Graph Theory in Quantum Mechanics and Thermodynamics

Ivan Contreras

University of Illinois at Urbana-Champaign

Beling Lectures
Wesleyan University, Illinois
September , 2017

Introduction

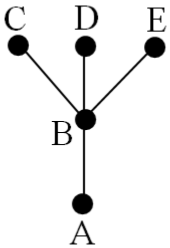
Based on the Illinois Geometry Lab project:
Quantum Mechanics on Graphs and CW-Complexes,
2016-2017.

Introduction

Based on the Illinois Geometry Lab project:
Quantum Mechanics on Graphs and CW-Complexes,
2016-2017.
Homework: Given the following graph:

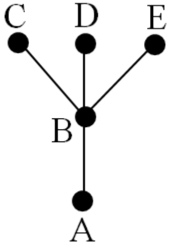
Introduction

Based on the Illinois Geometry Lab project:
Quantum Mechanics on Graphs and CW-Complexes,
2016-2017.
Homework: Given the following graph:



Introduction

Based on the Illinois Geometry Lab project:
Quantum Mechanics on Graphs and CW-Complexes,
2016-2017.
Homework: Given the following graph:



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.

Plan:

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

Plan:

- Describe the evolution of physical systems by the Laplace operator.
- Introduce a combinatorial model to understand such evolution.
- The enumerative problem: Generating function for the number of different types of walks on graphs.

Plan:

- Describe the evolution of physical systems by the Laplace operator.
- Introduce a combinatorial model to understand such evolution.
- The enumerative problem: Generating function for the number of different types of walks on graphs.
- Applications: Diffusion of information on social networks, heat diffusion, topology of networks.

Physical Motivation: Dynamics

Example

Classical Mechanics: A ball thrown from the International Space Station.

Physical Motivation: Dynamics

Example

Classical Mechanics: A ball thrown from the International Space Station.
Forces: Gravity from Earth ($-mg$).

Physical Motivation: Dynamics

Example

Classical Mechanics: A ball thrown from the International Space Station.
Forces: Gravity from Earth ($-mg$).
Dynamics: Lagrangian function $\mathcal{L}(q, \dot{q}, t) = \frac{1}{2}m(\dot{q})^2 - mgq$

- How to find the (classical) trajectory?

Physical Motivation: Dynamics

Example

Classical Mechanics: A ball thrown from the International Space Station.
Forces: Gravity from Earth ($-mg$).
Dynamics: Lagrangian function $\mathcal{L}(q, \dot{q}, t) = \frac{1}{2}m(\dot{q})^2 - mgq$

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

$$S(q) = \int_{t_0}^{t_1} \mathcal{L}(q, \dot{q}, t)\, dt$$

Theorem (Euler-Lagrange)

The dynamics is determined by solving the following equation:

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

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.

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.

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)?

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!

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?

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!

Quantum Mechanics

The usual classical mechanical approach fails to explain phenomena such as:

Quantum Mechanics

The usual classical mechanical approach fails to explain phenomena such as:

- Wave/Particle duality (Planck, de Broglie, Young)

Quantum Mechanics

The usual classical mechanical approach fails to explain phenomena such as:

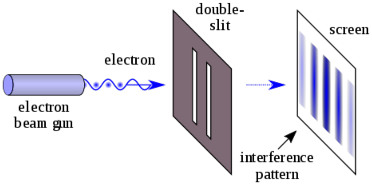
- Wave/Particle duality (Planck, de Broglie, Young)
- Uncertainty principle (Heisenberg)

Quantum Mechanics

The usual classical mechanical approach fails to explain phenomena such as:

- Wave/Particle duality (Planck, de Broglie, Young)
- Uncertainty principle (Heisenberg)
- Superposition of states (Schrödinger)

Two-slit experiment by Young



Source: Wikipedia.org

The mathematics of QM

- Configuration space $\mathbb{R}^n \Longrightarrow$ Space of states $\mathcal{H} = L_2(\mathbb{R}^n)$ (states of a quantum particle).

The mathematics of QM

- Configuration space $\mathbb{R}^n \Longrightarrow$ Space of states $\mathcal{H} = L_2(\mathbb{R}^n)$ (states of a quantum particle).
- Classical Measurement $\Longrightarrow$ Self adjoint operators on $\mathcal{H}$.

The mathematics of QM

- Configuration space $\mathbb{R}^n \Longrightarrow$ Space of states $\mathcal{H} = L_2(\mathbb{R}^n)$ (states of a quantum particle).
- Classical Measurement $\Longrightarrow$ Self adjoint operators on $\mathcal{H}$.
- Classical evolution $\Longrightarrow$ Schrödinger's equation.

Schrödinger's equation

The evolution of a quantum state Ψ is given by the solution of the differential equation

Schrödinger's equation

The evolution of a quantum state Ψ is given by the solution of the differential equation

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

where

- $\left|\Psi\right\rangle = \Psi(x,t)$ is the state.

Schrödinger's equation

The evolution of a quantum state Ψ is given by the solution of the differential equation

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

where

- $\left|\Psi\right\rangle = \Psi(x,t)$ is the state.
- $\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$ is the *Laplace operator*.

Schrödinger's equation

The evolution of a quantum state Ψ is given by the solution of the differential equation

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

where

- $|\Psi\rangle = \Psi(x,t)$ is the state.
- $\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$ is the *Laplace operator*.
- V is the classical potential.

Thermodynamics and Heat equation

A similar equation (with similar symbols!)describe the thermodynamics of a system, i.e. the distribution of heat of a region over time.

Thermodynamics and Heat equation

A similar equation (with similar symbols!)describe the thermodynamics of a system, i.e. the distribution of heat of a region over time.

$$\frac{\partial \Psi(x,t)}{\partial t} = k \Delta \Psi(x,t),$$

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.

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.

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

- Configuration space $\mathbb{R}^n \Longrightarrow$ Finite graph $\Gamma = (V, E)$.

Proposal: QM and TD on a graph

- Configuration space $\mathbb{R}^n \implies$ Finite graph $\Gamma = (V, E)$.
- Space of quantum states $\mathcal{H} = L_2(\mathbb{R}^n)$ (states of a quantum particle on $\mathbb{R}^n$) $\implies \mathcal{H}_\Gamma = \mathbb{C}^{|V|}$ (linear functions on Γ)

Proposal: QM and TD on a graph

- Configuration space $\mathbb{R}^n \Longrightarrow$ Finite graph $\Gamma = (V, E)$.
- Space of quantum states $\mathcal{H} = L_2(\mathbb{R}^n)$ (states of a quantum particle on $\mathbb{R}^n$) $\Longrightarrow \mathcal{H}_\Gamma = \mathbb{C}^{|V|}$ (linear functions on Γ)
- Quantum measurements $\Longrightarrow$ Self adjoint $|V| \times |V|$-matrices.

Proposal: QM and TD on a graph

- Configuration space $\mathbb{R}^n \implies$ Finite graph $\Gamma = (V, E)$.
- Space of quantum states $\mathcal{H} = L_2(\mathbb{R}^n)$ (states of a quantum particle on $\mathbb{R}^n$) $\implies \mathcal{H}_\Gamma = \mathbb{C}^{|V|}$ (linear functions on Γ)
- Quantum measurements $\implies$ Self adjoint $|V| \times |V|$-matrices.
- Quantum evolution $\implies$ Graph Schrödinger's equation.

The Graph Laplacian

Definition

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

$$\Delta_\Gamma(i,j) = \begin{cases} |\text{ Neighbors of } v_i| & \text{if } i = j \\ -1 & \text{if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

The Graph Laplacian

Definition

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

$$\Delta_\Gamma(i,j) = \begin{cases} |\text{ Neighbors of } v_i| & \text{if } i = j \\ -1 & \text{if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

Δ_Γ enjoys similar properties as Δ: self adjoint, non negative definite.

The Graph Laplacian

Definition

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

$$\Delta_\Gamma(i,j) = \begin{cases} |\text{ Neighbors of } v_i| & \text{if } i = j \\ -1 & \text{if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

Δ_Γ enjoys similar properties as Δ: self adjoint, non negative definite.
What does Δ_Γ do as an operator?

The Graph Laplacian

Definition

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

$$\Delta_\Gamma(i,j) = \begin{cases} |\text{ Neighbors of } v_i| & \text{if } i = j \\ -1 & \text{if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

Δ_Γ enjoys similar properties as Δ: self adjoint, non negative definite.

What does Δ_Γ do as an operator? Answ: Difference operator

The Graph Laplacian

Definition

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

$$\Delta_\Gamma(i,j) = \begin{cases} |\text{ Neighbors of } v_i| & \text{if } i = j \\ -1 & \text{if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

Δ_Γ enjoys similar properties as Δ: self adjoint, non negative definite.

What does Δ_Γ do as an operator? Answ: Difference operator

Why is Δ_Γ the right discrete Laplacian?

The Graph Laplacian

Definition

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

$$\Delta_\Gamma(i,j) = \begin{cases} |\text{ Neighbors of } v_i| & \text{if } i = j \\ -1 & \text{if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases}$$

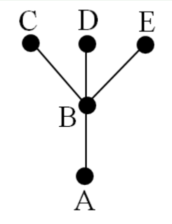
Δ_Γ enjoys similar properties as Δ: self adjoint, non negative definite.

What does Δ_Γ do as an operator? Answ: Difference operator

Why is Δ_Γ the right discrete Laplacian? Answ: Finite elements second derivative.

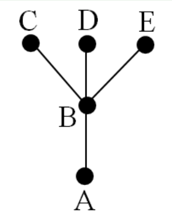
Example

For $\Gamma =$



Example

For $\Gamma =$



Then

$$\Delta_\Gamma = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & -1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 \end{bmatrix}.$$

Graph Schrödinger Equation (GSE)

Definition

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

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

Graph Schrödinger Equation (GSE)

Definition

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

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

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

When $V = 0$ the solution of the GSE exists, is unique and given by

$$\left|\Psi_{t_f}\right\rangle = e^{\frac{i\hbar(t_f - t_0)\Delta_\Gamma}{2m}}\left|\Psi_{t_0}\right\rangle$$

The enumerative problem: Main results

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

The enumerative problem: Main results

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

Definition

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

The enumerative problem: Main results

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

Definition

A generalized walk on a graph Γ 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

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

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)

The enumerative problem: Main results

This formula has been recently generalized for hypergraphs (higher dimensional generalizations of graphs)

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

A similar formula holds for generalized walks on hypergraphs.

The enumerative problem: Main results

This formula has been recently generalized for hypergraphs (higher dimensional generalizations of graphs)

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

A similar formula holds for generalized walks on hypergraphs.

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.

The enumerative problem: Main results

This formula has been recently generalized for hypergraphs (higher dimensional generalizations of graphs)

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

A similar formula holds for generalized walks on hypergraphs.

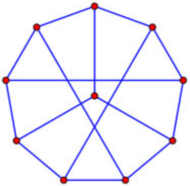
Definition

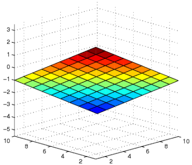
An edge-to-edge generalized walk is the *dual* of a generalized walk: the particle starts and ends at edges and travels through vertices.

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

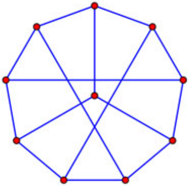
The solution of GSE for the space of states $\mathcal{H} = \mathbb{C}^{|V|} \oplus \mathbb{C}^{|E|}$ gives a generating function for the number of edge-to-edge generalized walks.

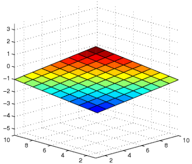
Summary: QM Versus GQM





Summary: QM Versus GQM

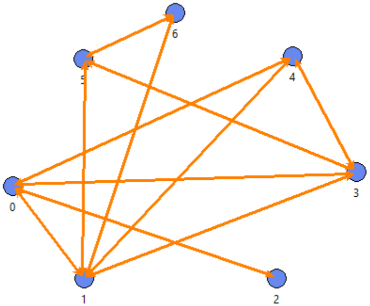




Physics	Graph QM	QM
Quantum Particle	point/wave	point/wave
Configuration Space	Γ	$\mathbb{R}^N$
States	$\|\Psi\rangle \in \mathbb{C}^{\|V\|}$	$\|\Psi\rangle \in L^2(\mathbb{R}^N)$
Evolve Ψ	$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\Delta_\Gamma \|\Psi\rangle$	$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\Delta \|\Psi\rangle$
Solution	$\Psi_t = e^{\frac{i\hbar}{2m}\Delta_\Gamma t/\hbar}\Psi_0$	$\Psi_t = e^{i\frac{\hbar}{2m}\Delta t/\hbar}\Psi_0$

- The Δ in each Schrödinger equation is different!!!

Graph Thermodynamics: Social Experiment on Twitter



- We analyze a Twitter network composed of members of the IGL group, and volunteers.
- The diffusion of information is modeled by

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

- $\mathcal{H} = \mathbb{C}^{|V|}$
- $\Psi(t) = e^{-\Delta t/\hbar}\Psi_0$, where $\Psi_0 = (1, 0, \ldots, 0)^T$

Twitter Simulation

Twitter Simulation

Graph Thermodynamics: Melting of Gallium

By using the software *Molecular Biology*, we were able to model the (combinatorial) heat diffusion of gallium while melting on a person's hand.

Graph Thermodynamics: Melting of Gallium

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!

Acknowledgements and References

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:

- C. Yu, *Super-Walk Formulae for Even and Odd Laplacians in Finite Graphs* , by Chengzheng Yu, Rose-Hulman Institute of Technology Mathematics Journal, Volume 18, No. 1 (2017).
- I. Contreras and B. Xu, *The Graph Laplacian and Morse Inequalities*,arXiv: 1704.08354 (2017).
- I. Contreras, S. Loeb and C. Yu, *Hyperwalk Formulae for Even and Odd Laplacians in Finite CW-Hypergraphs*, arXiv:1708.07995 (2017).