# Index theorems and trace formulas for quantum graphs

ISem 26 - Project F

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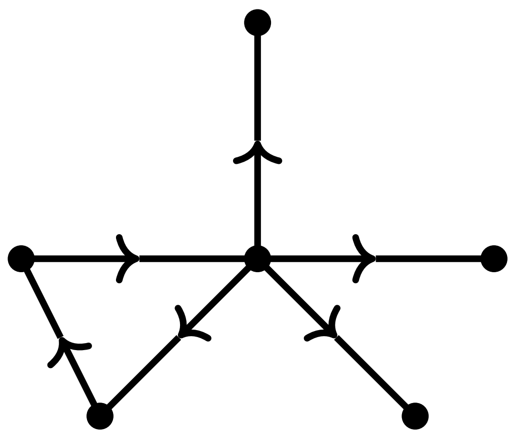
# Overview

Our presentation will focus on 4 main points which are:

1. Introduction to the setting
2. Heat Kernels
3. Trace Formula
4. Index theorem

# What is a metric graph or a network?



- set of vertices $V$
- set of edges $\mathcal{I}$
- boundary map $\partial$: edges $\mapsto$ initial and terminal vertex
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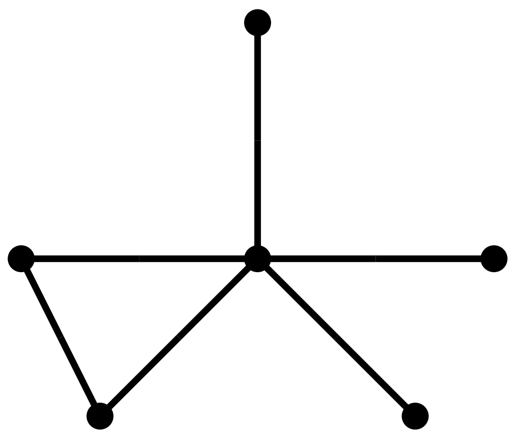

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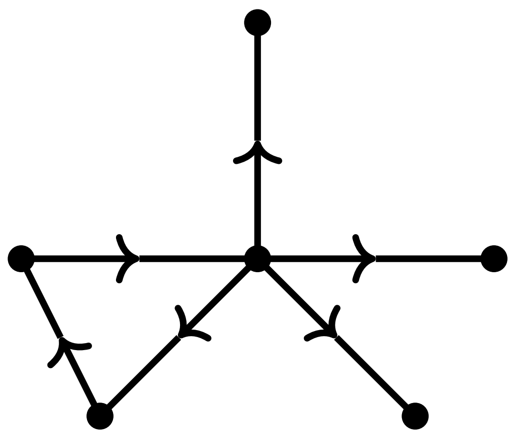

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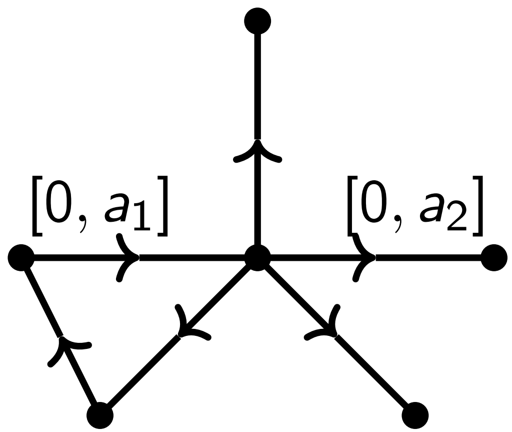


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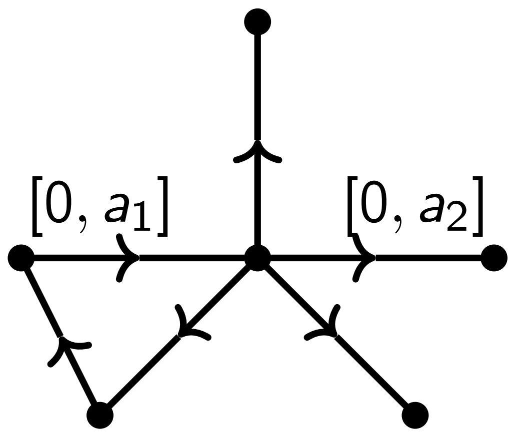
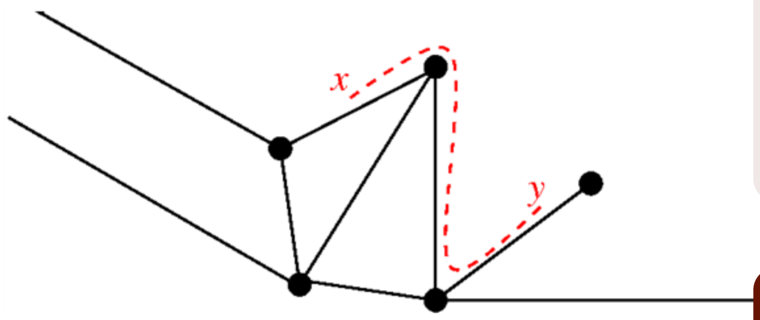



Metric via minimal path lengths

## Definition: Metric Graph $(\mathcal{G}, \underline{a})$

- set of vertices $V$
- set of edges $\mathcal{I}$
- boundary map $\partial$: edges $\mapsto$ initial vertex $\partial_-(j)$ and terminal vertex $\partial_+(j)$
- directed or not directed
- weights or lengths $a_j$ for $j \in \mathcal{I}$ and $\underline{a} = \{a_j\}_{j \in \mathcal{I}}$

## Remark:

Here, only compact graphs

# Prerequisites

- Let $\mathcal{H} = \bigoplus \mathcal{H}_j$ where $\mathcal{H}_j = L^2(I_j)$ on $I_j = [0, a_j]$. Analogously, define functions spaces "edgewise"
- $D = \{\psi \in \mathcal{H} | \psi, \psi' \text{absolutely continuous}, \psi'' \text{square integrable}\}$.
- A differential operator on the metric graph $(\mathcal{G}, \underline{a})$ is the differential operator that acts on a function $\psi$ in $D$.
- The Laplace operator denoted by $-\Delta$:

$$(-\Delta\psi)(x) = -\frac{\partial^2\psi}{\partial x^2}(x), \quad \psi \in D.$$

- Becomes self-adjoint with certain boundary conditions defined below.

# Maximal isotropic subspace

- A Hilbert space $\mathcal{K} \cong \mathbb{C}^{2|\mathcal{I}|}$, ${}^d\mathcal{K} = \mathcal{K} \times \mathcal{K}$.
- $\psi \in D$, $[\psi] = \underline{\psi} \bigoplus \underline{\psi}' \in \; {}^d\mathcal{K}$ with

$$[\psi] = \begin{pmatrix} \underline{\psi} \\ \underline{\psi}' \end{pmatrix}, \quad \underline{\psi} = \begin{pmatrix} \{\psi_i(0)\}_i \\ \{\psi_i(a_i)\}_i \end{pmatrix}, \quad \underline{\psi}' = \begin{pmatrix} \{\psi_i'(0)\}_i \\ \{-\psi_i'(a_i)\}_i \end{pmatrix}$$

$$\omega([\phi], [\psi]) = \langle -\Delta\phi, \psi \rangle_{{}^d\mathcal{K}} - \langle \phi, -\Delta\psi \rangle_{{}^d\mathcal{K}} \quad \phi, \psi \in D$$

## Definition

A linear subspace $\mathcal{M}$ of ${}^d\mathcal{K}$ is called isotropic if the form $\omega$ vanishes identically on $\mathcal{M}$, it is furthermore maximal if it is not a proper subspace of a larger isotropic subspace.

# Maximal Isotropic space

## Theorem

*$\mathcal{M} \subset {}^d\mathcal{K}$ is maximal isotropic if and only if there exist linear maps $A, B : \mathcal{K} \to \mathcal{K}$ such that:*

1. $\mathcal{M} = \mathcal{M}(A, B) := Ker(A, B)$,
2. $(\chi_1 \oplus \chi_2) \rightarrowtail (A, B)(\chi_1 \oplus \chi_2) := A\chi_1 + B\chi_2$, *has maximal rank* $2|\mathcal{I}|$,
3. $AB^\dagger = BA^\dagger$ .

If $M(A, B)$ is a maximal isotropic subspace then :

1. $(A + ikB)$ is invertible for $\Im k > 0$,
2. $\mathfrak{S}(A, B) = -(A + ikB)^{-1}(A - ikB)$ for $k > 0$ is unitary.

**Definition**

$(-\Delta(M, \underline{a}))$ is the Laplacian on $(\mathcal{G}, \underline{a})$ with

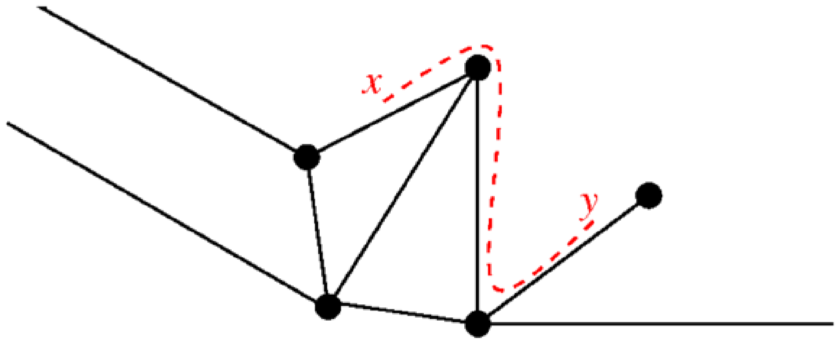
$$D(-\Delta(M, \underline{a})) := \{\psi \in \mathcal{D} \quad | \quad [\psi] \in M\}$$

**Remark :** $\psi \in D(-\Delta(M, \underline{a})) \quad \Longleftrightarrow \quad A\underline{\psi} + B\underline{\psi'} = 0.$

# What is Quantum graph?

**Definition**

A quantum graph $\Gamma = (\mathcal{G}, \underline{a}, H)$ is a metric graph $(\mathcal{G}, \underline{a})$ equipped with a differential operator $H$.




We consider the Laplacian $-\Delta$ which becomes self-adjoint with the boundary conditions such as Kirchhoff boundary conditions

$$\sum_{v} \frac{\partial \psi}{\partial x}(v) = 0 \quad \text{and} \quad \psi \text{ continuous at } v$$

with $x$ the distance from $v$ to a variable point on $G$.

# Scattering matrix

The spectrum of the operator $-\Delta$

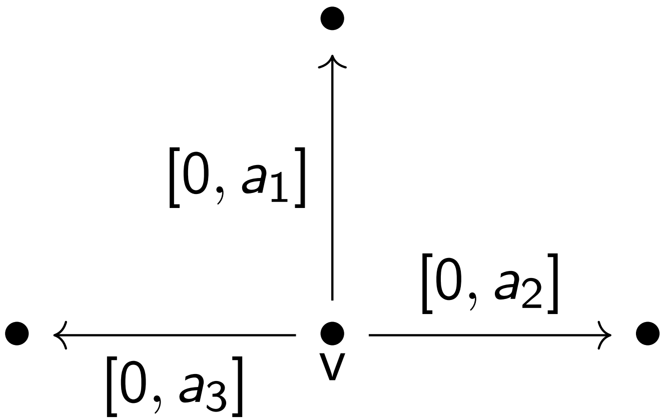
$$-\frac{\partial^2}{\partial^2 x}\psi(x) = k^2\psi(x) \Rightarrow \psi(x) = \mathfrak{s}\mathrm{e}^{-\mathrm{ikx}} + \hat{\mathfrak{s}}\mathrm{e}^{\mathrm{ikx}}.$$

$\mathfrak{s}$ and $\hat{\mathfrak{s}}$ coefficients of the local scattering matrix at vertex $v$ an unitary $d_v \times d_v$-matrix with entries $\mathfrak{S}^v_{e_i e_j}(k)$ for $e_i$, $e_j \in \mathcal{I}_v$.

$$\mathfrak{S}_v = -(A_v + \mathrm{ik}B_v)^{-1}(A_v - \mathrm{ik}B_v)$$

For $\psi \in D(-\Delta(M, \underline{a})) \quad \Longleftrightarrow \quad A_v\underline{\psi} + B_v\underline{\psi'} = 0$:
$\mathfrak{S}_v$ is independent of $k$ or scale invariant if it has the form $1 - 2P_v$ with $P_v$ an orthogonal projection.

# Example of a scattering matrix on a vertex




The scattering matrix on $v$ with Kirchhoff boundary conditions $A_v\underline{\psi} + B_v\underline{\psi\prime} = 0$, for

$$A_v = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$ and

$$B_v = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix}$$ is

computing in python here

# Computation of scattering matrix in Python

isem26.ipynb

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```
import numpy as np
A = np.array([[1,-1,0],
              [0,1,-1],
              [0,0,0]])

B = np.array([[0,0,0],
              [0,0,0],
              [1,1,1]])

i = complex(0,1)
for k in range(1,4):
  S = -i*(np.linalg.inv(A+k*i*B)).dot(A-k*i*B)
  print(f"S{k} =\n 1/3*{(S*3*i).real}\n")
```

```
S1 =
 1/3*[[ 1. -2. -2.]
 [-2.  1. -2.]
 [-2. -2.  1.]]

S2 =
 1/3*[[ 1. -2. -2.]
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S3 =
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```

isem26.ipynb
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A = np.array([[1,-1,0],
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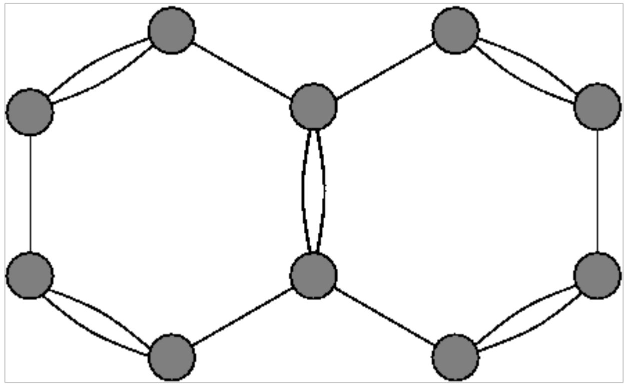
              [0,0,0]])

B = np.array([[0,0,0],
              [0,0,0],
              [1,1,1]])
```

```python
Span_KernelOrtho_B = np.array([[1,1,1]])
e = Span_KernelOrtho_B/ np.linalg.norm(Span_KernelOrtho_B)

P_ortho = e.T.dot(e)

n,m = P_ortho.shape
S = np.eye(n,m)-2*P_ortho

print(f'S=1/3*{3*S}')
```

```
S=1/3*[[ 1. -2. -2.]
 [-2.  1. -2.]
 [-2. -2.  1.]]
```

# Motivation



Naphthalene

- energy spectrum of free electrons
- nanotechnology
- ...

1-d Laplace operators

$$-\frac{\partial^2}{\partial x^2}$$

with couplings, e.g.

$$u \quad \text{continuity in know } v$$

$$\sum u_e'(v) = \gamma_v u(v)$$

sum over all adjacent $v$ and $\gamma_v \in \mathbb{R}$ given $\rightsquigarrow$ 1-d Schrödinger operator with $\delta$-potentials

$$-\frac{\partial^2}{\partial x^2} + \sum_v \gamma_v \delta_v$$

# Integral operator

## Definition

The operator $K$ on the Hilbert space $\mathcal{H}$ is called integral operator if

1. For all $j, j' \in \mathcal{I}$ there are measurable functions $K_{j,j'}(\cdot,\cdot) : I_j \times I_{j'} \to \mathbb{C}$ with the following properties:
   1. $K_{j,j'}\left(x_j,\cdot\right)\varphi_{j'}(\cdot) \in L^1\left(I_{j'}\right)$ for almost all $x_j \in I_j$,
   2. $\psi = K\varphi$ with
   $$\psi_j\left(x_j\right) = \sum_{j' \in \mathcal{I}} \int_{I_{j'}} K_{j,j'}\left(x_j, y_{j'}\right)\varphi_{j'}\left(y_{j'}\right) dy_{j'}$$
2. The $(|\mathcal{I}|) \times (|\mathcal{I}|)$ matrix-valued function $(x, y) \mapsto K(x, y)$ with
   $$[K(x, y)]_{j,j'} = K_{j,j'}\left(x_j, y_{j'}\right)$$
   is called the integral kernel of the operator $K$.

# Integral kernel of the resolvent

## Theorem

*For any maximal isotropic subspace* $\mathcal{M} \subset {}^d\mathcal{K}$

1. *The resolvent* $(-\Delta(\mathcal{M};\underline{a}) - k^2)^{-1}$ *is an integral operator*
2. *Its integral kernel is given by :*

$$r_{\mathcal{M}}(x,y;k,\underline{a}) = r^{(0)}(x,y,k) + \frac{\mathrm{i}}{2k}\Phi(x,k)R(k;\underline{a})^{-1}[\mathbb{I} - \mathfrak{S}(k;\mathcal{M})T(k;\underline{a})]^{-1} \circ \circ\, \mathfrak{S}(k;\mathcal{M})R(k;\underline{a})^{-1}\Phi(y,k)^T, \quad (2.1)$$

# Notations

Where :

1. $$r^{(0)}(x,y,k)_{j,j'} = i\delta_{j,j'}\frac{e^{ik|x_j-y_j|}}{2k},$$

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2. $$\Phi(x,k) = \begin{pmatrix} 0 & 0 \\ \phi_+(x,k) & \phi_-(x,k) \end{pmatrix}_{2|\mathcal{I}|\times 2|\mathcal{I}|}$$

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3. $$R(k,\underline{a}) = \begin{pmatrix} \mathrm{I} & 0 \\ 0 & e^{-ik\underline{a}} \end{pmatrix}_{2|\mathcal{I}|\times 2|\mathcal{I}|}$$

   where $[e^{\pm ik\underline{a}}]_{jk} = \delta_{jk}e^{\pm ika_j}$, and $\mathrm{I}$ is the $_{2|\mathcal{I}|\times 2|\mathcal{I}|}$ identity matrix.

5

$$T(k, \underline{a}) = \begin{pmatrix} 0 & e^{ik\underline{a}} \\ e^{ik\underline{a}} & 0 \end{pmatrix}_{2|\mathcal{I}|\times 2|\mathcal{I}|}$$

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6.
$$\mathfrak{S}(k;\mathcal{M}).$$

## Sketch of the proof

Let $M(k)$ be the integral operator with kernel given by 2.1.
Let $\varphi \in \mathcal{H}$. Set $\psi = M(k)\varphi$.

**Goal :** $(-\Delta(\mathcal{M}; \underline{a}) - k^2)^{-1} = M(k)$.

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**Steps :**

1. $(-\Delta(\mathcal{M};\underline{a}) - k^2)\psi = \varphi$,
2. $\psi \in \mathrm{Dom}(\Delta(\mathcal{M};a))$,
3. $r_{\mathcal{M}}(x,y;k,\underline{a}) = r_{\mathcal{M}}(y,x;\bar{k},\underline{a})^{\dagger}$.

# $\psi \in \mathrm{Dom}(\Delta(\mathcal{M}; a))$

On a dense subset of $\mathcal{H}$ we prove :

$$\psi \in \mathrm{Dom}(\Delta(\mathcal{M}; a)) \iff A\underline{\psi} + B\underline{\psi}' = 0$$

## $(-\Delta(\mathcal{M};\underline{a}) - k^2)\psi = \phi$

- For a continious $\varphi \in \mathcal{H}_j$, we have :

$$-\frac{\mathrm{i}}{2k}\left(\frac{d^2}{dx_j^2} + k^2\right)\int_{I_j} \mathrm{e}^{\mathrm{i}k|x_j - y_j|}\varphi_j\left(y_j\right)dy_j = \varphi_j\left(x_j\right), \quad x_j \in \overset{o}{I_j},$$

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- on the interval $I_j$ we have

$$\psi_j(x_j) = \int_{I_j} -\frac{\mathrm{i}}{2k}\mathrm{e}^{\mathrm{i}k|x_j - y_j|}\varphi_j\left(y_j\right)dy_j + e^{ikx_j}\int_{I_j} r_{A,B}\varphi_j dy_j$$

Applying $\left(\frac{d^2}{dx_j^2} + k^2\right)$ on both sides we get :

$$-\frac{\mathrm{i}}{2k}\left(\frac{d^2}{dx_j^2} + k^2\right)\psi_j\left(x_j\right) = \varphi_j\left(x_j\right)$$

- Because $M(k)$ is bounded and $\left(-\Delta(\mathcal{M};\underline{a}) - k^2\right)\psi = \varphi$ for all $\varphi$ in a dense subset of $\mathcal{H}$, then the claims follows .

# $r_{\mathcal{M}}(x, y; k, \underline{a}) = r_{\mathcal{M}}(x, y; \bar{k}, \underline{a})^\dagger$

- $r^{(0)}(y, x, k) = r^{(0)}(x, y, -\overline{k})^\dagger$

- $R_+(k; \underline{a})^\dagger = R_+(-\overline{k}; \underline{a})$,

- $T(k; \underline{a})^\dagger = T(-\overline{k}; \underline{a}) \quad$ and $\quad \Phi(x, k)^\dagger = \Phi(x, -\overline{k})^T$,

- $$\mathfrak{S}(k; \mathcal{M})[\mathbb{I} - T(k; \underline{a})\mathfrak{S}(k; \mathcal{M})]^{-1} = [\mathbb{I} - \mathfrak{S}(k; \mathcal{M})T(k; \underline{a})]^{-1}\mathfrak{S}(k; \mathcal{M}),$$

- $\mathfrak{S}(-\overline{k}; \mathcal{M})^\dagger = \mathfrak{S}(k; \mathcal{M})$.

# Walks on the graph

## Definition

A non trivial walk $w_{j,j'}$ from $j = j_0$ to $j' = j_{n+1}$ is an ordered sequence of vertices and edges

$$\{j, v_0, j_1, v_1, ..., v_n, j'\}$$

such that :

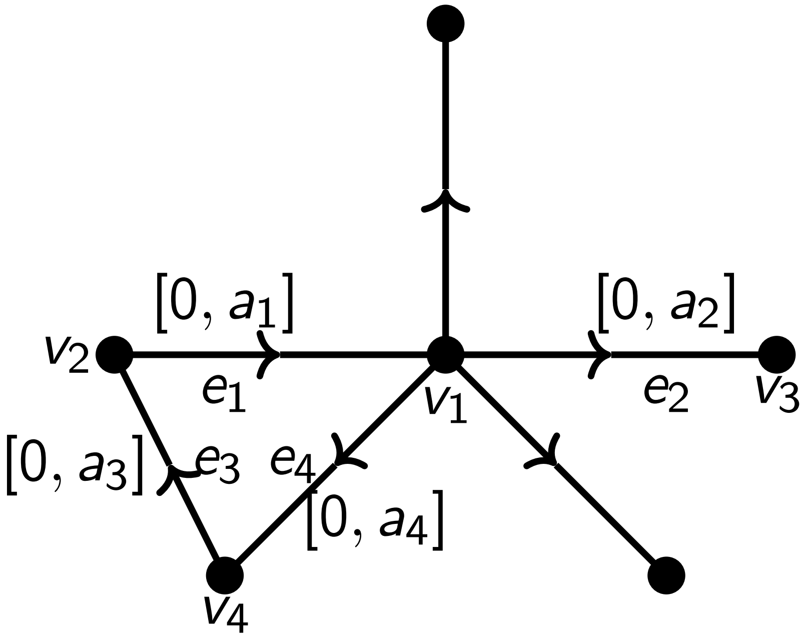
$$\forall k \in \{0, ..., n\}, v_k \in V, v_k \in \partial(j_k) \wedge v_k \in \partial(j_{k+1})$$

.

1. $v_-(w_{j,j'}) := v_0$ denotes the vertex from which $w_{j,j'}$ leaves $j$.
2. $v_+(w_{j,j'}) := v_n$ denotes the vertex from which $w_{j,j'}$ enters $j'$.
3. $|w|_{comb} := n$, $|w| := \sum_{k=1}^{n} a_{j_k}$.

4. $\mathcal{W}_{j,j'} := \{j - j' \text{ walks } w\}$.
5. $$\operatorname{dist}\left(x_j, v_-(\mathrm{w})\right) := \begin{cases} x_j & \text{if} \quad v_-(\mathrm{w}) = \partial^-(j), \\ a_j - x_j & \text{if} \quad v_-(\mathrm{w}) = \partial^+(j), \end{cases}$$
$$\operatorname{dist}\left(x_{j'}, v_+(\mathrm{w})\right) := \begin{cases} x_{j'} & \text{if} \quad v_+(\mathrm{w}) = \partial^-(j), \\ a_j - x_j & \text{if} \quad v_+(\mathrm{w}) = \partial^+(j). \end{cases}$$

# Walks on graphs

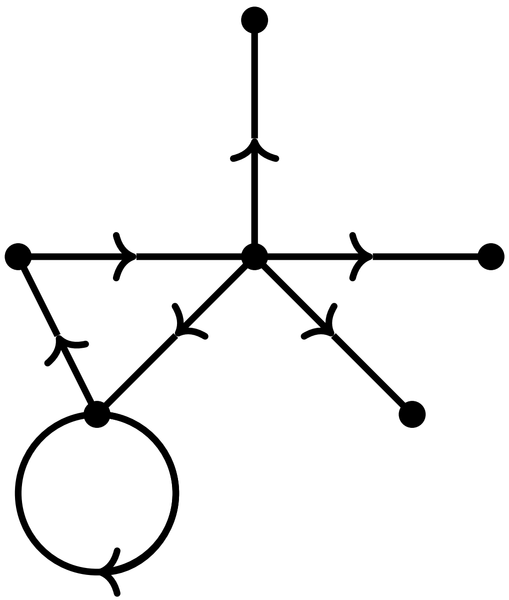



$w_{1,2} = \{e_1, v_2, e_1, v_1, e_2, v_3, e_2\}$, or
$w'_{1,2} = \{e_1, v_2, e_3, v_4, e_4, v_1, e_2, v_3, e_2\}$

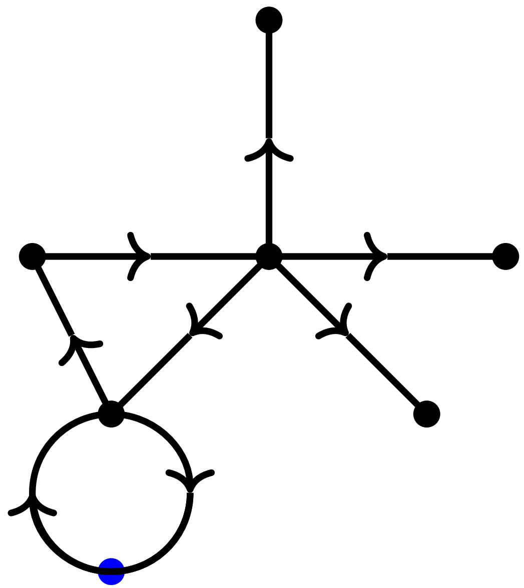
- $v_-(w_{1,2}) = v_-(w'_{1,2}) = v_2$ and
  $v_+(w_{1,2}) = v_+(w'_{1,2}) = v_3$
- $|w_{1,2}| = a_1 + a_2$ and
  $|w_{1,2}|_{comb} = 1 + 1$
- $|w'_{1,2}| = a_3 + a_4 + a_2$ and
  $|w'_{1,2}|_{comb} = 1 + 1 + 1$

# Walks on graphs

tadpole



no tadpole



# Combinatorial expansion of the resolvent

## Theorem

1. *Assume that $\mathcal{G}$ has no tadpoles.*
2. $0 < Im\ k$

$$[r_{\mathcal{M}}(x, y; k, \underline{a})]_{j,j'} = \frac{\mathrm{i}}{2k}\delta_{j,j'}\mathrm{e}^{\mathrm{i}k|x_j - y_j|}$$

$$+\frac{\mathrm{i}}{2k}\sum_{\mathrm{w}\in\mathcal{W}_{j,j'}} \mathrm{e}^{\mathrm{i}\,\mathrm{dist}\left(x_j, v_-(\mathrm{w})\right)} W_{\mathcal{M}}(\mathrm{w})\mathrm{e}^{\mathrm{i}k|\mathrm{w}|}\mathrm{e}^{\mathrm{i}k\,\mathrm{dist}\left(y_{j'}, v_+(\mathrm{w})\right)},$$

where $W_{\mathcal{M}}(\mathrm{w}) = \prod_{l=0}^{|\mathrm{w}|_{\mathrm{comb}}} \left[\mathfrak{S}\left(A\left(v_l\right), B\left(v_l\right)\right)\right]_{i_{l+1}, i_l}$.

- $T(k; \underline{a})$ is a uniform contraction,

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-

$$[\mathbb{I}-\mathfrak{S}(\mathrm{k};\mathcal{M})T(\mathrm{k};\underline{a})]^{-1}\mathfrak{S}(\mathrm{k};\mathcal{M})=\sum_{n=0}^{\infty}\mathfrak{S}(\mathrm{k};\mathcal{M})(T(\mathrm{k};\underline{a})\mathfrak{S}(\mathrm{k};\mathcal{M}))^{n}$$

- $T(k; \underline{a})$ is a uniform contraction,
-

$$[\mathbb{I} - \mathfrak{S}(\mathrm{k}; \mathcal{M}) T(\mathrm{k}; \underline{a})]^{-1} \mathfrak{S}(\mathrm{k}; \mathcal{M}) = \sum_{n=0}^{\infty} \mathfrak{S}(\mathrm{k}; \mathcal{M}) (T(\mathrm{k}; \underline{a}) \mathfrak{S}(\mathrm{k}; \mathcal{M}))^n$$

- $\mathrm{e}^{\mathrm{i}\,\mathsf{dist}\left(x_j, v_-(\mathrm{w})\right)}$

- $T(k;\underline{a})$ is a uniform contraction,
- $$[\mathbb{I}-\mathfrak{S}(\mathrm{k};\mathcal{M})T(\mathrm{k};\underline{a})]^{-1}\mathfrak{S}(\mathrm{k};\mathcal{M}) = \sum_{n=0}^{\infty}\mathfrak{S}(\mathrm{k};\mathcal{M})(T(\mathrm{k};\underline{a})\mathfrak{S}(\mathrm{k};\mathcal{M}))^{n}$$
- $\mathrm{e}^{\mathrm{i}\,\mathsf{dist}\left(x_j,v_-(\mathsf{w})\right)}$
- $W_{\mathcal{M}}(\mathsf{w})\mathrm{e}^{\mathrm{i}k|\mathsf{w}|}$

# Heat kernel expansion

## Theorem

*The heat kernel of* $-\Delta(\mathcal{M}, \underline{a})$ *has the absolutely convergent expansion*

$$[p_t(x, y; \mathcal{M}, \underline{a})]_{j,j'} = \delta_{j,j'} g_t\left(x_j - y_j\right)$$
$$+ \sum_{\mathrm{w} \in \mathcal{W}_{j,j'}} W_{\mathcal{M}}(\mathrm{w}) g_t\left(\mathrm{dist}\left(x_j, v_-(\mathrm{w})\right) + |\mathrm{w}| + \mathrm{dist}\left(y_{j'}, v_+(\mathrm{w})\right)\right)$$

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*The series converges uniformly in* $x, y \in \bigtimes_{j \in \mathcal{I}} I_j$.

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*The series converges uniformly in* $x, y \in \times_{j \in \mathcal{I}} I_j$.

Where

$$g_t(x_j - y_j) := \frac{1}{\sqrt{4\pi t}} \exp\left\{-(x_j - y_j)^2/4t\right\}$$

**Proof.**

- $$\mathrm{e}^{t\Delta(\mathcal{M},\underline{a})} = -\frac{1}{2\pi\mathrm{i}} \int_{\gamma} \mathrm{e}^{-t\lambda} (-\Delta(\mathcal{M},\underline{a}) - \lambda)^{-1} d\lambda$$

- $$\frac{1}{2\pi} \int_{-\infty+\mathrm{i}\varepsilon}^{+\infty+\mathrm{i}\varepsilon} \mathrm{e}^{-\mathrm{k}^2 t} \mathrm{e}^{\mathrm{i}\mathrm{k}u} d\mathrm{k} = g_t(u) := \frac{1}{\sqrt{4\pi t}} \exp\left\{-u^2/4t\right\},$$

$\square$

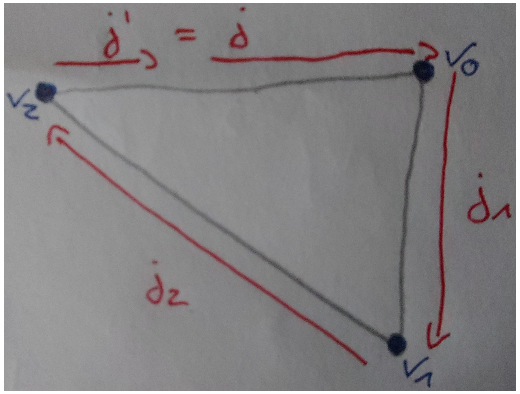
# Motivation

- Trace formulas link spectral properties with geometric properties
- e.g.the Selberg trace formula
  - applications in arithmetic geometry and number theory
- Applications to quantum graphs
  - e.g. quantum chaos, spectral statistics, inverse spectral and scattering problems.

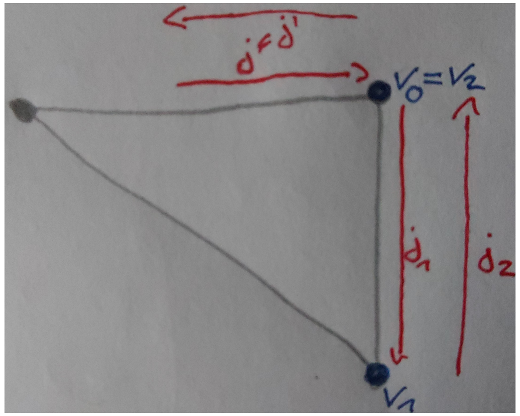
## Closed Walks

- A walk $w \in \mathcal{W}_{j,j}$ is called *closed*. It is called *properly closed* if $v_-(w) \neq v_+(w)$.
- For a properly closed walk w we denote by $j(w)$ its initial edge.
- Properly closed walks $w, w'$ are called *equivalent* , if they can be obtained from each other by successive application of the transformation

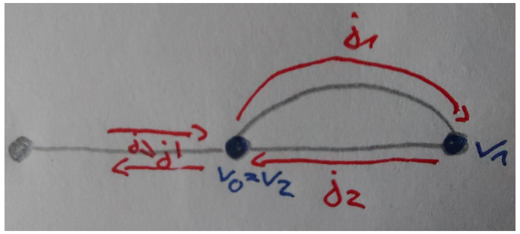
$$\{j, v_0, j_1, v_1, \ldots, v_n, j\} \to \{j_1, v_1, \ldots, j_n, v_n, j, v_0, j_1\}.$$




(properly closed walk)




(not properly closed)




(not properly closed walk)

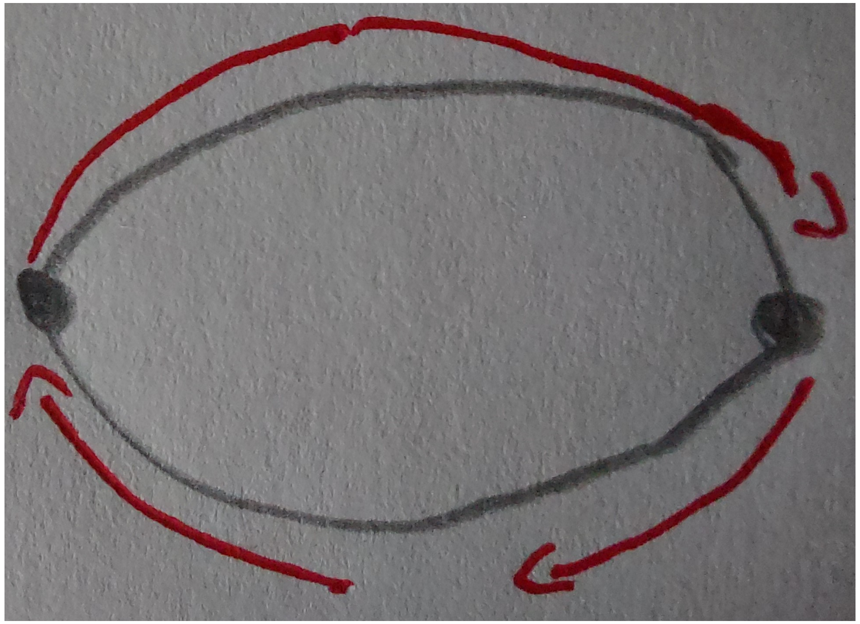
# Cycles

- A *cycle* $\mathfrak{c}$ is an equivalence class of properly closed walks.
- For $\mathrm{w} \in \mathfrak{c}$, $j = j(\mathrm{w})$, the *metric length* of $\mathfrak{c}$ is given by $|\mathfrak{c}| = |w| + a_j$.
- $\mathfrak{C}$ denotes the set of all cycles.
- For $\mathfrak{c} \in \mathfrak{C}$, $\mathfrak{c} \ni \mathrm{w} = \{j, v_0, j_1, v_1, \ldots, v_n, j\}$, $p \in \mathbb{N}$ we denote by $p\mathfrak{c}$ the unique cycle containing the following properly closed walk

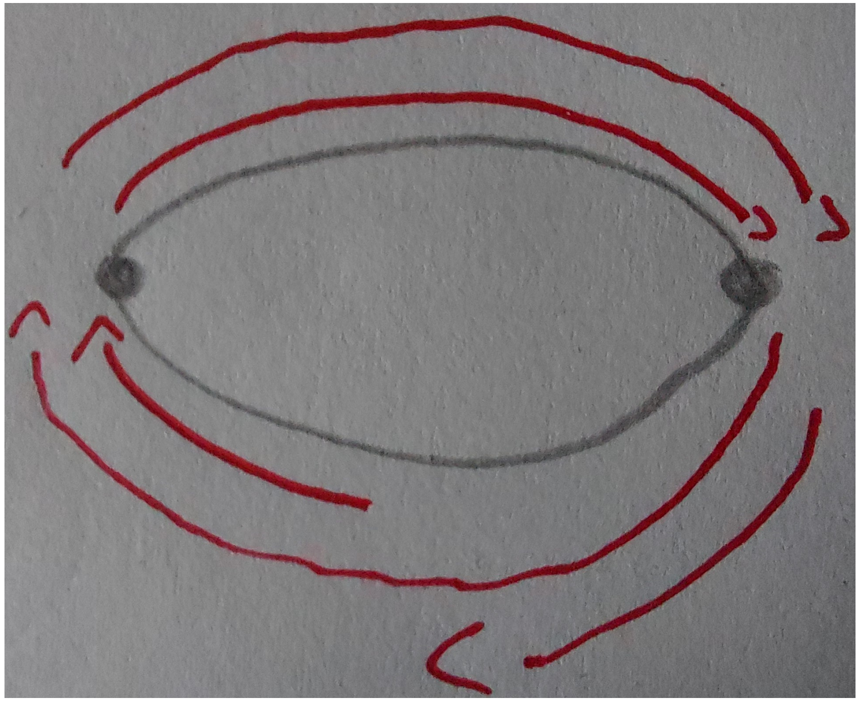
$$\underbrace{\{j, v_0, j_1, v_1, \ldots, v_n, j, v_0, j_1, v_1, \ldots, v_n, j, v_0, j_1, \ldots, v_n, j\}}_{\text{repeated } p \text{ times}}$$

- A cycle $\mathfrak{c}$ is called *primitive* if it is not of the form $\mathfrak{c} = p\mathfrak{c}'$ for any $p \geq 2$, $\mathfrak{c} \in \mathfrak{C}$
- $\mathfrak{C}_{\mathrm{prim}}$ denotes the set of all primitive cycles.
- Every cycle $\mathfrak{c}$ is either primitive or of the form $\mathfrak{c} = p\mathfrak{c}'$ for some $\mathfrak{c}' \in \mathfrak{C}_{\mathrm{prim}}$

# Cycles



primitive cycle $\mathfrak{c}$



non primitive cycle $2\mathfrak{c}$

# Trace Formula

**Theorem**

*Assume that the compact Graph $\mathcal{G}$ has no loops. Let the maximal isotropic subspace $\mathcal{M}$ define local and scale invariant vertex conditions. Then*

$$\operatorname{tr}_{\mathcal{H}}\left(e^{t\Delta(\mathcal{M},\underline{a})}\right) = \frac{L}{2\sqrt{\pi t}} + \frac{1}{4}\operatorname{tr}_{\mathcal{K}}\mathfrak{S}(\mathcal{M})$$
$$+ \frac{1}{2\sqrt{\pi t}} \sum_{\mathfrak{c}\in\mathfrak{C}_{\mathrm{prim}}} \sum_{p\in\mathbb{N}} W_{\mathcal{M}}(\mathfrak{c})^p |\mathfrak{c}| \exp\left(-\frac{p^2|\mathfrak{c}|^2}{4t}\right), \quad t > 0,$$

*where $L := \sum_{j\in\mathcal{I}} a_j$ and $W_{\mathcal{M}}(\mathfrak{c}) = W_{\mathcal{M}}(\mathrm{w})$ for any walk $\mathrm{w}$ in the cycle $\mathfrak{c}$.*

- For any trace class operator $K$ on $\mathcal{H}$ we have

$$\mathrm{tr}_{\mathcal{H}} K = \sum_{j \in \mathcal{I}} \mathrm{tr}_{\mathcal{H}_j} P_j K P_j,$$

- Each $P_j e^{t\Delta(\mathcal{M},\underline{a})} P_j$ is an integral operator on $L^2(I_j)$ with a kernel jointly continuous in $x_j, y_j \in \mathring{I}_j$

$$\Rightarrow \mathrm{tr}_{\mathcal{H}} \left( e^{t\Delta(\mathcal{M},\underline{a})} \right) = \sum_{j \in \mathcal{I}} \mathrm{tr}_{\mathcal{H}_j} \left( P_j e^{t\Delta(\mathcal{M},\underline{a})} P_j \right)$$

$$= \sum_{j \in \mathcal{I}} \int_{I_j} [p_t(x_j, x_j; \mathcal{M}, \underline{a})]_{j,j} dx_j$$

Heat kernel expansion

$$\begin{aligned}
&\Rightarrow \mathrm{tr}_{\mathcal{H}}\left(e^{t\Delta(\mathcal{M},\underline{a})}\right) \\
&\quad = \sum_{j\in\mathcal{I}} \int_{I_j} g_t(0)\,dx_j \\
&\qquad + \sum_{j\in\mathcal{I}} \sum_{\mathrm{w}\in\mathcal{W}_{j,j}} W_{\mathcal{M}}(\mathrm{w}) \int_{I_j} g_t(\mathrm{dist}(x_j, v_-(\mathrm{w})) + |\mathrm{w}| + \mathrm{dist}(x_j, v_+(\mathrm{w})))\,dx_j,
\end{aligned} \tag{3.1}$$

where the sum converges absolutely.

## Terms not associated with any walk

Remember $g_t(u) = \frac{1}{\sqrt{4\pi t}} \exp(-u^2/4t)$. So

$$\sum_{j \in \mathcal{I}} \int_{I_j} g_t(0) dx_j = \sum_{j \in \mathcal{I}} \frac{a_j}{\sqrt{4\pi t}} = \frac{L}{2\sqrt{\pi t}}.$$

## Terms associated with properly closed walks

- For a properly closed walk w from $j$ to $j$, $v_-(\mathrm{w}) \neq v_+(\mathrm{w})$.

$$\Rightarrow \ \operatorname{dist}(x_j, v_-(\mathrm{w})) + \operatorname{dist}(x_j, v_+(\mathrm{w})) = a_j.$$

- Summing over all walks in the cycle $\mathfrak{c} = \mathfrak{c}(\mathrm{w})$

$$\Rightarrow \sum_{\mathrm{w}\in\mathfrak{c}} W_{\mathcal{M}}(\mathrm{w}) \int_{I_{j(w)}} g_t(|\mathrm{w}|+a_{j(w)})dx_{j(w)} = W_{\mathcal{M}}(\mathfrak{c})g_t(|\mathfrak{c}|) \sum_{\mathrm{w}\in\mathfrak{c}} a_{j(\mathrm{w})}.$$

- If $\mathfrak{c} = p\mathfrak{c}'$ for some $p \in \mathbb{N}$ and some $\mathfrak{c}' \in \mathfrak{C}_{\mathrm{prim}}$, then $\sum_{\mathrm{w}\in\mathfrak{c}} a_{j(\mathrm{w})} = |\mathfrak{c}'|$ and $W_{\mathcal{M}}(\mathfrak{c}) = W_{\mathcal{M}}(\mathfrak{c}')^p$.

Thus the contribution from all properly closed walks to (3.1) is

$$\frac{1}{2\sqrt{\pi t}} \sum_{\mathfrak{c}\in\mathfrak{C}_{\mathrm{prim}}} \sum_{p\in\mathbb{N}} W_{\mathcal{M}}(\mathfrak{c})^p |\mathfrak{c}| \exp\left(-\frac{p^2|\mathfrak{c}|^2}{4t}\right), \quad t > 0.$$

# Terms associated with not properly closed walks

- For not properly closed walks $v_-(\mathrm{w}) = v_+(\mathrm{w})$, so

$$\mathrm{dist}(x_j, v_-(\mathrm{w})) + \mathrm{dist}(x_j, v_+(\mathrm{w})) = \begin{cases} 2x_j, & v_-(\mathrm{w}) \in \partial^-(j), \\ 2(a_j - x_j), & v_-(\mathrm{w}) \in \partial^+(j). \end{cases}$$

$$\Rightarrow \int_{I_j} g_t(\mathrm{dist}(x_j, v_-(\mathrm{w})) + \mathrm{dist}(x_j, v_+(\mathrm{w})) + |\mathrm{w}|)dx_j$$

$$= \int_{I_j} g_t(2x_j + |w|)dx_j.$$

- w is called of type $A$ if it is of the form

$$\mathrm{w} = \{j_p, v_p, j_{p-1}, v_{p-1}, \ldots, j_0, v_0, j_0, \ldots, v_{p-1}, j_{p-1}, v_p, j_p\},$$

otherwise, it is called type $B$.

# Terms associated with not properly closed walks

**Lemma**

$$\sum_{j\in\mathcal{I}}\sum_{\mathrm{w}\in W^{A}_{j,j}} W_{\mathcal{M}}(\mathrm{w})\int_{I_j} g_t(2x_j+|w|)dx_j=\frac{1}{4}\mathrm{tr}_{\mathcal{K}}\mathfrak{S}(\mathcal{M}).$$

**Lemma**

$$\sum_{j\in\mathcal{I}}\sum_{\mathrm{w}\in W^{B}_{j,j}} W_{\mathcal{M}}(\mathrm{w})\int_{I_j} g_t(2x_j+|w|)dx_j=0.$$

# Proof of the first Lemma

Let $\operatorname{erfc}(x) := \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du$ denote the complementary error function. Then

$$\int_0^a g_t(2x + |\mathrm{w}|)dx = \int_0^a \frac{1}{2\sqrt{\pi t}} \exp\left(-\frac{(2x+|\mathrm{w}|)^2}{4t}\right)$$

$$= \frac{1}{2\sqrt{\pi}} \int_0^{|\mathrm{w}|/\sqrt{t}^{(2a+|\mathrm{w}|)/2\sqrt{t}}} e^{-u^2} du = \frac{1}{4}\left(\operatorname{erfc}\left(\frac{|\mathrm{w}|}{2\sqrt{t}}\right) - \operatorname{erfc}\left(\frac{|\mathrm{w}|+2a}{2\sqrt{t}}\right)\right)$$

For $v_0 \in V$, $p \in \mathbb{N}_0$ arbitrary we set

$$\partial G_{v_0}(p) := \{\text{walks of the form}\{j_p, v_p, j_{p-1}, v_{p-1}, \ldots, j_0, v_0, j_0, \ldots, v_{p-1}, j_{p-1}, v_p, j_p\}\}$$

$$G_{v_0}(p) := \bigcup_{q=0}^{p} \partial G_{v_0}(q).$$

# Proof of the first Lemma

$$\sum_{\mathrm{w}\in G_{v_0}(0)} W_{\mathcal{M}}(\mathrm{w}) \int_{I_j} g_t(2x_j + |\mathrm{w}|)dx_j$$

$$= \sum_{j\in\mathcal{I}, v_0\in\partial(j)} [\mathfrak{S}(\mathcal{M}_{v_0}]_{j,j} \frac{1}{4}\left(\operatorname{erfc}(0) - \operatorname{erfc}\left(\frac{0+2a}{2\sqrt{t}}\right)\right)$$

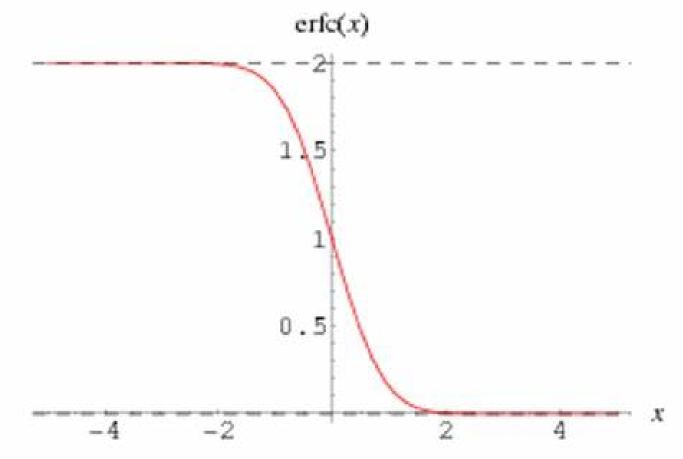
$$= \frac{1}{4}\operatorname{tr}_{\mathcal{L}_{v_0}}[\mathfrak{S}(\mathcal{M}_{v_0})] - \frac{1}{4}\sum_{\mathrm{w}\in\partial G_{v_0}(0)} W_{\mathcal{M}}(\mathrm{w})\operatorname{erfc}\left(\frac{|\mathrm{w}|+2a_{j(\mathrm{w})}}{2\sqrt{t}}\right)$$

By Induction we get

$$\sum_{\mathrm{w}\in G_{v_0}(p)} W_{\mathcal{M}}(\mathrm{w}) \int_{I_{j(\mathrm{w})}} g_t(2x_{j(\mathrm{w})} + |\mathrm{w}|)dx_{j(\mathrm{w})} = \frac{1}{4}\operatorname{tr}_{\mathcal{L}_{v_0}}[\mathfrak{S}(\mathcal{M}_{v_0})]$$

$$-\frac{1}{4}\sum_{\mathrm{w}\in\partial G_{v_0}(p)} W_{\mathcal{M}}(\mathrm{w})\operatorname{erfc}\left(\frac{|\mathrm{w}|+2a_{j(\mathrm{w})}}{2\sqrt{t}}\right)$$

# Proof of the first Lemma




$$\mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du \leq Ce^{-x^2}$$

$$\sum_{\mathrm{w} \in \partial G_{v_0}(p)} \left| W_{\mathcal{M}}(\mathrm{w}) \mathrm{erfc}\left( \frac{|\mathrm{w}| + 2a_{j(\mathrm{w})}}{2\sqrt{t}} \right) \right| \leq |\mathcal{I}|^{p+1} |V|^p \mathrm{erfc}\left( \frac{pa_{\min}}{\sqrt{t}} \right)$$

Letting $p \to \infty$ and summing over all $v_0 \in V$ yields the claim.

# Proof of the second Lemma

Any walk of type B is of the form

$$\{j_p, v_p, j_{p-1}, \dots, j_0, v_0, \mathfrak{s}, v_0, j_0, \dots, j_{p-1}, v_p, j_p\}.$$

For $p \in \mathbb{N}_0$ we set

$$\partial F_{\mathfrak{s},v_0}(p) := \{\text{walks of the form}\{j_p, v_p, j_{p-1}, \dots, j_0, v_0, \mathfrak{s}, v_0, j_0, \dots, j_{p-1}, v_p, j_p\}\}$$

$$F_{\mathfrak{s},v_0}(p) := \bigcup_{q=0}^{p} \partial F_{\mathfrak{s},v_0}(q).$$

By induction we get

$$\sum_{\mathrm{w}\in F_{\mathfrak{s},v_0}(p)} W_{\mathcal{M}}(\mathrm{w}) \int_{I_{j(\mathrm{w})}} g_t(2x_{j(\mathrm{w})} + |\mathrm{w}|)dx_{j(\mathrm{w})}$$

$$= -\frac{1}{4} \sum_{\mathrm{w}\in \partial F_{\mathfrak{s},v_0}(p)} W_{\mathcal{M}}(\mathrm{w})\mathrm{erfc}\left(\frac{|\mathrm{w}| + 2a_{j(\mathrm{w})}}{2\sqrt{t}}\right)$$

# Introduction

Two important Laplacians with scale-invariant vertex conditions are the Laplacian $\Delta_{\mathrm{K}}$ with *Kirchhoff conditions*

$$\psi_1(v) = \ldots = \psi_{d_v}(v), \qquad \sum_{i=1}^{d_v} \psi_i'(v) = 0$$

for a $\psi \in H^2(\mathcal{G})$, and the dual version, the Laplacian $\Delta_{\mathrm{aK}}$ with *anti-Kirchhoff conditions*

$$\psi_1'(v) = \ldots = \psi_{d_v}'(v), \qquad \sum_{i=1}^{d_v} \psi_i(v) = 0.$$

The difference in the corresponding traces is only a constant stemming from the different kernels of these Laplacians:

$$\mathrm{tr}_{\mathcal{H}}\left(e^{t\Delta_{\mathrm{K}}}\right) - \mathrm{tr}_{\mathcal{H}}\left(e^{t\Delta_{\mathrm{aK}}}\right) = \dim\ker\Delta_{\mathrm{K}} - \dim\ker\Delta_{\mathrm{aK}}$$

# Factorization

- We want to better understand the Laplacians $\Delta_{\mathrm{K}}$ and $\Delta_{\mathrm{aK}}$ by factorizing them into two first-order derivative operators $\Delta_{\mathrm{K}} = -A^*A$, and $\Delta_{\mathrm{aK}} = -AA^*$.
- Here, $A\psi = \frac{\partial\psi}{\partial x}$ with Kirchhoff continuity conditions on $\psi$ (not on $\psi'$).
- We then investigate $A$, especially its index, as

$$\begin{aligned}
\mathrm{ind} A &= \dim\ker A - \dim\operatorname{coker} A \\
&= \dim\ker A - \dim\ker A^* \\
&= \dim\ker \Delta_{\mathrm{K}} - \dim\ker \Delta_{\mathrm{aK}} \\
&= \mathrm{tr}_{\mathcal{H}}\left(e^{t\Delta_{\mathrm{K}}}\right) - \mathrm{tr}_{\mathcal{H}}\left(e^{t\Delta_{\mathrm{aK}}}\right)
\end{aligned}$$

# Index Theorem - First Variant

**Theorem**

*Let $\Delta$ denote a self-adjoint Laplacian on metric graph $(\mathcal{G}, \underline{a})$ with scale-invariant boundary conditions. Then $\Delta = -A^*A$ where $A$ is given by $A\psi = \frac{\partial \psi}{\partial x}$ with boundary conditions on $\psi$ encoded in its domain.*
*Further, the index of $A$ is given by*

$$\mathrm{ind} A = E - p$$

*where $E$ is the number of edges of $\mathcal{G}$ and $p$ is the number of vertex conditions of $\Delta$ on $\psi$ (not those on $\psi'$).*

# Proof of First Index Theorem

- Let $\frac{\partial}{\partial x} : \bigoplus_{j \in \mathcal{I}} H^1(I_j) \to \mathcal{H}$ be the derivative operator on the edges without vertex conditions.
- Let $A$ be the restriction of $\frac{\partial}{\partial x}$ onto a subspace of codimension $p$ given by vertex conditions on $\psi$ (not on $\psi'$).

**Lemma**

The operators $\frac{\partial}{\partial x}$ and $A$ are Fredholm operators with indices $\mathrm{ind}\frac{\partial}{\partial x} = E$ and $\mathrm{ind}A = E - p$.

# Proof of First Index Theorem

## Proof of the lemma.

- $\frac{\partial}{\partial x}$ is surjective
- kernel is given by functions which are constant on each edge, dimension is $E$
- $\mathrm{ind}\frac{\partial}{\partial x} = E$
- Restriction reduces index by codimension $p$
- $\mathrm{ind}A = E - p$

$\square$

# Proof of the First Index Theorem

**Proof of the first index theorem.**

- Let $A$ be the restriction of $\frac{\partial}{\partial x} : \bigoplus_{e \in E} H^1(e) \to \mathcal{H}$ onto a subspace of codimension $p$ given by the vertex conditions of $\Delta$ on $\psi$.
- Writing $\Delta = -A^* A$ gives correct boundary conditions on $\psi$ and $\psi'$.
- Apply the lemma.

$\square$

The detail not to be overlooked is implementing the boundary conditions into the operator $A$.

# Example for $A$

Let $A$ be given by the Kirchhoff boundary conditions on $\psi$, i.e.

$$\psi_1(v) = \ldots = \psi_{d_v}(v),$$

Then $A^*$ is given by $A\psi = -\frac{\partial \psi}{\partial x}$ with boundary condition

$$\sum_{i=1}^{d_v} \psi_i(v) = 0$$

This is because the boundary term in the integration by parts formula

$$\sum_{v \in V} \sum_{i=1}^{d_v} f_i(v) g_i(v)$$

has to be 0 for any $f, g \in \bigoplus_{e \in E} H^1(e)$. See also the isotropic subspaces earlier.

# Index Theorem - Second Variant

## Theorem

*Let $\Delta_{\mathrm{K}}$ and $\Delta_{\mathrm{aK}}$ denote the (self-adjoint) Laplacian on a metric graph $(\mathcal{G}, \underline{a})$ with Kirchhoff (resp. anti-Kirchhoff) boundary conditions. Then $\Delta_{\mathrm{K}} = -A^*A$ and $\Delta_{\mathrm{aK}} = -AA^*$ where $A$ is given by $A\psi = \frac{\partial \psi}{\partial x}$ with boundary conditions on $\psi$ encoded in its domain. Further, the index of $A$ is given by*

$$\mathrm{ind} A = \chi(\mathcal{G})$$

*where $\chi(\mathcal{G}) = V - E$ is the Euler characteristic of $\mathcal{G}$.*

# Proof of the Second Index Theorem

**Proof.**

- Recall the Kirchhoff conditions:

$$\psi_1(v) = \ldots = \psi_{d_v}(v)$$

- They define $\deg v - 1$ conditions per vertex, thus $\sum_v (\deg v - 1) = 2E - V$ conditions in total.
- Thus, $\operatorname{ind} T = E - (2E - V) = V - E = \chi(\mathcal{G})$.

$\square$

# Outlook on generalizations

- Atiyah-Singer theorem: For an $n$-dimensional manifold $X$,

$$\mathrm{ind} A = (-1)^n \langle \mathrm{ch}(A)\mathrm{Td}(X), X\rangle.$$

- Riemann-Roch theorem: For a Riemannian surface $X$ with genus $g$ and canonical divisor $K$,

$$\ell(D) - \ell(K - D) = \deg D + g - 1.$$

- Gauss-Bonnet theorem: For a compact surface $X$,

$$\frac{1}{2\pi}\int_X K = \chi(X).$$

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