Quantizing graphs, one way or two?

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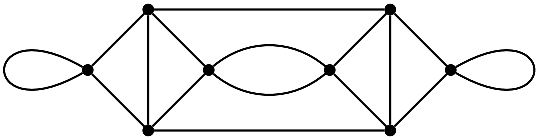
FernUniversität in Hagen 26/4/23

Outline

1. Quantum graph operators
2. Wave propagation
3. Comparison
4. Dirac operator model

Graphs



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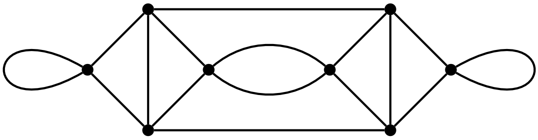

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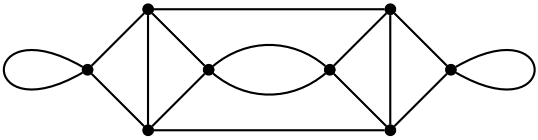

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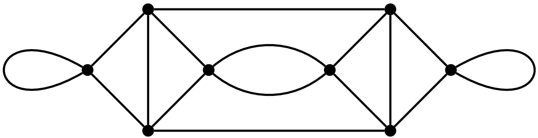

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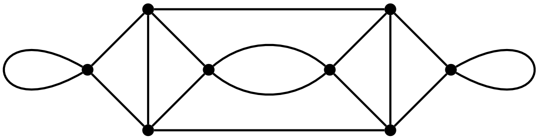

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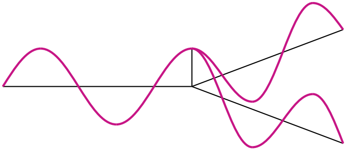
- $|\mathcal{E}| = E$
- *Degree* of v is no. of edges incident with v.
- G is *simple* if it has no loops or multiple edges.

Quantum graphs

Self-adjoint Hamiltonians acting on functions defined on a quasi-one-dimensional network of intervals.



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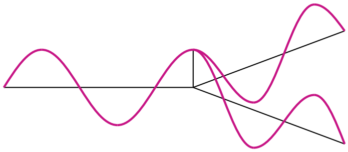
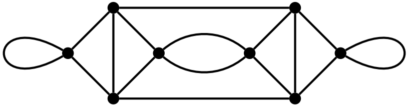


- Free electrons in organic molecules (Pauling '36)
- Superconducting networks
- Photonic crystals
- Nanotechnology
- Quantum chaos
- Anderson localization

Metric graphs



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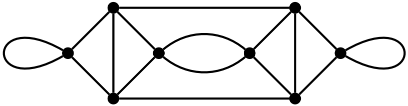
Metric graphs



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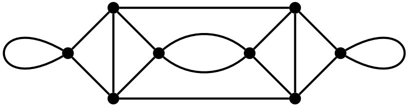
- *Laplace equation* on $[0, L_e]$,

$$-\frac{\mathrm{d}^2}{\mathrm{d}x_e^2} f_e(x_e) = k^2 f_e(x_e) \ . \tag{1}$$

Metric graphs



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- *Hilbert space* $\bigoplus_{e \in \mathcal{E}} L^2([0, L_e])$.

Domain of Laplace operator

Vertex conditions

$$\mathbb{A}_v \mathbf{F}(v) + \mathbb{B}_v \mathbf{F}'(v) = \mathbf{0}$$

$$\mathbf{F}(v) = (f_{e_1}(0), \ldots, f_{e_l}(0), f_{e_{l+1}}(L_{e_{l+1}}), \ldots, f_{e_d}(L_{e_d})))^T$$
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Domain: subspace of $\bigoplus_{e\in\mathcal{E}} W^{2,2}([0,L_e])$ satisfying vertex conditions.

Theorem 1 (Kostrykin-Schrader '99)

Laplacian self-adjoint iff $(\mathbb{A}_v, \mathbb{B}_v)$ *maximal rank and*

$$\mathbb{A}_v \mathbb{B}_v^\dagger = \mathbb{B}_v \mathbb{A}_v^\dagger \qquad \forall\, v \in \mathcal{V}.$$

Example

Standard (Neumann like) conditions

f continuous at v and $\sum_{e\sim v} f_e'(v) = 0$.

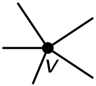
$$\mathbb{A}_v \mathbf{F}(v) + \mathbb{B}_v \mathbf{F}'(v) = \mathbf{0}$$

$$\mathbb{A}_v = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 \\ 0 & 1 & -1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & 1 & -1 \\ 0 & \dots & 0 & 0 & 0 \end{pmatrix} \qquad \mathbb{B}_v = \begin{pmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 0 \\ 1 & 1 & \dots & 1 \end{pmatrix}$$

Wave propagation

Solution of Laplace equation on $[0, L_e]$,

$$f_e(x_e) = a_e^{\mathrm{in}} \mathrm{e}^{-\mathrm{i}kx_e} + a_{\bar{e}}^{\mathrm{out}} \mathrm{e}^{\mathrm{i}kx_e} \ . \quad (2)$$



Substituting in vertex condition $\vec{a} = \sigma^{(v)}(k) \overleftarrow{a}$.

$$\sigma^{(v)}(k) = -\left(\mathbb{A}_v + \mathrm{i}k\mathbb{B}_v\right)^{-1}\left(\mathbb{A}_v - \mathrm{i}k\mathbb{B}_v\right) \quad (3)$$

$\sigma^{(v)}(k)$ unitary *vertex scattering matrix*.

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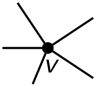

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Example: Standard conditions

$$[\sigma^{(v)}]_{ij} = \frac{2}{d_v} - \delta_{ij}$$

Secular equation

Use pairs of directed edges $e = (u, v)$, $\bar{e} = (v, u)$ to label plane-wave coefficients, $o(e) = u$ and $t(e) = v$.

Graph scattering matrix

$$\Sigma_{e\,e'}(k) = \delta_{t(e'),o(e)}\,\sigma^{(o(e))}_{e,e'}(k)$$

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$\mathbf{a} = (a_1, \dots a_E, a_{\bar{1}}, \dots, a_{\bar{E}})$ defines an eigenfunction if,

$$D(k)\Sigma(k)\mathbf{a} = \mathbf{a}\ , \tag{4}$$

where $D(k) = \mathrm{diag}\{\mathrm{e}^{\mathrm{i}kL_1}, \dots, \mathrm{e}^{\mathrm{i}kL_E}, \mathrm{e}^{\mathrm{i}kL_1}, \dots, \mathrm{e}^{\mathrm{i}kL_E}\}$.

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Secular equation (Kottos-Smilansky '97)

$$\det\left(\mathrm{I} - D(k)\Sigma(k)\right) = 0$$

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- Freedom to choose scattering matrices to simplify analysis.

Examples

- FFT scattering matrices with democratic transition probabilities $|\sigma_{ij}^{(v)}|^2 = 1/d$ where d degree of v and $w = \exp(2\pi\mathrm{i}/d)$.

$$\sigma^{(v)} = \frac{1}{\sqrt{d}} \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & w & w^2 & \dots & w^{d-1} \\ 1 & w^2 & w^4 & \dots & w^{2(d-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & w^{d-1} & w^{2(d-1)} & \dots & w^{(d-1)(d-1)} \end{pmatrix} \tag{5}$$

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- Equi-transmitting scattering matrices $|\sigma_{ii}^{(v)}|^2 = 0$ and $|\sigma_{ij}^{(v)}|^2 = 1/(d-1)$ for $i \neq j$.
(H-Smilansky-Winn '07, Kurasov-Ogik-Rauf '14)

Energy independence

Theorem 2 (Kostrykin-Potthoff-Schrader '07, Fulling-Kuchment-Wilson '07)

At a vertex v the following are equivalent.

1. *The scattering matrix* $\sigma^{(v)}(k)$ *is independent of* k .
2. $\mathbb{A}_v \mathbb{B}_v^\dagger = 0$.
3. *There exists* $k \neq 0$ *such that* $\left(\sigma^{(v)}(k)\right)^2 = \mathrm{I}$.
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Example: Standard conditions $\mathbb{A}_v \mathbb{B}_v^\dagger = 0$ and $[\sigma^{(v)}]_{ij} = \frac{2}{d_v} - \delta_{ij}$.

$$\mathbb{A}_v = \begin{pmatrix} 1 & -1 & 0 & 0 & \dots \\ 0 & 1 & -1 & 0 & \dots \\ & & \ddots & \ddots & \\ 0 & \dots & 0 & 1 & -1 \\ 0 & \dots & 0 & 0 & 0 \end{pmatrix} \qquad \mathbb{B}_v = \begin{pmatrix} 0 & \dots & 0 \\ \vdots & & \vdots \\ 0 & \dots & 0 \\ 1 & \dots & 1 \end{pmatrix}$$

Consequences for wave-propagation quantization

- Only vertex scattering matrices that square to the identity correspond to scattering matrices of the Laplace (or Schrödinger) operators.
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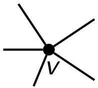
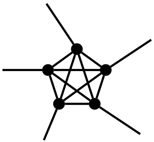
Approximating vertex scattering matrices

Theorem 3 (Cheon-Exner-Turek '10)

Self-adjoint vertex conditions parametrized by $\mathbb{A}_v, \mathbb{B}_v$ can be approximated by replacing v with K_{d_v}, with delta conditions at the vertices of K_{d_v} and delta potentials on the edges of K_{d_v}.





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Scattering matrix for delta conditions

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$$\sigma^{(v)}(k) = \frac{2}{d_v - \mathrm{i}\frac{\alpha_v}{k}}\mathrm{J} - \mathrm{I} \qquad (6)$$

where J is a matrix of 1's.
In high energy limit $\sigma^{(v)}(k)$ approaches k-independent scattering matrix of standard conditions $\sigma^{(v)} = \frac{2}{d_v}\mathrm{J} - \mathrm{I}$.

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In high energy limit the scattering matrix of general vertex scattering conditions can be approximated by a larger graph with k-independent scattering matrices.

Dirac equation in 1d

Time independent Dirac equation on $[0, L_e]$,

$$-\mathrm{i}\hbar c\alpha \frac{\mathrm{d}}{\mathrm{d}x_e}\mathbf{f}_e(x_e) + mc^2\beta\mathbf{f}_e(x_e) = k\mathbf{f}_e(x_e)\ . \qquad (7)$$

- Dirac algebra $\alpha^2 = \beta^2 = \mathrm{I}$ and $\alpha\beta + \beta\alpha = 0$.

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- Dirac algebra $\alpha^2 = \beta^2 = \mathrm{I}$ and $\alpha\beta + \beta\alpha = 0$.
- Faithful irreducible representation 2×2 matrices.
- Physical interpretation of spin: restrict Dirac equation in 3d.
- e.g.

$$\alpha = \begin{pmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & \mathrm{i} & 0 \\ 0 & -\mathrm{i} & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Domain of Dirac op.

Vertex conditions

$$\mathbb{A}_v \mathbf{F}^+(v) + \mathbb{B}_v \mathbf{F}^-(v) = \mathbf{0}$$

$$\mathbf{F}^+(v) = \Big(f_1^{e_1}(0), f_2^{e_1}(0), \ldots, f_1^{e_l}(0), f_2^{e_l}(0), f_1^{e_{l+1}}(L_{e_{l+1}}), f_2^{e_{l+1}}(L_{e_{l+1}}), \ldots, f_1^{e_d}(L_{e_d}), f_2^{e_d}(L_{e_d}) \Big)^T$$

$$\mathbf{F}^-(v) = \Big(-f_4^{e_1}(0), f_3^{e_1}(0), \ldots, -f_4^{e_l}(0), f_3^{e_l}(0), f_4^{e_{l+1}}(L_{e_{l+1}}), -f_3^{e_{l+1}}(L_{e_{l+1}}), \ldots, f_4^{e_d}(L_{e_d}), -f_3^{e,d}(L_{e_d}) \Big)^T$$

Domain: subspace of $\bigoplus_{e \in \mathcal{E}} W^{1,2}([0, L_e]) \otimes \mathbb{C}^4$.

Theorem 4 (Bolte-H. '03)

Dirac op. self-adjoint iff $rk(\mathbb{A}_v, \mathbb{B}_v)$ *maximal and* $\mathbb{A}_v \mathbb{B}_v^\dagger = \mathbb{B}_v \mathbb{A}_v^\dagger$.

Wave propagation of spinors

$$\mathbf{f}_e(x_e) = a^e_\alpha \begin{pmatrix} 1 \\ 0 \\ 0 \\ \mathrm{i}\gamma(k) \end{pmatrix} \mathrm{e}^{\mathrm{i}kx_e} + a^e_\beta \begin{pmatrix} 0 \\ 1 \\ -\mathrm{i}\gamma(k) \\ 0 \end{pmatrix} \mathrm{e}^{\mathrm{i}kx_e} + a^{\bar{e}}_\alpha \begin{pmatrix} 1 \\ 0 \\ 0 \\ -\mathrm{i}\gamma(k) \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx_e} + a^{\bar{e}}_\beta \begin{pmatrix} 0 \\ 1 \\ \mathrm{i}\gamma(k) \\ 0 \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx_e} \qquad (8)$$

$$\gamma(k) = \frac{E - mc^2}{\hbar ck} \qquad E = \sqrt{(\hbar ck)^2 + m^2c^4} \qquad (9)$$

Zero mass $\gamma(k) = 1$ and $\gamma(k) \to 1$ as $k \to \infty$.

Scattering matrices

$$\overrightarrow{a} = \big(a_\alpha^{e_1}, a_\beta^{e_1}, \dots, a_\alpha^{e_l}, a_\beta^{e_l}, \\ a_\alpha^{\bar{e}_{l+1}} \mathrm{e}^{-\mathrm{i}kL_{e_{l+1}}}, a_\beta^{\bar{e}_{l+1}} \mathrm{e}^{-\mathrm{i}kL_{e_{l+1}}}, \dots, a_\alpha^{\bar{e}_d} \mathrm{e}^{-\mathrm{i}kL_{e_d}}, a_\beta^{\bar{e}_d} \mathrm{e}^{-\mathrm{i}kL_{e_d}}\big)^T$$

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From vertex condition $\overrightarrow{a} = \sigma^{(v)} \overleftarrow{a}$.

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- Scattering at vertices rotates spin.

Scattering matrices

$$\overrightarrow{a} = \big(a_\alpha^{e_1}, a_\beta^{e_1}, \dots, a_\alpha^{e_l}, a_\beta^{e_l}, \\ a_\alpha^{\bar{e}_{l+1}} \mathrm{e}^{-\mathrm{i}kL_{e_{l+1}}}, a_\beta^{\bar{e}_{l+1}} \mathrm{e}^{-\mathrm{i}kL_{e_{l+1}}}, \dots, a_\alpha^{\bar{e}_d} \mathrm{e}^{-\mathrm{i}kL_{e_d}}, a_\beta^{\bar{e}_d} \mathrm{e}^{-\mathrm{i}kL_{e_d}} \big)^T$$

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From vertex condition $\overrightarrow{a} = \sigma^{(v)} \overleftarrow{a}$.

$$\sigma^{(v)}(k) = -\big(\mathbb{A}_v - \mathrm{i}\gamma(k)\mathbb{B}_v\big)^{-1}\big(\mathbb{A}_v + \mathrm{i}\gamma(k)\mathbb{B}_v\big) \qquad (10)$$

- Scattering at vertices rotates spin.
- For zero mass or in high energy limit $\sigma^{(v)}$ k-independent.

Dirac op. model

Let U_v be a $2d_v \times 2d_v$ unitary matrix. Consider the zero mass self-adjoint Dirac op. with vertex conditions defined by,

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- But 2 incoming and 2 outgoing plane waves on each edge.

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- This form prevents spin rotation during scattering.
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- Secular equation $\det \left(\mathrm{I} - (D(k)\widehat{\Sigma}) \otimes \mathrm{I}_2\right) = 0$.
- Reduces to $\det \left(\mathrm{I} - (D(k)\widehat{\Sigma})\right) = 0$.

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- For massive particles this agreement is obtained in the high energy limit.
- Wave-propagation quantization a subset of quantum graphs described by self-adjoint Hamiltonians.
- 2-component spinor construction - Berkolaiko '08.

Conclusions

- Spectra of graphs quantized by specifying vertex scattering matrices can be regarded as spectra of Hamiltonians on metric graphs.
- The correspondence is observed for Dirac operators with vertex conditions that do not rotate spin and zero mass or in the high energy limit.

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