Quantum theory on graphs

with an application to the

Traveling Salesman Problem

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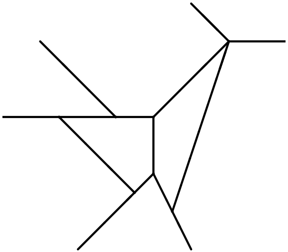
The first basic concept is given by the

Definition: A metric graph $\mathcal{G}$ is a finite collection of halflines and intervals of given lengths with an identification of some of its endpoints (=vertices)



A graph with $n = 6$ external lines and $m = 8$ internal lines

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There is the unique notion of a distance between two points

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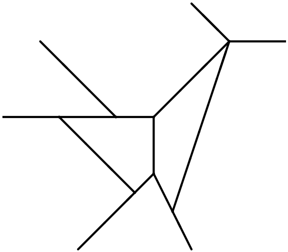

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$\mathcal{G}$ is a metric space:

There is the unique notion of a distance between two points

Quantum Mechanics

In order to do quantum mechanics on a given graph we have to specify

1. the state space, a Hilbert space $\mathcal{H} = \mathcal{H}(\mathcal{G})$ with elements ψ called wave functions,
2. an operator on this Hilbert space, the Hamiltonian $\mathbf{H}$.
3. This will define a dynamics in form of the time dependent Schrödinger equation

$$\mathrm{i}\hbar\partial_t\psi(t) = \mathbf{H}\psi(t)$$

giving rise to a flow in Hilbert space.

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Wave Functions

Definition: **The Hilbert space $\mathcal{H}$ is the space of square integrable, complex valued functions ψ on $\mathcal{G}$. The scalar product is**

$$\langle \phi, \psi \rangle = \int_{\mathcal{G}} \overline{\phi(x)} \psi(x) dx$$

where dx is the canonical Lebesgue measure on $\mathcal{G}$.

Laplace Operators

The simplest dynamics is where there is free flow away from any vertex. Thus the Schrödinger equation should take the form

$$i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t)$$

as long as $x \in \mathcal{G}$ is not a vertex v of the graph.

Question

What happens at the vertices?

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Question

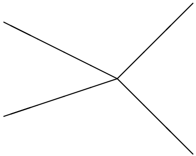
What happens at the vertices?

Answer: Specify Boundary conditions at the vertices

The general one vertex case:

$$\psi = \{\psi_e(x)\}_{e \in \mathcal{E}} \in \oplus_{e \in \mathcal{E}} L^2(\mathbb{R}_+)$$

$\mathcal{E}$ = set of external half-lines $e \cong [0_e, \infty_e) \cong \mathbb{R}_+$, $n = |\mathcal{E}|$



The 1-vertex graph with $n = 4$ external lines

The boundary values $\psi(0) = \{\psi_e(0_e)\}_{e \in \mathcal{E}} \in \mathbb{C}^n$ and $\psi'(0) = \{\psi'_e(0_e)\}_{e \in \mathcal{E}} \in \mathbb{C}^n$ combined define a linear space $\mathbb{C}^{2n}$.

Laplace Operators: Boundary conditions

Green's Theorem (= partial integration)

gives a hermitean symplectic form on this $2n$ dim. linear space

$$\langle \Delta\psi, \phi\rangle - \langle \psi, \Delta\phi\rangle = \langle \begin{bmatrix} \psi(0) \\ \psi'(0) \end{bmatrix}, J \begin{bmatrix} \phi(0) \\ \phi'(0) \end{bmatrix} \rangle_{\mathbb{C}^{2n}}$$

$$J = \begin{pmatrix} 0 & -\mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}.$$

For selfadjoint extensions of the *Laplace* operator this has to vanish for ϕ and ψ in the domain of definition. Consequence for the choice $\psi = \phi$: The sum of the quantum probability currents at the vertex has to vanish. This is the quantum version of the **local** *Kirchhoff law* **at the vertex.**

The domain of a given s.a. extension of the Laplace operator consists of those ψ whose boundary values lie in a given, fixed maximal isotropic subspace $\mathcal{M}$ of $\mathbb{C}^{2n}$.

Boundary conditions and Selfadjointness

Let $\mathcal{M} = \mathcal{M}(A, B)$ be given by the linear relation

$$A\psi(0) + B\psi'(0) = 0$$

with A and B being $n \times n$ matrices.
Theorem: The boundary condition (A, B) defines a selfadjoint Laplace operator $\Delta = \Delta(A, B)$ on the graph $\mathcal{G}$

1. iff $\mathcal{M}(A, B)$ is a maximal isotropic subspace of $\mathbb{C}^{2n}$
2. iff $AB^\dagger$ is selfadjoint and the $n \times 2n$ matrix (A, B) has maximal rank

and then

$$\mathcal{M}(A, B) = \mathcal{M}(A', B')$$

iff there is invertible C with $A' = CA, \; B' = CB$. All maximal isotropic subspaces can be written as $\mathcal{M} = \mathcal{M}(A, B)$.

This approach gives all selfadjoint Laplace operators on the graph and is equivalent to *von Neumann*'s theory of selfadjoint extensions.

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Scattering Theory: Single vertex graphs (Ansatz)

Consider an incoming plane wave with wave vector $\mathbf{k} = \sqrt{E}$ in channel $l \in \mathcal{E}$ (in units where $\hbar = 2m = 1$) superposed with an outgoing plane wave in each channel $j \in \mathcal{E}$ thus giving a solution ψ^l of the stationary Schrödinger equation at energy E,

$$-\Delta\psi^l = E\psi^l$$

of the form

$$\psi_j^l(x) = e^{-\mathrm{i}\mathbf{k}x}\delta_{jl} + S_{jl}(\mathbf{k})e^{\mathrm{i}\mathbf{k}x}$$

and which satisfies the boundary condition. The diagonal parts of the $n \times n$ matrix $S(\mathbf{k})$ give the n reflection amplitudes and the off-diagonal parts the transmission amplitudes.

Scattering Theory: Single vertex graphs (Solution)

Solution

$$S_{A,B}(\mathbf{k}) = -\,(A + \mathrm{i}\mathbf{k}B)^{-1}\,(A - \mathrm{i}\mathbf{k}B)$$

is unitary and satisfies the relations

$$\begin{aligned}
S_{CA,CB}(\mathbf{k}) &= S_{A,B}(\mathbf{k}) && \text{for invertible} \quad C,\\
S_{\bar{A},\bar{B}}(\mathbf{k}) &= S_{A,B}(\mathbf{k})^t && \text{(time reversal)},\\
S_{A,B}(-\mathbf{k}) &= S_{A,B}(\mathbf{k})^{-1} && \text{(hermitian analyticity)},\\
S_{AU,BU}(\mathbf{k}) &= U^{-1} S_{A,B}(\mathbf{k}) U && \\
\Delta(AU, BU) &= U^{-1}\Delta(A,B)U && \text{(gauge covariance)},
\end{aligned}$$

where $\bar{A}$ is the complex conjugate of A, ^{t} denotes transposition and U is any $n \times n$ unitary.

Scattering Theory: Single vertex graphs (S-matrix and Boundary conditions)

$$S_{CA,CB}(\mathbf{k}) = S_{A,B}(\mathbf{k}) \quad \text{for invertible} \quad C,$$

implies that $S_{A,B}(\mathbf{k})$ depends only on the maximal isotropic subspace $\mathcal{M} = \mathcal{M}(A, B)$.

Conversely: The S-matrix at any energy $\mathbf{k}_0^2 = E_0$ uniquely fixes the boundary condition, where A and B may be chosen to be given by

$$A = \frac{1}{2}(S(\mathbf{k}_0) - \mathbb{I}), \quad B = \frac{1}{2\mathrm{i}\mathbf{k}_0}(S(\mathbf{k}_0) + \mathbb{I}).$$

Also

$$S(\mathbf{k}) = ((\mathbf{k} - \mathbf{k}_0)S(\mathbf{k}_0) + (\mathbf{k} + \mathbf{k}_0))^{-1}((\mathbf{k} + \mathbf{k}_0)S(\mathbf{k}_0) + (\mathbf{k} - \mathbf{k}_0)).$$

In addition: Choosing $S(\mathbf{k}_0) = U$ arbitrarily unitary gives all selfadjoint Laplace operators.

Applications in quantum computing?

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Scattering Theory: Single vertex graphs (Consequences)

Consequences

1. There is a one – to – one correspondence between
   a) maximal isotropic subspaces,
   b) $n \times n$ unitaries (see also Arnold),
   c) Laplacians.
2. a) The bound states correspond to poles in $\mathbf{k}$ of $S(\mathbf{k})$ on the positive imaginary axis
   b) The number of bound states ($=$ positive eigenvalues of the corresponding Laplace operator) equals the number of positive eigenvalues of $AB^\dagger$ or equivalently of $\frac{1}{\mathrm{i}}(S(\mathbf{k}_0) - S(\mathbf{k}_0)^\dagger), \quad \mathbf{k}_0 > 0$.
3. The notion *for almost all* boundary conditions makes sense.
4. Choose $U = S(\mathbf{k}_0)$ with non – vanishing entries. Then no matrix element of the resulting single vertex S-matrix vanishes identically.

Scattering Theory: General Graphs

General graphs $\mathcal{G}$ with

1. A set $\mathcal{E}$ of $n = \mid \mathcal{E} \mid$ external lines (=half lines),
2. An additional set $\mathcal{I}$ of $m = \mid \mathcal{I} \mid$ internal lines $i \cong [0_i, a_i]$, i.e. with a set of lengths $\underline{a} = \{a_i\}_{i \in \mathcal{I}}$
3. Function on these intervals: $\psi = \{\psi_j\}$, $j \in \mathcal{E} \cup \mathcal{I}$,
4. Boundary values: $[\psi]$, $[\psi'] \in \mathbb{C}^{|\mathcal{E}|+2|\mathcal{I}|}$,
5. Boundary conditions: $A[\psi] + B[\psi'] = 0$,
6. $A, B = (\mid \mathcal{E} \mid +2 \mid \mathcal{I} \mid) \times (\mid \mathcal{E} \mid +2 \mid \mathcal{I} \mid)$ matrices with (A, B) has maximal rank and $AB^\dagger = BA^\dagger$ thus leading to *local Kirchhoff laws* at each vertex and therefore defining a Laplace operator $\Delta_{A,B,\underline{a}}$
7. Actually (A, B) defines the graph uniquely.

Scattering Theory: General Graphs

Definition of the S-matrix and internal amplitudes α and β for incoming plane wave of momentum $\mathbf{k}$ in channel $l \in \mathcal{E}$:

$$\psi_j^l(x) = \begin{cases} e^{-\mathrm{i}\mathbf{k}x}\delta_{jl} + S_{jl}(\mathbf{k})e^{\mathrm{i}\mathbf{k}x} & \text{for} \quad j \in \mathcal{E} \\ \\ \alpha_{jl}(\mathbf{k})e^{\mathrm{i}\mathbf{k}x} + \beta_{jl}(\mathbf{k})e^{-\mathrm{i}\mathbf{k}x} & \text{for} \quad j \in \mathcal{I} \end{cases}$$

has to satisfy the boundary conditions at each vertex.

Interpretation of α and β: $|\alpha_{jl}(\mathbf{k})|^2 - |\beta_{jl}(\mathbf{k})|^2$ is the quantum probability current on the interior line j.

Scattering Theory: General Graphs

Theorem

:

The quantum version of *Kirchhoff*'s law:

1. $S = S_{A,B,\underline{a}}(\mathbf{k})$ is well defined, continuous and unitary for all *all* $\mathbf{k} > 0$,
2. $S(\mathbf{k})$ is a meromorphic function in $\mathbf{k}$ in the complex plane,
3. In the upper half plane it has at most a finite number of poles which are located on the imaginary semiaxis $\Re e\ k = 0$,

Scattering Theory: General Graphs

More explicitly: There is a matrix representation in the form

$$\begin{pmatrix} S(\mathbf{k}) \\ \alpha(\mathbf{k}) \\ \beta(\mathbf{k}) \end{pmatrix} = -Z(\mathbf{k})^{-1}(A - \mathrm{i}\mathbf{k}B)\begin{pmatrix} \mathbb{I}_{n\times n} \\ 0_{m\times n} \\ 0_{m\times n} \end{pmatrix}$$

with A and B being $(n+2m)\times(n+2m)$ matrices defining the boundary conditions on the space $\mathbb{C}^{n+2m}$ of boundary values (or boundary values of derivatives) at the vertices.
$Z(\mathbf{k})$ is also an $(n+2m)\times(n+2m)$ matrix of the form

$$Z(\mathbf{k}) = Z(\mathbf{k}; A, B, \underline{a}) = A\begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & \mathbb{I} \\ 0 & e^{\mathrm{i}\mathbf{k}\underline{a}} & e^{-\mathrm{i}\mathbf{k}\underline{a}} \end{pmatrix} + \mathrm{i}\mathbf{k}B\begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & -\mathbb{I} \\ 0 & -e^{\mathrm{i}\mathbf{k}\underline{a}} & e^{-\mathrm{i}\mathbf{k}\underline{a}} \end{pmatrix}$$

The two diagonal $m\times m$ matrices $\exp(\pm\mathrm{i}\mathbf{k}\underline{a})$ are given by
$\exp(\pm\mathrm{i}\mathbf{k}\underline{a})_{jk} = \delta_{jk}e^{\pm\mathrm{i}\mathbf{k}a_j}$ for $j,k\in\mathcal{I}$.

Path Sum representation

of the S-matrix

Definition: $\mathcal{W}_{ee'}$ is the set of walks $\mathbf{w}$ from e' to e ($e, e' \in \mathcal{E}$).

Then as a reflection of the quantum superposition principle there is a *Selberg-Gutzwiller* type representation for any S-matrix element

$$S(\mathbf{k})_{ee'} = \sum_{\mathbf{w} \in \mathcal{W}_{ee'}} \mathsf{S}(\mathbf{k}; \mathbf{w})_{ee'} e^{\mathrm{i}\, \mathbf{k}\, \mathrm{length}(\mathbf{w})}$$

The weight factor $\mathsf{S}(\mathbf{k}; \mathbf{w})_{ee'}$ is given as

$$\mathsf{S}(\mathbf{k}; \mathbf{w})_{ee'} = \prod_r S(\mathbf{k}; v(r))_{j_{out}(r), j_{in}(r)}$$

with $S(\mathbf{k}; v)$ being the S-matrix at the vertex v. The $v(r)$ are the vertices visited during the walk $\mathbf{w}$ and $j_{in}(r)$ and $j_{out}(r)$ the lines by which $v(r)$ is entered and left respectively. [1]

[1] Read from right to left

Theorem

For

1. lengths $\{a_i\}_{i\in\mathcal{I}}$ of the intervals, which are linearly independent over the rationals
2. and generic boundary conditions

the metric graph $\mathcal{G}$ and the boundary conditions can be recovered from the knowledge of the scattering matrix

Formulation

of the Traveling Salesman Problem

The Traveling Salesman Problem (TSP):

For given external lines $e, e' \in \mathcal{E}$ find a walk from e' to e of shortest length which visits each vertex of the graph

(i) at least once

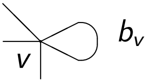
or

(ii) exactly once

TSP is NP complete

For given graph

1. Introduce penalty laps (see Biathlon) at each vertex v (=shooting range) of length b_v



2. Introduce suitable boundary conditions at the vertices
3. resulting in an S-matrix which can be written as

$$S(\mathrm{k}; \underline{a}, \underline{b})_{e,e'} = \sum_{(\underline{n},\underline{m})} S(\mathrm{k}; \underline{n}, \underline{m})_{e,e'} \; e^{\mathrm{ik}\, \underline{n}\cdot\underline{a}} \; e^{\mathrm{ik}\, \underline{m}\cdot\underline{b}}$$

($S(\mathrm{k}; \underline{n}, \underline{m})_{e,e'}$ is the sum of contributions from the walks with $n_i =$ transversals of the line i and $m_v =$ transversals of the lap at v)

The procedure

1. Calculate the scattering matrix by Linear algebra
2. Do Fourier analysis:
   Look only at contributions to $\underline{m} = \underline{1}$, which means
   Each lap is traversed exactly once
   $$\Downarrow$$
   Each vertex is visited at least once!
3. Again do Fourier analysis:
   Among the contributions to $\underline{m} = \underline{1}$ determine
   which non-vanishing contribution $\underline{n}$ has shortest length $\underline{a} \cdot \underline{n}$

Open problem: What is the computing time ?