The Mathematics of Quantum Mechanics and Networks

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A little story

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It is a win-win game!

Playing the game

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- **Answer:** It's like a piñata party!

Quantum Mechanics

- Piñata: Nucleus

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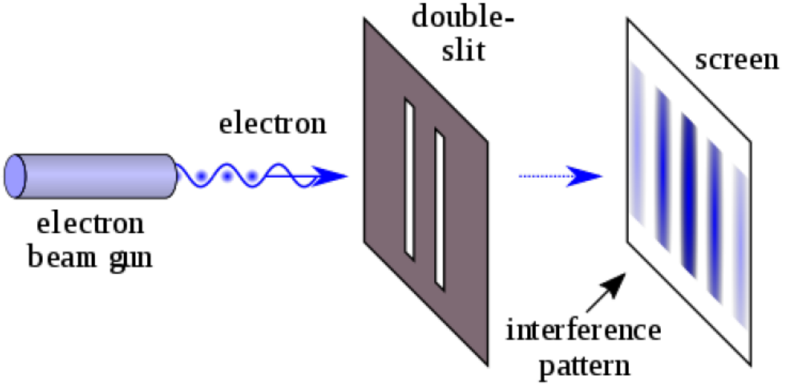
- **Duality:** A particle behaves both as a particle and as a wave.

Experimental Evidence



Mathematical Formulation of QM

Definition (The Schrödinger Equation of a free particle)

For a quantum state, $|\Psi(t)\rangle$, the **Schrödinger Equation** is given by

$$\frac{\partial\,|\Psi(t)\rangle}{\partial t} = i\hbar\Delta\,|\psi(t)\rangle$$

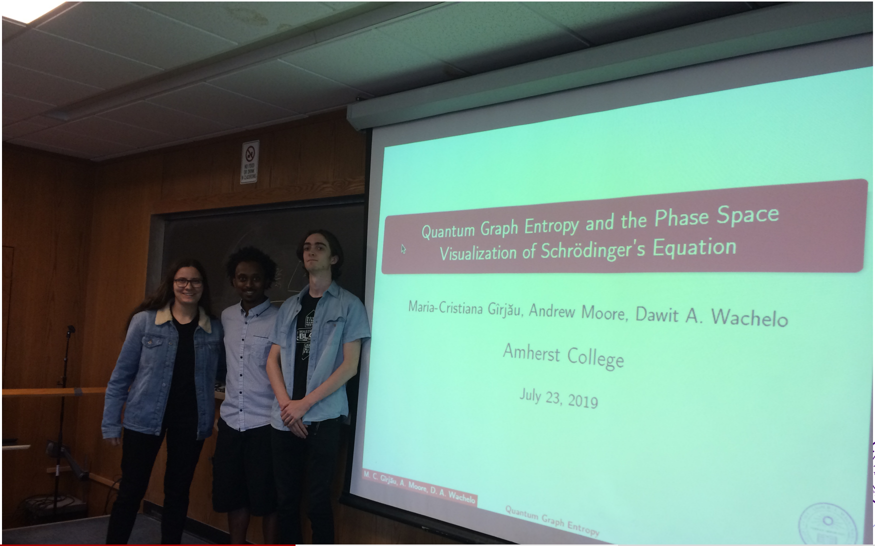
where Δ is the **Laplacian Operator**

$$\Delta = \sum_{i}^{n} \frac{\partial^2}{\partial x_i^2}$$

- The space of quantum states is huge (an infinite dimensional Hilbert space).
- The solutions depend on initial conditions, and the shape of the space

Our Summer Research

THE TEAM: Kitty Girjau, Andrew Moore, Andrew Rosevear, Andrew Tawfeek, Matt Sanders, Dawit Wachelo



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- The Laplace operator becomes a matrix!
- The study of the geometry of the configuration space becomes much simpler.
- We want to relate the solutions of this equation and the complexity of the graph.

Spectral Graph Theory

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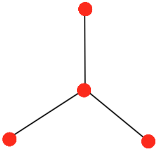
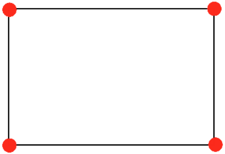
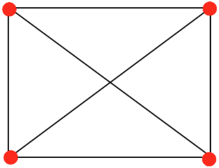






$$\begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

Definition (The Laplacian Matrix)

Given the **adjacency matrix, A**, and the **degree matrix, D**, for a given graph Γ, the **Laplacian**, $\Delta(\Gamma)$ of the graph is defined as a graph operator that is represented as a symmetric, non-invertible matrix with non-negative diagonal elements and whose rows and columns sum to zero:

$$\Delta = D - A$$

Example (for K_4):

$$\begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix}$$

Von Neumann Entropy of Graphs

Definition (The Von Neumann Graph Entropy (VNGE))

Given a Laplacian, Δ, for a graph Γ, the VNGE of Γ is given as

$$S(\Gamma) = -\sum_i \lambda_i \log_2 \lambda_i$$

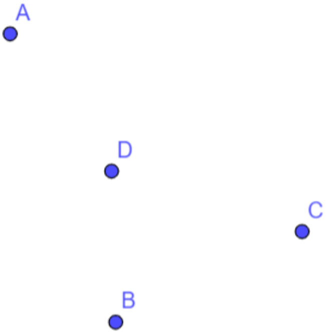
where λ_i are the nonzero eigenvalues of Δ.

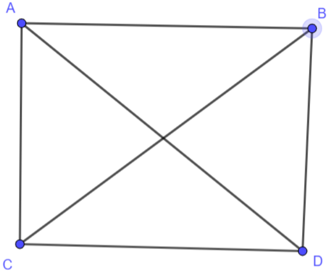
Understanding Von Neumann Entropy

Informally, entropy is a measure of the disorder within a system.

Information entropy (**Shannon**) vs **Quantum entropy** (**Von Neumann**)

Although an exact interpretation of the Von Neumann entropy is still an open question, it is a rough measure of the **complexity** of a graph.





Definition (The Discrete Schrödinger Equation)

Given a graph, Γ, and a quantum state, $|\Psi(t)\rangle$, the **Discrete Schrödinger Equation** is given by

$$\frac{\partial |\Psi(t)\rangle}{\partial t} = i\Delta |\psi(t)\rangle$$

where Δ is the **Graph Laplacian Matrix**.

Main Results

- We developed a polynomial approximation of the graph entropy.

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- We studied the geometry of the solutions of the Discrete Schrödinger Equation.
- There is a connection between the linear algebra of the graph Laplacian and the shape of the graph (graph topology).

Future Directions

* Build a rigorous link between entropy and the solutions of the Discrete Schrödinger Equation.

* Find a general formula for the entropy of the gluing of two graphs.

* Explore further the link between quantum mechanics and the shape of graphs.

Thank You!

Thanks for your attention!