# A Brief Introduction to Quantum Graphs

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# Quantum Graph

## Definition

A *quantum graph* is a triple $(\Gamma, L, \mathrm{MC})$, where

- $\Gamma$ is a *metric graph*,
- $L$ is a *differential expression* defined on functions on $\Gamma$, and
- MC (*matching conditions*) is a set of conditions relating the limit values of the functions defined on the edges of $\Gamma$.

# Metric Graph

## Definition

A *metric graph* is a tuple $(E, V)$ where:

- $E = \{e_n\}_{n=1}^{N}$ is a set of intervals (*edges*) $[x_{2n-1}, x_{2n}] \subset \mathbb{R}$.
- $V = \{v_m\}_{m=1}^{M}$ is a partition of the set $\{x_j\}_{j=1}^{2N}$.
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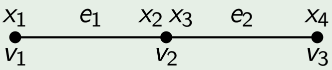
## Example




$$E = \{e_1, e_2\} = \{[x_1, x_2], [x_3, x_4]\}$$
$$V = \{v_1, v_2, v_3\} = \big\{\{x_1\}, \{x_2, x_3\}, \{x_4\}\big\}$$

# Functions on Metric Graphs

## Definition

Metric graph $\Gamma$, define the Hilbert space $L_2(\Gamma)$ by

$$L_2(\Gamma) = \bigoplus_{e \in E} L_2(e), \qquad \langle f, g \rangle^2_{L_2(\Gamma)} = \int_\Gamma f(x)\overline{g}(x)\, dx.$$

# Differential Expressions

Electric potential $q(x)$ and magnetic potential $a(x)$.
Magnetic Schrödinger Operator

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The equation

$$Lu = \lambda u.$$

# Differential Operators

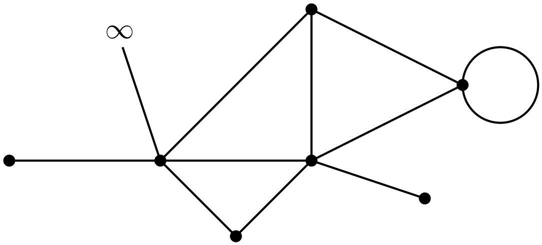
We are insterested in studying self-adjoint differential operators.
This is a rather technical discussion, essentially one requires symmetry,

$$\langle Lu, v \rangle = \langle u, Lv \rangle.$$

This implies that the energy of the system is preserved, since a symmetric operator has real eigenvalues. Furthermore the corresponding eigenfunctions form an orthonormal basis.

# Questions Arise

So far everything makes sense for single-line graphs.
What about general graphs?




How to "connect" the equations at the vertices? *Matching conditions.*

# Matching Conditions

Let us consider under which conditions a differential operator associated with the differential expression $L = -\frac{d^2}{dx^2}$ is symmetric.

$$
\begin{aligned}
\langle Lu, v\rangle_{L_2(\Gamma)} &= \sum_{e_n \in E} \int_{e_n} (-u'')\overline{v}\, dx \\
&= \sum_{e_n \in E} \left( \int_{e_n} u'\overline{v}'\, dx - \Big[ u'\overline{v} \Big]_{x_{2n-1}}^{x_{2n}} \right) \\
&= \sum_{e_n \in E} \left( \int_{e_n} u(-\overline{v}'')dx + \Big[ u\overline{v}' - u'\overline{v} \Big]_{x_{2n-1}}^{x_{2n}} \right) \\
&= \langle u, Lu\rangle_{L_2(\Gamma)} + \sum_{e_n \in E} \Big[ u\overline{v}' - u'\overline{v} \Big]_{x_{2n-1}}^{x_{2n}} \\
&= \langle u, Lu\rangle_{L_2(\Gamma)} + \sum_{m=1}^{M} \sum_{x \in v_m} \partial u(x)\overline{v}(x) - u(x)\partial \overline{v}(x)
\end{aligned}
$$

# Matching Conditions

That is, we require

$$0 = \langle Lu, v\rangle - \langle u, Lv\rangle = \sum_{m=1}^{M} \sum_{x_j \in v_m} \partial u(x_j)\overline{v}(x_j) - u(x_j)\partial\overline{v}(x_j).$$

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## Definition

The *standard matching conditions*, for a vertex $v$, are given by

$$\begin{cases} u(x_j) = u(x_i) \text{ for all } x_j, x_i \in v \\ \displaystyle\sum_{x_j \in v} \partial u(x_j) = 0. \end{cases}$$

1. Defining Quantum graphs
   - Metric graphs
   - Differential operators
   - Matching conditions

2. Properties of Quantum Graphs
   - First example
   - Scattering: Inverse problems
   - Star graph: Calculating the spectrum

# First Example

One-dimensional time-independent Schrödinger equation with no potential

$$-u''(x) = \lambda u(x) \iff u(x) = A\overrightarrow{e^{ikx}} + B\overleftarrow{e^{-ikx}}, \quad k^2 = \lambda.$$

$A$ and $B$ are determined by the boundary conditions.

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## Example (Particle in a Box)

Infinite potential in the region $x < 0, x > \ell$ is modeled by allowing the particle to exist only on the interval $[0, \ell]$.

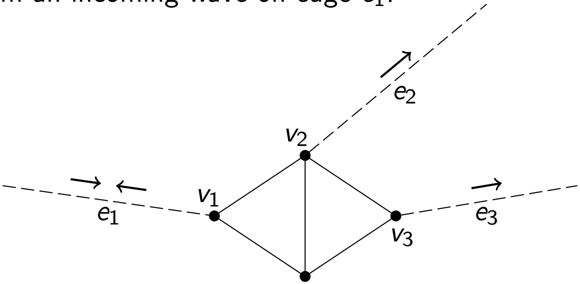

Figure : Finite line graph of length $\ell$, parametrized from 0 to $\ell$.

The boundary condition $u(0) = u(\ell) = 0$ (Dirichlet condition) gives

$$u(x) = A \sin kx, \quad \lambda = k^2 = \frac{\pi^2}{\ell^2} n^2, \quad n = 1, 2, \ldots.$$

# Scattering: Inverse problems

Scattering from an incoming wave on edge $e_1$.



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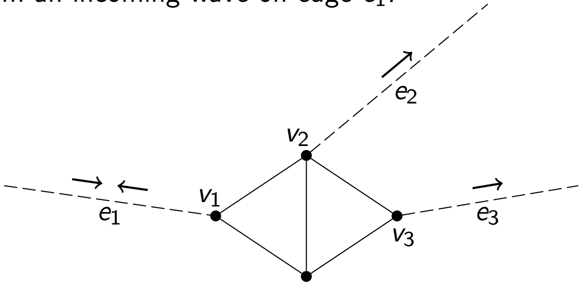
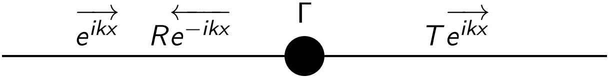


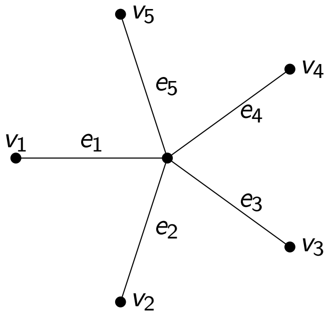

More generally,




$$|R|^2 + |T|^2 = 1$$

# Defining the star graph

Consider a star graph with $d$ edges, all having the same length $\ell$ and standard matching conditions at all vertices.



# Star graph: Calculating the spectrum

$$Lu_j = \lambda u_j \iff u_j(x) = A_j \cos kx + B_j \sin kx,\ j = 1, \ldots, d,\ \lambda = k^2 > 0$$

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Parametrize every edge so that $x = 0$ at the outer vertices and $x = \ell$ at the inner vertex. Matching conditions at the outer verices require the derivative to vanish,

$$u_j'(0) = kB_j \cos 0 = 0 \implies B_j = 0.$$

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At the inner vertex, $x = 0$, the continuity condition require

$$A_j \cos k\ell = A_{j'} \cos k\ell, \quad \text{for all } j \neq j'.$$

Assume first $\cos k\ell \neq 0$, then

$$A_j = A, \quad \text{for all } j,$$

for some constant $A$.

# Star graph: Calculating the spectrum

The derivative condition require

$$\sum_{j=1}^{d} \partial u_j(\ell) = -dkA\sin(k\ell) = 0 \implies \sin k\ell = 0,$$

since $k \neq 0$ and $A \neq 0$ to avoid the trivial solution. This gives the possible eigenvalues $\lambda_n$ with corresponding eigenfunctions $f_n$;

$$\lambda_n = k_n^2 = \left(\frac{n\pi}{\ell}\right)^2, \quad n = 1, 2, \ldots$$
$$f_n(x) = A\cos k_n x.$$

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Next, if $\cos k\ell = 0$, the continuity condition for the inner vertex,

$$A_j \cos k\ell = A_{j'} \cos k\ell, \quad \text{for all } j \neq j',$$

is trivially satisfied. Hence the constants $A_j$ on each vertex need not coincide.

# Star graph: Calculating the spectrum

The condition on the derivatives now reads

$$0 = \sum_{j=1}^{d} \partial u_j(\ell) = -k \sin(k\ell) \sum_{j=1}^{d} A_j \implies \sum_{j=1}^{d} A_j = 0,$$

since we are assuming $k \neq 0$ and $\cos k\ell = 0$. This equation has $d - 1$ linearly independent solutions. This is a degenerate energy level, there are $(d - 1)$ eigenstates with the same energy, given by $\cos k\ell = 0$, that is

$$\lambda_n = k_n^2 = \left(\frac{\pi}{2\ell} + \frac{n\pi}{\ell}\right)^2, \quad n = 1, 2, \ldots$$

Finally, one easily calculates the eigenfunction for $\lambda = 0$, the ground state at zero energy, to be a constant function on the entire graph.

# Star graph: Calculating the spectrum

To sum up, we can order all eigenvalues in an increasing sequence,

$$\lambda_0 = 0$$

$$\lambda_{dn} = \left(\frac{dn\pi}{\ell}\right)^2, \quad n = 1, 2, \ldots$$

$$\lambda_{dn+j} = \left(\frac{\pi}{2\ell} + \frac{dn\pi}{\ell}\right)^2, \quad j = 1, \ldots, (d-1), \quad n = 1, 2, \ldots$$

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\end{aligned}$$

Hence the $m$:th eigenvalue grows as

$$\lambda_m \sim \frac{\pi^2}{(d\ell)^2} m^2 \quad \text{as} \quad m \to \infty.$$

Note that $d\ell$ is the total length of the graph. The growth of the eigenvalues is an example of the the Weyl asymptotic law.