The discrete Laplacian on d-regular graphs : Trace Formula, Random Waves and Spectral Statistics

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### Work done with Yehonatan Elon, Idan Oren, and Amit Godel

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

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- II Idan Oren and Uzy Smilansky J. Phys. A: Math. Theor. 43 (2010) 225205
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## The Discrete Schroedinger Operator on d-Regular Graphs

# PLAN

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   The G(n,d) ensemble combinatorial and spectral properties.
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# **1. Introduction**

A graph  $\mathcal{G}$  is a set  $\mathcal{V}$  of vertices connected by a set  $\mathcal{E}$  of edges. The number of vertices :  $V = |\mathcal{V}|$ The number of edges :  $E = |\mathcal{E}|$ . 2E directed edges: from o(e) to  $\tau(e)$ .  $\hat{e}$  the reverse of e :  $o(\hat{e}) = \tau(e), \tau(\hat{e}) = o(e)$ . Simple graphs: at most 1 edge connects any 2 vertices.



A walk:  $\{i_0, i_1, \dots, i_n\}, i_k \in \mathcal{V}$  with  $i_k$  connected to  $i_{k+1}$ . Or:  $\{e_1, e_2, \dots, e_n\}, e_k \in \mathcal{E}$  with  $o(e_1) = i_0, \tau(e_n) = i_n$  and  $o(e_{k+1}) = \tau(e_k)$ Non back tracking walk:  $e_{k+1} \neq \hat{e}_k$ .



t-cycle: A non back tracking walk which starts and ends at the The same vertex (edge).

The  $V \times V$  adjacency (connectivity) matrix A:  $A_{i,j} = 1$  if the vertices i, j are connected and 0 otherwise,  $A_{i,i} = 0$ .

**degree**  $d_i$  (valency):  $\sharp$  { edges emanating from the vertex},  $d_i = \sum_{j=1}^{V} A_{i,j}$ 

### Examples:







Tree graph

Complete graph

d=4 regular graph

The first Betti number:  $\beta = \mathcal{E} - \mathcal{V} + \mathcal{C}$ 

- $\beta$  = number of independent cycles on the graph
  - = number of edges that should be deleted to get a tree.
- $\mathcal{C}$  = number of connected components (For a connected graphs  $\mathcal{C} = 1$ ).



# The Laplacian and its spectrum

Definition:

$$(L\mathbf{f})_i = -\sum_{j\sim i} (f_j - f_i) = -\sum_{j\sim i} f_j + d_i f_i$$
  
Where  $D = \text{diag}\{d_1, \cdots, d_V\}$  so,  $L = -A + D$ .

For the discrete Laplacian on d-regular graphs:

$$(L\mathbf{f})_i = -\sum_{j\sim i} (f_j - f_i) = -\sum_{j\sim i} f_j + df_i$$

In other words, for a *d* regular graph:  $L = -A + d I^{(V)}$ .

This is the generalization of the discretized Laplacian. In 2-d e.g., :

$$-\Delta f(x,y) = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) f(x,y)$$

$$\approx -\frac{(f(x+\delta,y) + f(x,y+\delta) + f(x-\delta,y) + f(x,y-\delta) - 4f(x,y))}{\delta^2}$$

## basic properties of the Laplacian

1. The Laplacian is a positive operator:

$$\sum_{i} f_i(Lf)_i = \sum_{i} d_i f_i^2 - \sum_{i,j} f_i A_{i,j} f_j \ge \sum_{i} d_i f_i^2 - \sum_{i,j} |f_i| A_{i,j} |f_j| \ge \sum_{i} (d_i - 1) f_i^2 \ge 0$$

- 2. The lowest eigenvalue is 0 corresponding to the eigenvector  $(1, \dots, 1)$ .
- 3. Let  $\mathcal{G}$  and  $\mathcal{G}'$  be two graphs whose Laplacians have the same spectrum. Then:  $V_{\mathcal{G}} = V_{\mathcal{G}'}$ ,  $E_{\mathcal{G}} = E_{\mathcal{G}'}$

#### Exercise

(a) Prove statement 3. above.

Does 3. imply that graphs which have the same spectrum are isomorphic?

#### **Isospectral (co-spectral) graphs**

Non isomorphic graphs whose Laplace (or Adjacency) spectra are the same



G and G' are isospectral

#### **Denote**:

Center vertex "0", the vertices on the ring i=1,..,N; N=2m (even) The number of radial edges in G and in G' is m and they do not overlap.

 $|1\rangle=(1,1,\cdots,1)^T$  (vector of length N)<br/> $|c\rangle=(c_1,\cdots,c_N)^T, c_i=1$   $\;$  if vertex i is connected to 0 in G, otherwise<br/>  $c_i=0$ 

$$\begin{split} |c'\rangle &= (c'_1, \cdots, c'_N)^T, c'_i = 1 \quad \text{if vertex i is connected to } 0 \text{ in G', otherwise} c'_i = 0 \\ |c'\rangle &= |1\rangle - |c\rangle \end{split}$$

#### **Proof:**

Denote  $|f\rangle = (f_1, \dots, f_N)^T$  the eigenvector entries on the N ring vertices,  $f_0$  the entry on the center vertex.

The Adjacency eigenvalue problem for the graph G reads:

$$\langle c|f\rangle = \lambda f_0$$
 and  $(f_{i+1} + f_{i-1}) + c_i f_0 = \lambda f_i$   $\forall i \in [1, N]$ 

Denote by  $A_R$  the Adjacecy matrix for the ring graph without the center vertex. The above can be written as:

$$(A_R - \lambda I)|f\rangle = -f_0|c\rangle \rightarrow |f\rangle = -f_0(A_R - \lambda I)^{-1}|c\rangle$$
  
$$\langle c|f\rangle = -f_0\langle c|(A_R - \lambda I)^{-1}|c\rangle = \lambda f_0$$

The secular equation reads:  $\lambda + \langle c | (A_R - \lambda I)^{-1} | c \rangle = 0$ , if  $f_0 \neq 0$ .

Denote:  $|k\rangle$  and  $\alpha_k$  the eigenvectors and corresponding eigenvalues of  $A_R$ .

In particular  $|1\rangle = (1, \dots, 1)^T$  is the (not normalized) eigenvector with  $\alpha_1 = 2$ 

$$\lambda + \left(\frac{\langle c|1\rangle^2}{N(\lambda - 2)} + \sum_{k=2}^N \frac{\langle c|k\rangle^2}{(\lambda - \alpha_k)}\right) = 0 \; .$$

The secular equation is invariant under  $|c\rangle \rightarrow |c'\rangle$  Since:

$$|c'\rangle = |1\rangle - |c\rangle, \langle 1|c'\rangle = \langle 1|c\rangle = m, \ \langle k|c'\rangle = -\langle k|c\rangle, k \ge 2, \ \text{Hence } \sigma(G) = \sigma(G') \ .$$

#### In general:

# Switching theorem Seidel (1974), Godsil-McKay (1982), Dam-Haemers, (2003).

Let B and C be symmetric matrices of dimensions  $b \times b$  and  $c \times c$ , such that B has constant row (and hence column) sums. Then the matrices

$$M = \begin{pmatrix} B & N \\ N^T & C \end{pmatrix} \text{ and } M' = \begin{pmatrix} B & N' \\ N'^T & C \end{pmatrix}$$

are cospectral if N is a (0, 1)-matrix where each column sum is either  $0, \frac{b}{2}$ , or b, and N' is the matrix obtained from N by replacing each column  $\langle v |$  with column sum  $\frac{b}{2}$  by  $\langle 1 | - \langle v |$ .

Comment: We can define graph Laplacians L = -M, L' = -M' (with the off-diagonal entries of M, M' from (0, 1)). These graphs are isospectral.

**Proof:** Define  $Q = (\frac{2}{b}E_b - I_b) \oplus I_c$  where  $I_b$  and  $I_c$  are the unit matrices of

dimensions resp. b, c and  $E_b$  is the all 1 matrix in dimension b.

Direct computation shows:  $M' = QMQ^{-1}$ .

Exercise: Construct a non-trivial pair of graphs with isospectral Laplacians.

## d-regular graphs :

Graphs where all the vertices have the same degree. Examples:

- 1. Complete graphs
- 2. Lattices
- 3. d-regular infinite trees.

d-regular graphs are an expanding family.

$$E = \frac{Vd}{2} \rightarrow V$$
 or  $d$  must be even  
 $\beta = V(\frac{d}{2} - 1)$ 

 $\mathcal{G}_{V,d}$ . The ensemble of all the *d* regular graphs with *V* vertices .

For fixed d and 
$$V \to \infty$$
 :  $|\mathcal{G}_{V,d}| \approx \sqrt{2} e^{\frac{1-d^2}{4}} \left(\frac{d^d V^d}{e^d (d!)^2}\right)^{\frac{V}{2}}$ 

 $\langle \cdots \rangle_{\mathcal{G}}$  : Ensemble average taken with uniform probability distribution.

$$C_t$$
: Number of  $t$  - periodic cycles with no back tracking  
 $\langle C_t \rangle_{\mathcal{G}} = \frac{V \cdot d \cdot (d-1)^{t-1} \cdot \frac{d-1}{dV}}{2t} = \frac{(d-1)^t}{2t}$ 

Hence, short t - perioic cycles with  $t < \log_{d-1} V$  are  $\mathbf{rare}$  .

The *R*-neighbourhood of every vertex for  $R \leq \log_{d-1} \frac{V}{2}$  is almost surely a d-regular tree.

The diameter of a G(V, d) graph, i.e. the maximal distance between vertices in G, is given by

$$diam(G) = \log_{d-1}(V \log_{d-1} V) + O(1)$$

Therefore, the typical distance between vertices along the boundary of the 'local tree' is of the same magnitude as the distance between two arbitrary vertices in G.

Denote by  $C_t$  the number of t- cycles (prinitive, non backscatter, non self intersecting t-periodic orbits).

For  $t < \log_{d-1} \frac{V}{2}$ , the  $C_t$  distribute as independent Poisson variables with a mean:  $\langle C_t \rangle_{\mathcal{G}} = \frac{(d-1)^t}{2t}$ 

Reminder : For d-regular graphs the spectra of A and L are the same but for a shift by d and sign change.

#### Spectral properties of d-regular graphs

The spectral density 
$$\rho(\lambda) = \frac{1}{V-1} \sum_{k=1}^{V-1} \delta(\lambda - \lambda_k)$$

The mean spectral density for d regular graphs,  $(V \to \infty, d = const)$ Kesten MacKay limit distribution: (Supported in  $|\lambda| < 2\sqrt{d-1}$ ):



(a) Cubic graph on 2000 vertices. (b) 5-valent graph on 500 vertices.
Figure 1. Eigenvalue distributions of random graphs vs McKay's law

#### EIGENVALUE SPACINGS FOR REGULAR GRAPHS

DMITRY JAKOBSON, STEPHEN D. MILLER, IGOR RIVIN AND ZEÉV RUDNICK

Unfolding the spectrum with the Kesten-McKay density using  $\mathcal{N}_{KM}$ : The mean spectral counting function.

$$s_j = \mathcal{N}_{KM}(\lambda_j) \quad ; \quad \frac{\mathrm{d}\mathcal{N}_{KM}}{\mathrm{d}\lambda} = \rho_{KM}(\lambda) \quad ; \ \mathrm{d}s = \rho_{KM}(\lambda)\mathrm{d}\lambda = \frac{\mathrm{d}\lambda}{\langle \mathrm{d}\lambda \rangle}$$



Figure 2. Level spacing distribution of a cubic graph on 2000 vertices vs GOE

# Spectral properties and mixing

The mattix  $M = \frac{1}{d}A$  is a bi-stocastic matrix.

M is the evolution operator for a random walk on the graph:

Denote by  $\mathbf{p}(t)$  the vector of vertex probabilities after t steps.

 $\mathbf{p}(t) = M^t \mathbf{p}(0).$ 

The largest eigenvector of M is 1 with eigenvector corresponding to uniform distribution.

The spectral gap s(G) gives an estimate for the speed at which any initial distribution reaches equidistribution.

$$s(G) = \frac{1}{\lambda_{max}} \left( \lambda_{max} - \max\{|\lambda_1|, \lambda_{n-1}\} \right)$$

Alon Boppana: 
$$s(G) < 1 - \frac{2\sqrt{d-1}}{d} + \frac{2}{d \log n}$$

Cheeger inequalities  $\frac{s(G)}{2} \le h(G) \le \sqrt{2s(G)}$ 

h(G) is the expansion factor explained in the next page

## Expanding family of graphs

Intuition: expanding graphs are extremely well connected graphs.

Definition: For a graph  $G = (\mathcal{V}, \mathcal{E})$  and a subset of vertices  $\mathcal{S} \subset \mathcal{V}$ , the boundary  $\partial \mathcal{S}$  is defined as the set of edges which connects  $\mathcal{S}$  to  $G \setminus \mathcal{S}$ . The expansion parameter of a graph is defined as

$$h(G) = \min_{\mathcal{S} \subset \mathcal{V}} \frac{|\partial \mathcal{S}|}{\min\{\sum_{v_i \in \mathcal{S}} d_i, \sum_{v_j \in \mathcal{V} \setminus \mathcal{S}} d_j\}}$$

Thus, in order to disassemble a set S out of the graph which contains E edges, one has to remove at least  $E \cdot h(G)$  edges. In particular, for a regular graph, one has to disconnect at least  $d|S| \cdot h(G)$  edges.

A family of graphs  $\{G_k\}_{k=1}^{\infty}$  with increasing  $V(G_k)$  is defined as a (geometrical) expanding family of graphs, if there exists a positive constant c > 0, so that  $\liminf_{k\to\infty} h(G_k) = c$ .

Note that in an expanding graph, the volume of any ball is proportional to that of its boundary, which implies that the growth rate of the graph is exponential, hence the name 'expander'.

### **Exercise:**

Compute the expansion parameter for a finite tree which is d-regular but for its canopy.

## Ramanujan graphs

A *d*-regular graph is Ramanujan if  $\forall 1 \le j \le V - 1 : |\lambda_j| \le 2\sqrt{d-1}$ .

Number Theory: Ramanujan graphs exist for d = p - 1. (A. Lubotsky, R. Philips and P. Sarnak)

# Numerical experiments: (Hoory)

A finite fraction of the graphs in  $\mathcal{G}(V, d)$  are Ramanujan.

The fraction is  $\approx 2/3$  independent of V or d.

$$\langle \lambda_1 - 2\sqrt{d-1} \rangle_{\mathcal{G}} \approx V^{-\alpha} \\ \alpha \approx 0.6$$

Conjecture:

The distribution near the spectrum edge follows Tracy - Widom.



FIGURE 9. (a) Distribution of  $\lambda(G)$  for 1000 random 4-regular graphs in the permutation model. Four 40 bin histograms of  $\lambda(G)$ for graph sizes 10000, 400000, 1000000, 4000000. (b) Median, mean and standard deviation of  $2\sqrt{d-1} - \lambda(G)$  as a function of the graph size *n*. A log-log graph, along with the best linear interpolations.