Graph Theory in Quantum Mechanics and Thermodynamics

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Introduction

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**Homework:** Given the following graph:

How many paths from A to C of length 4 are there? Of length $k$?
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![Graph](image)

How many paths from A to C of length 4 are there? Of length 6? length $k$?
Plan:

- Describe the evolution of physical systems by the Laplace operator.
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- Introduce a combinatorial model to understand such evolution.

Applications: Diffusion of information on social networks, heat diffusion, topology of networks.
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Physical Motivation: Dynamics

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Forces: Gravity from Earth \((-mg)\).
Dynamics: Lagrangian function \(L(q, \dot{q}, t) = \frac{1}{2} m(\dot{q})^2 - mgq\)

- How to find the (classical) trajectory?
  Principle of Minimal Action: The classical trajectory is a critical point for the function

\[
S(q) = \int_{t_0}^{t_1} L(q, \dot{q}, t) \, dt
\]
Theorem (Euler-Lagrange)

*The dynamics is determined by solving the following equation:*

\[
\frac{\partial}{\partial q} \mathcal{L}(q, \dot{q}, t) = \frac{d}{dt} \left( \frac{\partial}{\partial \dot{q}} \mathcal{L}(q, \dot{q}, t) \right)
\]

*The solutions depend on initial conditions. Under nice properties of \( \mathcal{L} \) the solution exists and is unique.*

**Question:** What about systems at a very small scale (e.g. subatomic particles)?

**Answer:** Quantum phenomena are observed!

**Question:** How about systems with millions of interacting particles?

**Answer:** Thermodynamics!
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- Uncertainty principle (Heisenberg)
- Superposition of states (Schrödinger)
Two-slit experiment by Young

Source: Wikipedia.org
The mathematics of QM

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- Configuration space $\mathbb{R}^n \mapsto$ Space of states $\mathcal{H} = L^2(\mathbb{R}^n)$ (states of a quantum particle).
- Classical Measurement $\mapsto$ Self adjoint operators on $\mathcal{H}$.
- Classical evolution $\mapsto$ Schrödinger’s equation.
Schrödinger’s equation

The evolution of a quantum state $\Psi$ is given by the solution of the differential equation

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = \left(-\frac{\hbar^2}{2m} \Delta + V\right) |\Psi\rangle,$$

where $|\Psi\rangle = \Psi(x,t)$ is the state. $\Delta = \sum_{n,i=1}^{\infty} \frac{\partial^2}{\partial x^2}$ is the Laplace operator. $V$ is the classical potential.
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\[ \frac{\partial \Psi(x, t)}{\partial t} = k \Delta \Psi(x, t), \]

where \( k \in \mathbb{R} \).
Challenges

These two are non trivial PDE’s, dependent on the geometry (e.g. metric) and topology (e.g. genus) of the configuration space.
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Challenges

- These two are non trivial PDE’s, dependent on the geometry (e.g. metric) and topology (e.g. genus) of the configuration space.
- Sensitive to boundary conditions.
- Schödinger’s equation is quite sensitive to the choice of potential $V$. 
Proposal: QM and TD on a graph

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- Quantum measurements $\Rightarrow$ Self adjoint $|V| \times |V|$-matrices.
- Quantum evolution $\Rightarrow$ Graph Schrödinger’s equation.
The Graph Laplacian

Definition

If $\Gamma = (V, E)$ is a finite graph, the graph Laplacian $\Delta_\Gamma$ is the $|V| \times |V|$-matrix defined by

$$\Delta_\Gamma(i, j) = \begin{cases} 
| \text{Neighbors of } v_i | & \text{if } i = j \\
-1 & \text{if } i \text{ and } j \text{ are neighbors} \\
0 & \text{otherwise}
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What does $\Delta_{\Gamma}$ do as an operator? Answ: Difference operator

Why is $\Delta_{\Gamma}$ the right discrete Laplacian? Answ: Finite elements second derivative.
Example

For $\Gamma =$

\[
\begin{bmatrix}
1 & -1 & 0 & 0 & 0 \\
-1 & 4 & -1 & -1 & -1 \\
0 & -1 & 1 & 0 & 0 \\
0 & -1 & 0 & 1 & 0 \\
0 & -1 & 0 & 0 & 1
\end{bmatrix}
\]
Example

For $\Gamma =$

Then

$$
\Delta_\Gamma = \begin{bmatrix}
1 & -1 & 0 & 0 & 0 \\
-1 & 4 & -1 & -1 & -1 \\
0 & -1 & 1 & 0 & 0 \\
0 & -1 & 0 & 1 & 0 \\
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\end{bmatrix}.
$$
Graph Schrödinger Equation (GSE)

Definition

The combinatorial evolution of a quantum system on a graph is given by the solutions of

\[ i\hbar \frac{\partial |\psi\rangle}{\partial t} = \left( -\frac{\hbar^2}{2m} \Delta \Gamma + V \right) |\psi\rangle , \]

Theorem (Del Vecchio(2012), Mnev (2016))

When \( V = 0 \) the solution of the GSE exists, is unique and given by

\[ |\psi_{tf}\rangle = e^{i\hbar \left( \frac{1}{2m} \Delta \Gamma + V \right)} |\psi_{t0}\rangle . \]
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*When* \( V = 0 \) *the solution of the GSE exists, is unique and given by*

\[ |\Psi_{t_f}\rangle = e^{i\frac{\hbar(t_f-t_0)\Delta_{\Gamma}}{2m}} |\Psi_{t_0}\rangle \]
The enumerative problem: Main results

The matrix valued function $Z(t) = e^{\frac{i\hbar(t_f - t_0)\Delta r}{2m}}$ is counting something!
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**Definition**

A generalized walk on a graph \( \Gamma \) allows for the particle to stay at a vertex after an edge has been chosen.
The enumerative problem: Main results

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Definition

A generalized walk on a graph \( \Gamma \) allows for the particle to stay at a vertex after an edge has been chosen.

Theorem (Del Vecchio (2012), C-Yu (2017))

The coefficients \( C^k(i, j) \) of the Taylor expansion

\[
Z(t) = \sum_{k=0}^{\infty} \left( \frac{i\hbar}{2m} \right)^k t^k C^k(i, j)
\]

is the number of signed generalized walks of length \( k \) starting at \( i \) and ending \( j \).
The enumerative problem: Main results

This formula has been recently generalized for hypergraphs (higher dimensional generalizations of graphs)
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Theorem (C-, Loeb, Yu (2017))

A similar formula holds for generalized walks on hypergraphs.
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An edge-to-edge generalized walk is the dual of a generalized walk: the particle starts and ends at edges and travels through vertices.
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Definition

An edge-to-edge generalized walk is the dual of a generalized walk: the particle starts and ends at edges and travels through vertices.

Theorem (C-, Loeb, Yu (2017))

The solution of GSE for the space of states $\mathcal{H} = \mathbb{C}^{|V|} \oplus \mathbb{C}^{|E|}$ gives a generating function for the number of edge-to-edge generalized walks.
Summary: QM Versus GQM

Physics

Graph QM

QM

Quantum Particle

point/wave

point/wave

Configuration Space

$\Gamma$

$R$

$N$

States

$|\Psi\rangle \in C$

$|V|$

$|\Psi\rangle \in L^2(R^N)$

Evolve

$i\hbar \frac{\partial}{\partial t} \Psi = -\frac{\hbar}{2m} \Delta \Gamma |\Psi\rangle$

Solution

$\Psi(t) = e^{i\frac{\hbar}{2m} \Delta \Gamma t} \Psi_0$

$\Psi(t) = e^{i\frac{\hbar}{2m} \Delta t} \Psi_0$

The $\Delta$ in each Schrödinger equation is different!!!
**Summary: QM Versus GQM**

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<td>Quantum Particle</td>
<td>point/wave</td>
<td>point/wave</td>
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<tr>
<td>Configuration Space</td>
<td>$\Gamma$</td>
<td>$\mathbb{R}^N$</td>
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<tr>
<td>States</td>
<td>$</td>
<td>\Psi\rangle \in \mathbb{C}^{</td>
</tr>
<tr>
<td>Evolve $\Psi$</td>
<td>$i\hbar \frac{\partial}{\partial t} \Psi = -\frac{\hbar^2}{2m} \Delta_{\Gamma}</td>
<td>\Psi\rangle$</td>
</tr>
<tr>
<td>Solution</td>
<td>$\Psi_t = e^{i\frac{\hbar}{2m} \Delta_{\Gamma} t/\hbar} \Psi_0$</td>
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</tbody>
</table>

*The $\Delta$ in each Schrödinger equation is different!!!
We analyze a Twitter network composed of members of the IGL group, and volunteers. The diffusion of information is modeled by

\[
\frac{\partial \Psi(x, t)}{\partial t} = -\Delta \Psi(x, t),
\]

\[
\mathcal{H} = \mathbb{C}^{|\mathcal{V}|}
\]

\[
\Psi(t) = e^{-\Delta t/\hbar}\Psi_0, \text{ where } \Psi_0 = (1, 0, \ldots, 0)^T
\]
Twitter Simulation
By using the software *Molecular Biology*, we were able to model the (combinatorial) heat diffusion of gallium while melting on a person’s hand.
By using the software *Molecular Biology*, we were able to model the (combinatorial) heat diffusion of gallium while melting on a person’s hand. *Heat Diffusion on Gallium*
Thanks for your attention!
IGL Team members: Sarah Loeb (Grad student), Rodrigo Araiza, Andrew Eberlein, Zhe Hu, Mateo Muro, Leonardo Rodriguez, Michael Toriyama, Boyan Xu, Chengzheng Yu, Yunting Zhang.

Papers and Preprints:

