

Interactions Between Quantum Graphs and Harmonic Analysis

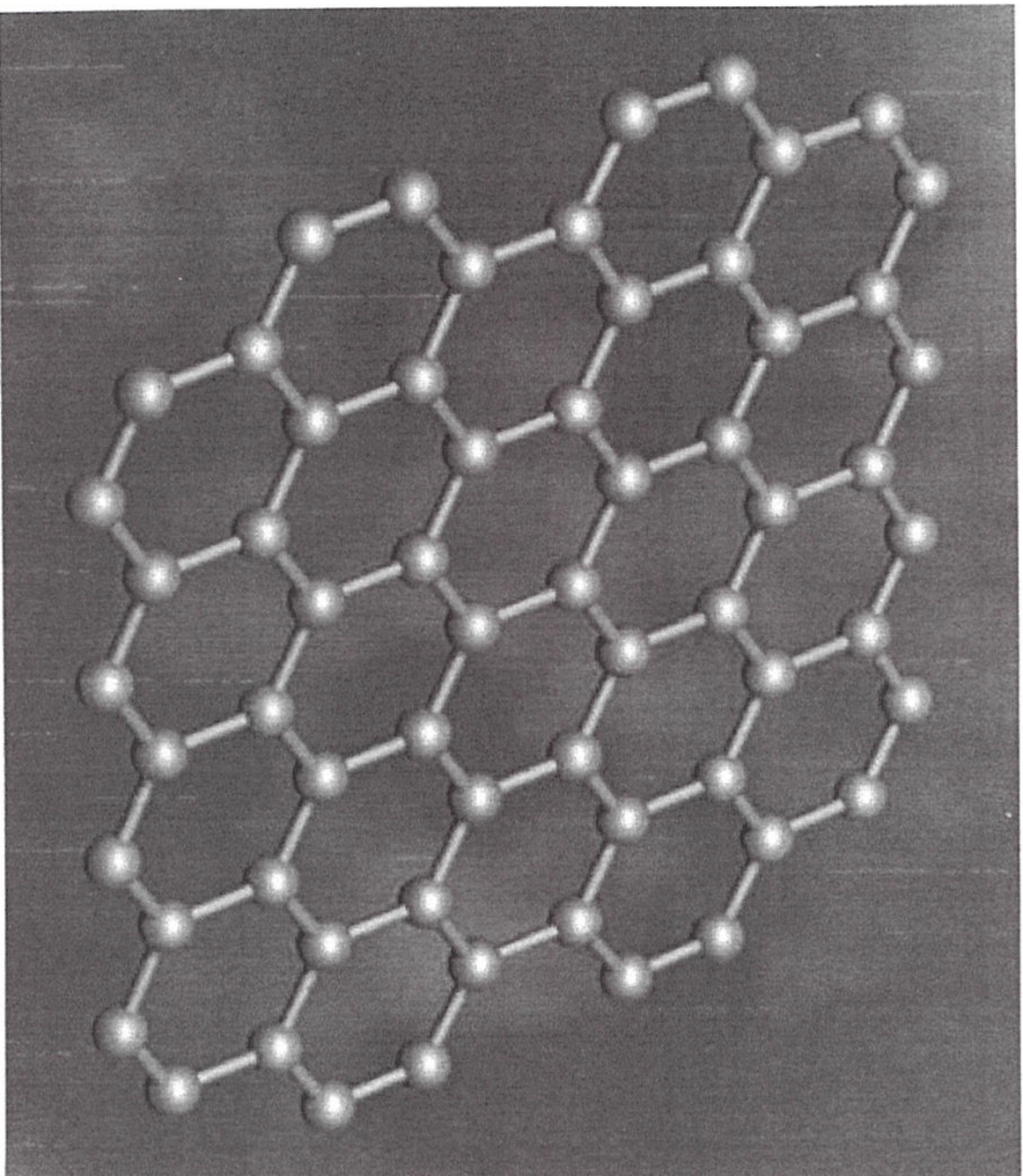
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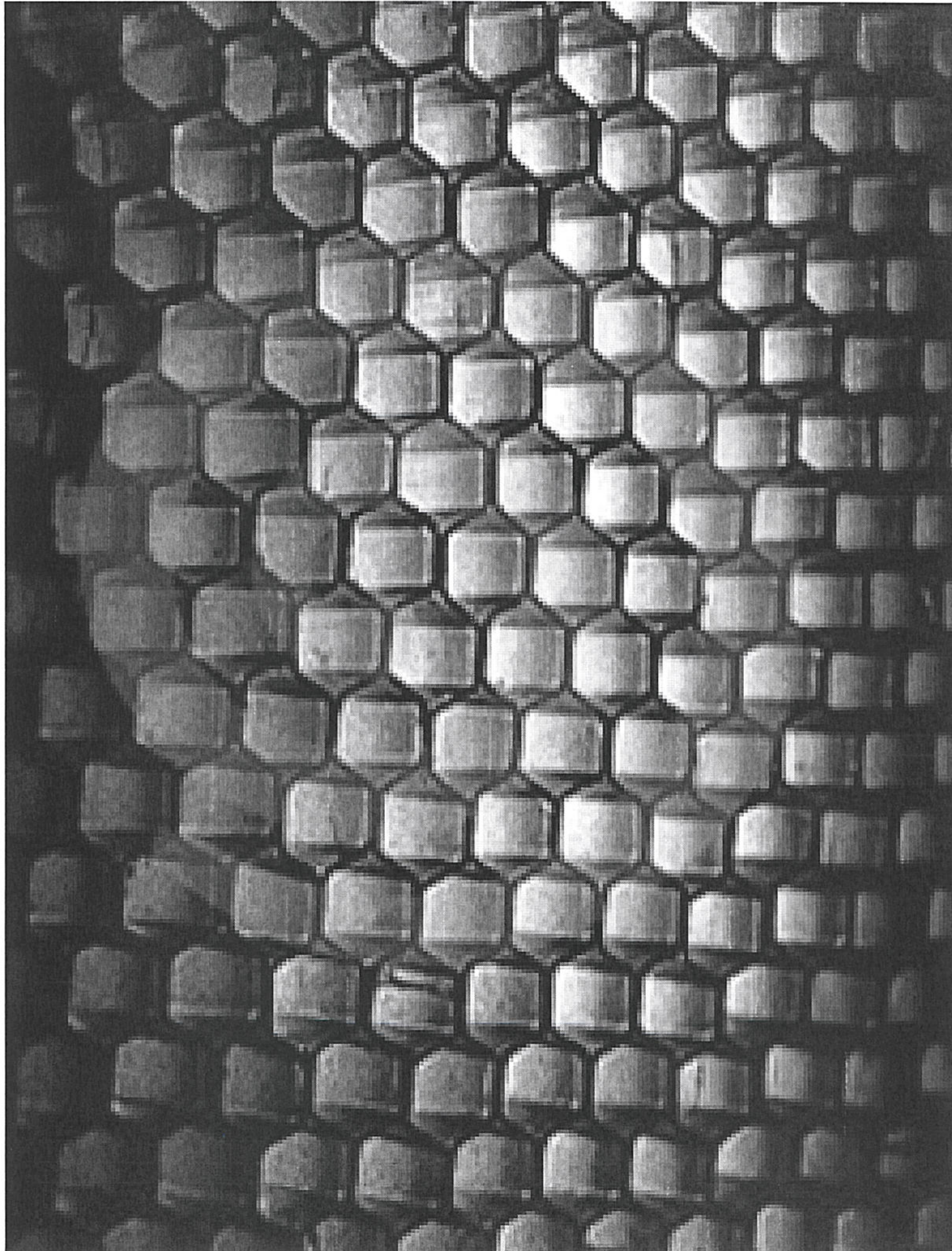
Abstract

Quantum graphs arise as models for thin physical networks. Their Laplace operators blend a one dimensional local structure with a graphical global structure through junction coupling conditions. When edge lengths are equal, or rationally related, the eigenvalues and trigonometric eigenfunctions have a surprisingly simple structure. As a consequence, they exhibit aspects of function theory usually associated with the circle, including a continuous graph Fast Fourier Transform.

molecule-graphene.jpg (JPEG Image, 450x385 pixels)



<http://www.theglitteringeye.com/images/>



Two pictures
Mention less regular networks -
road networks
river systems
human arterial tree

1 Differential equations on graphs

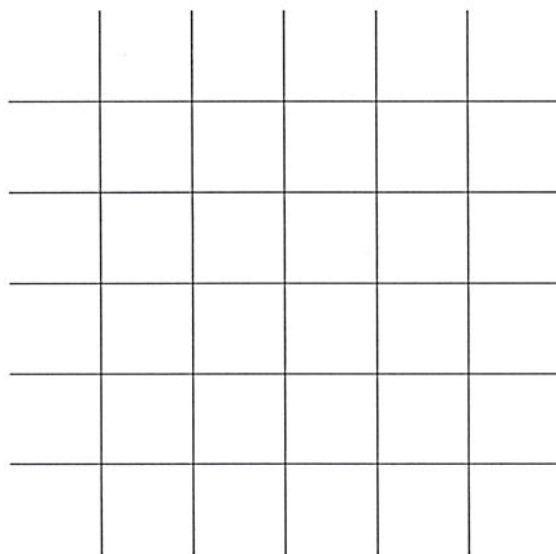


Figure 1. Wire screen

Use the 1-d heat equation for each wire,

$$\frac{\partial u}{\partial t}(t, x) = \frac{\partial^2 u}{\partial x^2}(t, x), \quad u(0, x) = f(x).$$

Couple edges e_j and e_k meeting at v ,

$$f_j(v) = f_k(v), \quad \sum f'_j(v) = 0,$$

the sum over all edges meeting at v , and derivatives computed with outward pointing local coordinates.

2 Quantum graph framework

Finite graph, finite length edges.

Edges are identified with intervals $e = [a_e, b_e]$.

Hilbert space $\oplus_j L^2(e_j)$ with inner product

$$\langle f(x), g(x) \rangle = \frac{1}{\sum_e (b_e - a_e)} \sum_e \int_{a_e}^{b_e} f_e(x) \overline{g_e(x)} dx.$$

Laplace operator $-\partial^2/\partial x^2$ with above domain is a nonnegative self adjoint operator with compact resolvent.

Eigenfunctions are trigonometric on each edge.

The 'Sturm-Liouville' or 'Fourier series' theory extends (beyond L^2) (M. Baker and R. Rumely)

Literature disclaimer

By inserting 'invisible' vertices and rescaling, make rational edge length graphs have edge lengths 1.

3 Discrete Graph Operators

With vertices v_1, \dots, v_N the adjacency matrix A is

$$A_{jk} = \begin{cases} 1, & \{v_j, v_k\} \in \mathcal{E}, \\ 0, & \{v_j, v_k\} \notin \mathcal{E} \end{cases}.$$

There is also an inner product

$$\langle f, g \rangle = \sum_{v \in \mathcal{V}} \text{deg}(v) f(v) \overline{g(v)},$$

$\text{deg}(v)$ = number of incident edges.

A self adjoint discrete Laplacian with this inner product is

$$\Delta_1 = I - D^{-1}A, \quad Df(v) = \text{deg}(v)f(v).$$

4 Edge lengths 1 - Remarkable facts

(von Below, Cattaneo, Friedman-Tillich)

The eigenspace $E(\lambda)$ for $-\partial^2/\partial x^2$ has 'periodicity':

Proposition 4.1. *If $\omega = \sqrt{\lambda} > 0$,*

$$\dim E(\omega^2) = \dim E([\omega + 2m\pi]^2), \quad m = 1, 2, 3, \dots$$

Using 'vertex evaluation map' we find

Theorem 4.2. *If $\lambda \notin \{n^2\pi^2 \mid n = 0, 1, 2, \dots\}$, then λ is an eigenvalue of $-\partial^2/\partial x^2$ if and only if $\mu = 1 - \cos(\sqrt{\lambda})$ is an eigenvalue of Δ_1 , with the same multiplicity.*

The cases $\lambda \in \{n^2\pi^2 \mid n = 1, 2, \dots\}$ are also 'combinatorial'. The edge space has the cycle subspace $Z_0(\mathcal{G})$. Let Z_1 be the set of functions $f : \mathcal{E} \rightarrow \mathbb{C}$ with

$$\sum_{e \simeq v} f(e) = 0, \quad v \in \mathcal{V}.$$

Let $E_0(n^2\pi^2) \subset E(n^2\pi^2)$ be the eigenfunctions of $\partial^2/\partial x^2$ vanishing at the vertices.

Theorem 4.3.

$$\dim(Z_0(\mathcal{G})) = \dim E_0((2n\pi)^2).$$

$$\dim(Z_1) = \dim E_0((2n-1)\pi)^2).$$

5 Graph refinements

Thinking like a numerical analyst, let's sample the length 1 graph edges uniformly.

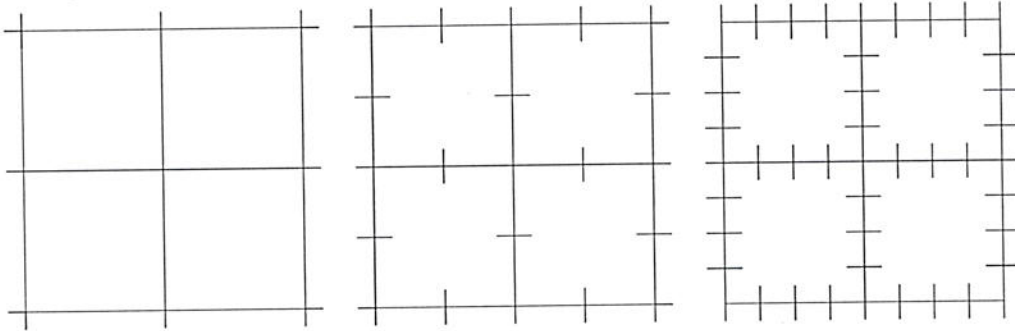


Figure 3.1: Refinement of a graph

The operator $\Delta_\infty = -\partial^2/\partial x^2$ stays fixed since the new vertex conditions do not change the domain.

The graphs have changed, giving new adjacency matrices and degree operators.

By the v.B,C.,F.-T. theorem orthogonal eigenspaces of $-\partial^2/\partial x^2$ descend by sampling to orthogonal eigenspaces of the 'new Δ_1 ' if the corresponding eigenvalues are distinct.

This generalizes the Fourier series - DFT coupling of S^1 .

6 Discrete Graph Fourier analysis

After sampling edge $e \in \mathcal{G}_1$ becomes N edges in \mathcal{G}_N with vertex space \mathbb{H}_N , discrete Laplacian

$$\Delta_N = N^2(I - D^{-1}A), \quad \Delta_N : \mathbb{H}_N \rightarrow \mathbb{H}_N,$$

and inner product

$$\langle f, g \rangle_N = \frac{1}{2NN_{\mathcal{E}}} \sum_v \deg(v) f(v) \overline{g(v)}.$$

Eigenspaces are $E_N(\lambda)$, resp. $E_{\infty}(\lambda)$. Let $E_p(n^2\pi^2)$ be the subspace having the form $C \cos(n\pi x)$ on each edge. Let $\mathbb{S}_N \subset L^2(\mathcal{G}_{\infty})$ denote the subspace

$$\mathbb{S}_N = \text{span}\{E_p(N^2\pi^2), E_{\infty}(\lambda), 0 \leq \lambda < N^2\pi^2\}.$$

Proposition 6.1. *The restriction $R_N : \mathbb{S}_N \rightarrow \mathbb{H}_N$ is a bijection. For $0 \leq \lambda < N^2\pi^2$ this map takes distinct orthogonal eigenspaces $E_{\infty}(\lambda)$ of Δ_{∞} onto distinct orthogonal eigenspaces $E_N(N^2(1 - \cos(\sqrt{\lambda}/N)))$ of Δ_N , and R_N takes $E_p(N^2\pi^2)$ onto $E_N(2N^2)$.*

We'd like an FFT using sampled Δ_∞ eigenfunctions.
 Good bases generated by 'frequency increase'.
 Multiplicity of eigenvalues complicates image orthogonality within eigenspaces.

Theorem 6.2. *There is a Fourier transform*

$$\mathcal{F}_N : \mathbb{H}_N \rightarrow \mathbb{C}^M, \quad M = \dim(\mathbb{H}_N)$$

satisfying

$$\mathcal{F}_N(\Delta_N f) = \{\mu_{m,k} \mathcal{F}(f)_{m,k}\},$$

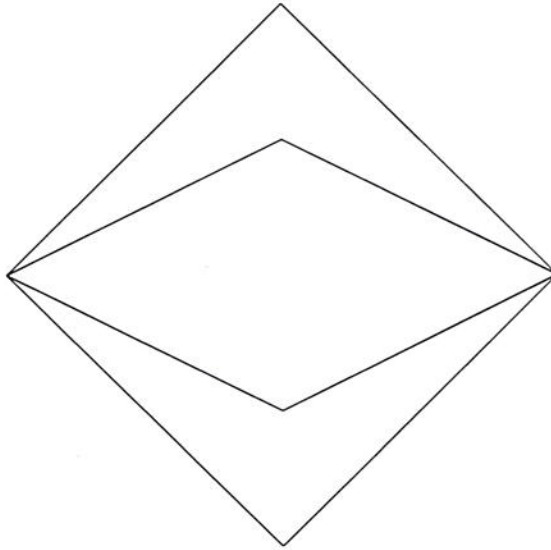
isometric on \mathbb{C}^M with a modified inner product.

If N is a power of 2, then $\mathcal{F}_N(f)$ and its inverse can be computed in time $O(N \log_2(N))$.

Question: Are leafless equilateral graph eigenspaces $E(\lambda)$ for $\lambda \neq n^2\pi^2$ 'generically' simple? Friedlander: arbitrary positive real lengths.

7 A family of examples

Basic examples - complete bipartite graphs $K(m, 2)$ on $m, 2$ vertices.



The graph $K_{4,2}$

Local model for any graph.

Obtain from the polar coordinate 2-sphere by uniform angular sampling.

Rotationally symmetric eigenfunctions $\cos(k\pi x)$.

Rest $\sin(k\pi x) \exp(2\pi i \frac{jm}{M})$.

8 Rework S^2 trapezoidal rule analysis

'Continuum limit' of $K(m, 2)$ Laplacians leads to polar S^2 Laplacian $\Delta_p = \partial^2/\partial x^2 + \partial^2/\partial y^2$ with nonlocal polar condition

$$\int_0^1 \partial_x f(0, y) dy = 0 = \int_0^1 \partial_x f(1, y) dy.$$

Trapezoidal rule

$$T(M, N, f) = \frac{1}{MN} \sum_{m=0}^{M-1} \sum_n'' f(x_n, y_m) \simeq \int_{I^2} f(x, y)$$

exact on eigenfunctions with corresponding index range.

Sobolev spaces H^s from domain of $\Delta_p^{s/2}$ provide rates,

Theorem 8.1. *If $f(x, y) \in H^s$ and $L = \min(M, N)$, then*

$$\int_{I^2} f(x, y) - T(M, N, f) = O(L^{2-s}).$$

Novelty for singular function estimates. The singular function $\cos(2\pi y)$ on S^2 , which is not continuous at the poles, converts to the polar integrand $f(x, y) = 2\pi^2 \sin(\pi x) \cos(2\pi y)$, which is in all H^s .

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