d}{2\pi}\cdot\frac{2\sin\phi-\frac{\mathrm{d}\phi}{\mathrm{d}\mu}[\mu^2+d(d-2)-2(d-1)\mu\cos\phi]}{\mu^2+d^2-2\mu d\cos\phi}=\rho_{\mathrm{KM}}(\mu), \tag{54}$$

where the lhs of this differential equation is the general expression for the smooth part of the spectral density function, normalized by the number of eigenvalues V, or equivalently

$$\frac{2k}{V}+\frac{d}{2}\left(\frac{1}{2}-\frac{\phi(\mu)}{\pi}\right)+\frac{\phi(\mu)}{\pi}\mp\frac{1}{\pi}\arccos\left(\frac{\mu\cos\phi(\mu)-d}{\sqrt{\mu^2+d^2-2\mu d\cos\phi(\mu)}}\right)-(-1\mp 1)=N_{\mathrm{KM}}(\mu), \tag{55}$$

where the lhs is the general expression for the phase of $(1-\mathrm{e}^{2\mathrm{i}\phi})^{-E}(\mu-d\,\mathrm{e}^{\mathrm{i}\phi})^V$ divided by πV, $N_{\mathrm{KM}}(\mu)=\int_{-2\sqrt{d-1}}^{\mu}\rho_{\mathrm{KM}}(\mu)$ is the Kesten–McKay counting function and $\mp$ refers to the sign of $\mu\sin\phi$. The parameter $k\in\mathbb{Z}$ arises from the fact that $(1-\mathrm{e}^{2\mathrm{i}\phi})^{-E}(\mu-d\,\mathrm{e}^{\mathrm{i}\phi})^V$ is defined up to an integer multiplicity of 2π. Note that if $\phi_{\mathrm{KM}}^{(\frac{2k}{V})}(\mu)$ is the kth solution to (55), then $\phi_{\mathrm{KM}}^{(\frac{2k}{V})}(\mu)+2\pi$ is the $k+\frac{(d-2)V}{2}$ solution, so in fact there are at most $\frac{(d-2)V}{2}$ distinct solutions to (54) and (55), where all the rest result by an addition of multiples of 2π. Figure 3 shows the numerical solution of (54).

Assuming very large d and scaling the spectral parameter, $u=\frac{\mu}{2\sqrt{d-1}}$, one can expand in powers of $\frac{1}{\sqrt{d-1}}$ so that (54) takes the form

$$\frac{\mathrm{d}\phi}{\mathrm{d}u}=-\frac{4}{d-1}\sqrt{1-u^2}+\mathcal{O}\left(\left(\frac{1}{d-1}\right)^{\frac{3}{2}}\right)$$

and solve to first order

$$\phi_{\mathrm{KM}}^{(\frac{2k}{V})}(\mu)=C_k-\frac{1}{2(d-1)^2}\mu\sqrt{4(d-1)-\mu^2}-\frac{2}{d-1}\arcsin\frac{\mu}{2\sqrt{d-1}}\qquad \text{where}\qquad C_k=\frac{\pi}{2}+\frac{2\pi}{d-2}\left(1+\frac{2k}{V}\right). \tag{56}$$

To every distinct solution corresponds a set of continuous operators $U_{\mathrm{KM}}^{(r)}(\mu)=U\big(\mu,\phi_{\mathrm{KM}}^{(r)}(\mu)\big)$ for which the smooth part is the Kesten–McKay measure $\big(r\equiv\frac{2k}{V}\big)$. Thus, the fluctuating part must vanish after averaging over the ensemble, as V goes to infinity. Although a solution $\phi_{\mathrm{KM}}^{(r)}$ can cross the value $\phi_{\mathrm{KM}}^{(r)}(\mu_0)=\pi k$ for $\mu_0\neq\pm d$, hence is not a valid solution

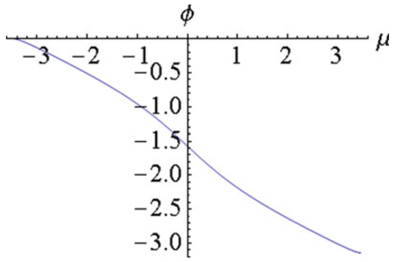

Figure 3. The numerical solution of (54) for $d = 4$ and $\frac{2k}{V} = -2$.

under the construction above, a continuous set of unitary operators can still be defined using this solution by

$$U^{(r)}(\mu) = \begin{cases} \dfrac{1 - e^{2i\phi_{KM}^{(r)}(\mu)}}{\mu - d\, e^{i\phi_{KM}^{(r)}(\mu)}} B - e^{i\phi_{KM}^{(r)}(\mu)} J & \text{if } \mu \neq \mu_0 \\ (-1)^k J & \text{if } \mu = \mu_0 \end{cases} \tag{57}$$

with the desired property.

5. Discussion

The novel feature which emerges from the present work is the fact that the *same* spectral density can be expressed by trace formulae which are based on *different* sets of periodic walks. Moreover, the form of the smooth part and the weight associated with periodic walks depend continuously on the parameters w and ϕ in (25) and (51), respectively. This is most prominent in the case $w = 1$ where the contributing walks are non-backscattering. For any $w \neq 1$, back-scattering walks are contributing, so the weights and the phases associated with each periodic walk are w dependent.

The choice $w = 1$ was beneficial for several reasons. First, it serves as a new and independent proof of the Kesten–McKay formula (12), where the tree approximation is not taken explicitly. Second, we were able to derive a leading-order correction for large, but finite, V.

The trace formulae we have derived provide new insight into the question raised in the introduction: Can we distinguish among the periodic orbits on the graph distinct subsets, each responsible to a different feature in the spectral density? As we have mentioned, the smooth part (the Kesten–McKay measure) stems from periodic walks restricted to tree-like subgraphs. We can now identify the nb-periodic orbits as the subset which is responsible for the fluctuating part of the spectral density. It is therefore conjectured that for $w \neq 1$, the back-scattered walks give opposite contributions to the smooth and oscillatory parts of $\rho(\mu)$. This sheds a new light on the puzzle regarding the re-summation which is required in (13).

We have chosen to write the fluctuating part of the spectral density, (29), in a slightly peculiar way. Usually in trace formulae, the summands in the sum over periodic orbits can be written as an amplitude times an exponent. The exponent plays the role of classical action. We can thus identify the quantity $\arccos \frac{\mu}{2\sqrt{d-1}}$ as an 'action' per unit step, of the quantum evolution on the graph. The amplitude is proportional to y_t, which is a measure of the number of t-periodic nb-orbits.

As we have shown, the w-trace formula can be used as a tool for turning spectral information about graphs into combinatorial information. This is one of the advantages of the w-trace formula over that specialized for $w = 1$.

In the last section, we have proven that a set of unitary evolution operators, which govern the quantum evolution on the graph, exists, and that they reproduce the density of states for the discrete Laplacian. This stands in contrast to the non-unitary 'evolution operators' which were used in the preceding sections. As was shown, a specific choice can be made, in order to reproduce the Kesten–McKay measure (or the semi-circle distribution, for large d).

In the following paper in the series, we shall use the fluctuating part of (29) in order to investigate the spectral fluctuations of discrete Laplacians on regular graphs. We shall show that these fluctuations are given by the appropriate ensembles of random matrix theory and establish some interesting connections between spectral and combinatorial graph theory.

Acknowledgments

The authors wish to express their gratitude to Mr Sasha Sodin for many insightful discussions and for his assistance in overcoming obstacles along the way. Professor Nati Linial is also acknowledged for explaining to us some results from graph theory. We are indebted to Dr I Sato for reading the manuscript and for several critical remarks and suggestions.

This work was supported by the Minerva Center for nonlinear Physics, the Einstein (Minerva) Center at the Weizmann Institute and the Wales Institute of Mathematical and Computational Sciences) (WIMCS). Grants from EPSRC (grant EP/G021287), BSF (grant 2006065) and ISF (grant 166/09) are acknowledged.

Appendix. The Bartholdi identity

The basis for the work presented in this paper is an identity proved recently by Bartholdi [20] which reveals a number of interesting connections between the spectral properties of the graph and its set of periodic orbits. This identity generalizes a previous result by Bass [21]. For general graphs, the Bartholdi identity is

$$\det(I^{(2E)} - s(B - wJ)) = (1 - w^2 s^2)^{E-V} \det(I^{(V)} + ws^2(D - wI^{(V)}) - sA). \tag{A.1}$$

The parameters s and w are arbitrary real or complex numbers, $I^{(2E)}$ and $I^{(V)}$ are the identity matrices in dimensions $2E$ and V, respectively, and the matrices A, B, D and J were defined in (1). For d-regular graphs, the Bartholdi identity reads

$$\det(I^{(2E)} - s(B - wJ)) = (1 - w^2 s^2)^{E-V} \det(I^{(V)}(1 + w(d - w)s^2) - sA). \tag{A.2}$$

Its importance in the present context comes from the fact that it connects the spectrum of the adjacency matrix A with that of the matrices B and J, which can be used to count various types of cycles and walks on the corresponding graph.

Bartholdi's original proof of this identity is based on combinatorial considerations. Proofs which are algebraic in nature were provided by various authors, and we quote here the version given by Mizuno and Sato [22] to make this paper self-contained, and to provide a base for the derivation of the trace formula for the discrete Laplacian.

Proof of Bartholdi's identity

The proof of Bartholdi's identity follows almost *verbatim* the proof presented in [22].

Define the two $2E \times V$ rectangular matrices

$$B^{(+)}_{e,i} := \begin{cases} 1 & \text{if } t(e) = i \\ 0 & \text{otherwise.} \end{cases}; \qquad B^{(-)}_{e,i} := \begin{cases} 1 & \text{if } o(e) = i \\ 0 & \text{otherwise.} \end{cases} \tag{A.3}$$

Denoting by $\widetilde{X}$ the transpose of X, one can easily prove that

$$\begin{aligned} &B^{(+)}\widetilde{B^{(-)}} = B; \qquad \widetilde{B^{(-)}}B^{(+)} = A \\ &\widetilde{B^{(+)}}B^{(+)} = dI^{(V)}; \qquad B^{(+)}\widetilde{B^{(+)}} = YJ + I^{(2E)}. \end{aligned} \tag{A.4}$$

Construct the two $(2E + V) \times (2E + V)$ square matrices

$$L = \begin{bmatrix} (1 - w^2s^2)I^{(V)} & -\widetilde{B^{(-)}} + ws\widetilde{B^{(+)}} \\ 0 & I^{(2E)} \end{bmatrix}; \qquad M = \begin{bmatrix} I^{(V)} & \widetilde{B^{(-)}} - ws\widetilde{B^{(+)}} \\ sB^{(+)} & (1 - w^2s^2)I^{(2E)} \end{bmatrix}. \tag{A.5}$$

Using the identities (A.4) one can compute the matrices LM and ML, and since their determinants are equal, one finally gets the desired identity (16).

Generalizations of the Bartholdi identity

The Bartholdi identity can easily be generalized to three interesting cases: ‘magnetic’ graphs, multigraphs and weighted graphs. The proof always follows the same steps shown above, and for each case, one has to define the four matrices, A, B, D, J, properly.

- *Magnetic regular graphs:* We replace the adjacency matrix A by its ‘magnetic’ analog (10), and the edge connectivity matrix B by

$$(B^{(M)})_{e,e'} = B_{e,e'}\,\mathrm{e}^{\frac{\mathrm{i}}{2}(\phi_e + \phi_{e'})}. \tag{A.6}$$

  The matrix J is not modified since $\phi_e = -\phi_{\hat{e}}$. The ‘magnetic’ Bartholdi identity now reads

$$\det(I^{(2E)} - s(B^{(M)} - wJ)) = (1 - w^2s^2)^{E-V}\det(I^{(V)}(1 + w(d - w)s^2) - sA^{(M)}). \tag{A.7}$$

  The proof follows the same steps as above, after modifying $B^{(\pm)}_{e,i}$ by multiplying them by $\mathrm{e}^{\pm\frac{\mathrm{i}}{2}\phi_e}$, and, by replacing the transpose operation $(\widetilde{\ })$ by Hermitian conjugation. For non-regular magnetic graphs, the matrix D is the same as the non-magnetic case.
- *Multigraphs:* The adjacency matrix is defined as explained in the introduction (section 1). B is still a (0, 1) matrix where we must list *all* the edges, including parallel ones and loops. J does not change and in D we must count the degree of a vertex including parallel edges and counting loops as two edges.
- *Weighted graphs:* The weighted adjacency matrix was defined in section 1. J is not changed, and we redefine B, D in the following way:

$$(B^{(W)})_{e,e'} = B_{e,e'}\sqrt{W_e W_{e'}} \tag{A.8}$$

$$(D^{(W)})_{i,j} = \delta_{ij}\sum_{e:t(e)=i} W_e. \tag{A.9}$$

These are three canonical generalizations. Obviously, one can make further generalization by combining them (magnetic multigraph, for example).

References

[1] Imry Y 1997 *Introduction to Mesoscopic Physics* (Oxford: Oxford University Press)
[2] Grimmett G 1999 Grundlehren der mathematischen Wissenschaften *Percolation* 2nd edn, vol 321 (Berlin: Springer)
[3] Grimmett G and Stirzaker D 2001 *Probability and Random Processes* (Oxford: Oxford University Press)
[4] Jakobson D, Miller S, Rivin I and Rudnick Z 1999 Level spacings for regular graphs *IMA Vol. Math. Appl.* **109** 317–29
[5] Bohigas O, Giannoni M-J and Schmit C 1984 Characterization of chaotic quantum spectra and universality of level fluctuation laws *Phys. Rev. Lett.* **52** 1–4
[6] Gutzwiller M C 1971 *J. Math. Phys.* **12** 343
[7] Berry M V 1985 Semiclassical theory of spectral rigidity *Proc. R. Soc.* A **400** 229–51
[8] Sieber M and Richter K 2001 Correlations between periodic orbits and their Rôle in spectral statistics *Phys. Scr.* **T90** 128–33
[9] Heusler S, Muller S, Braun P and Haake F 2004 Universal spectral form factor for chaotic dynamics *J. Phys. A: Math. Gen.* **37** L31
[10] Hashimoto K 1989 Zeta functions of finite graphs and representations of *p*-adic groups automorphic forms and geometry of arithmetic varieties (*Adv. Stud. Pure Math.* vol 15) (Boston, MA: Academic) pp 211–80
[11] Avron J E, Raveh A and Zur B 1988 Adiabtaic quantum transport in multiply connected systems *Rev. Mod. Phys.* **60** 873–915
[12] Kesten H 1959 Symmetric random walks on groups *Trans. Am. Math. Soc.* **92** 336–54
[13] McKay B D 1981 The expected eigenvalue distribution of a random labelled regular graph *Linear Algebr. Appl.* **40** 203–16
[14] Brooks R 1991 The spectral geometry of k-regular graphs *J. Anal.* **57** 120–51
[15] Alon N, Benjamini I, Lubetzky E and Sodin S 2006 Non-backtracking random walks mix faster arXiv:math/0610550v1
[16] Harrison J M, Smilansky U and Winn B 2007 Quantum graphs where back-scattering is prohibited *J. Phys. A: Math. Theor.* **40** 14181–93
[17] Smilansky U 2007 Quantum chaos on discrete graphs *J. Phys. A: Math. Theor.* **40** F621–30
[18] Kottos T and Smilansky U 1997 Quantum chaos on graphs *Phys. Rev. Lett.* **79** 4794–7
Kottos T and Smilansky U 1999 Periodic orbit theory and spectral statistics for quantum graphs *Ann. Phys.* **274** 76–124
[19] Roth J P 1985 *Lecture Notes in Mathematics: Theorie de Potential* ed A Dold and B Eckmann (Berlin: Springer) p 521
[20] Bartholdi L 1999 Counting paths in graphs *Enseign. Math.* **45** 83–131
[21] Bass H 1992 The Ihara–Selberg zeta function of a tree lattice *Int. J. Math.* **3** 717–97
[22] Mizuno H and Sato I 2005 A new proof of Bartholdi's theorem *J. Algebr. Comb.* **22** 259–71
[23] Murty M Ram 2003 Ramanjuan graphs *J. Ramanujan Math. Soc.* **18** 1–20
[24] Mizuno H and Sato I 2008 The scattering matrix of a graph *Electron. J. Comb.* **15** R96
[25] Shnirelman A I 1974 Ergodic properties of eigenfunctions *Uspehi Mat. Nauk* **29** 181–2
[26] Blümel R and Smilansky U 1990 Random matrix description of chaotic scattering: semi classical approach. *Phys. Rev. Lett.* **64** 241–4
[27] Gutzwiller M 1991 *Chaos in Classical and Quantum Mechanics* (New York: Springer)
[28] Haake F 2001 *Quantum Signatures Of Chaos* (Berlin: Springer)
[29] Stoeckmann H J 1990 *Quantum Chaos—An Introduction* (Cambridge: Cambridge University press)
[30] Gnutzmann S and Smilansky U 2006 Quantum graphs: applications to quantum chaos and universal spectral statistics *Adv. Phys.* **55** 527–625
[31] Bollobas B 1985 *Random Graphs* (London: Academic)
[32] Chung F R K 1997 Spectral graph theory *Regional Conference Series in Mathematics* vol 92 (Providence, RI: American Mathematical Society)
[33] Terras A A 1999 Fourier analysis on finite groups and applications *London Mathematical Society Student Texts* vol 43 (Cambridge: Cambridge University Press)
[34] Terras A A 2002 Arithmetic quantum chaos *IAS/Park City Math. Ser.* **12** 333–75
[35] Hurt N E 2001 The prime geodesic theorem and quantum mechanics on finite volume graphs: a review *Rev. Math. Phys.* **13** 1459–503
[36] Ihara Y 1966 On discrete subgroups of the two by two projective linear group over a p-adic field *J. Mat. Soc. Japan* **18** 219–35
[37] Stark H M and Terras A A 1996 Zeta functions of finite graphs and coverings *Adv. Math.* **121** 124–65

[38] Kotani M and Sunada T 2000 Zeta functions on finite graphs *J. Math. Sci. Univ. Tokyo* **7** 7–25

[39] Stark H M 1999 Multipath zeta functions of graphs *Emerging Applications of Number Theory (Minneapolis, MN, 1996) (IMA Vol. Math. Appl.* vol 109*)* (New York: Springer) pp 601–15

[40] Janson S, Łuczak T and Ruciński A 2000 *Random Graphs* (New York: Wiley)

[41] Mnëv P 2007 Discrete path integral approach to the Selberg trace formula for regular graphs *Commun. Math. Phys.* **274** 233–41

[42] Hoory S, Linial N and Wigderson A 2006 Expander graphs and their applications *Bull. Am. Math. Soc.* **43** 439–561

[43] Sodin S 2009 The Tracy–Widom law for some sparse random matrices arXiv:0903.4295v2 [math-ph]