Thesis Proposal:
Adapting Particle Transport Monte Carlo Code to Solve the Simple 1D Time Independent Schrodinger Equation

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Introduction

- Ways to solve the 1D time independent Schrodinger equation

1) Analytic Solution

2) Deterministic Numerical Solution
   - Finite difference method
   - Inverse power method

Topic

- Ways to solve the 1D time independent Schrodinger equation

3) Probabilistic Monte Carlo Solution

   - Specifically a Particle Transport Monte Carlo Solution

Idea

- The following differential equations have the same form.

< 1D time independent Schrödinger equation >

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

< Steady state neutron diffusion equation >

$$-D\frac{d^2}{dx^2}\phi(x) + \Sigma_a\phi(x) = \frac{1}{k}\nu\Sigma_f\phi(x)$$

($\phi(x)$: neutron flux, D: diffusion coefficient, Σ_a: macroscopic absorption cross section,
K: multiplication factor of reactor, Σ_f: macroscopic fission cross section,
ν: average number of neutrons released per fission)

Idea

- The particle transport Monte Carlo code already exists for neutron diffusion.

  ex) MCNP (Monte Carlo N-Particle)

- We can intrepret the result of the Monte Carlo simulation as the solution of the Schrodinger equation.

Importance

- The Monte Carlo method is highly effective for solving problems with **complicated internal geometries.**
- Existing particle transport codes (MCNP, OpenMC, etc.) have been developed and validated in nuclear engineering. **Adapting these codes allows for efficient reuse of mature algorithms** and demonstrates their versatility in addressing new problems, such as quantum mechanics.
- While Quantum Monte Carlo (QMC) methods are well-established for solving the Schrödinger equation, the direct adaptation of particle transport Monte Carlo codes for quantum problems remains **a relatively unexplored approach.**

To Do List

1) Study Monte Carlo particle transport method
2) Implement code
3) Interpret to Schrodinger Equation solution
4) Add more quantum effects to code
5) Apply to more complex situations
   - Various potentials
   - Higher dimensions
   - Different systems (atoms, inside of materials, etc.)

Resources and Tools

- Alex F Bielajew . (2020). *Fundamentals of the Monte Carlo method for neutral and charged particle transport*.
- Brown, F. B. (n.d.). *FUNDAMENTALS OF MONTE CARLO PARTICLE TRANSPORT*. Lecture.
- Leppänen, J. (2007). *Development of a new Monte Carlo Reactor Physics Code* (thesis). *Development of a new Monte Carlo reactor physics code*. VTT, Espoo.
- Shentu, J., Yun, S.-H., & Cho, N.-Z. (2007). A Monte Carlo method for solving heat conduction problems with complicated geometry. *Nuclear Engineering and Technology*, *39*(3), 214. https://doi.org/10.5516/net.2007.39.3.207
- The MCNP code website: https://mcnp.lanl.gov