Capstone Project Review #2

(Project Requirements Specification and Literature Survey)

Comparison of classical Monte Carlo and QMC of 2D and 3D lattice for Energy minimization

Project Title : Quantum Monte Carlo Algorithm

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Monte Carlo Simulation of a 2D/3D Electron Lattice for Energy Minimization

The Ising model is a well-established framework in statistical physics used to study magnetic materials. In this study, we apply the model to a **finite 2D/3D electron lattice**, where each electron is represented as a spin variable . The objective is to understand how the system evolves toward an energy-minimized state using Monte Carlo and QMC simulations.

The steps involved in the process of energy minimization

- **The Ising Model Hamiltonian**

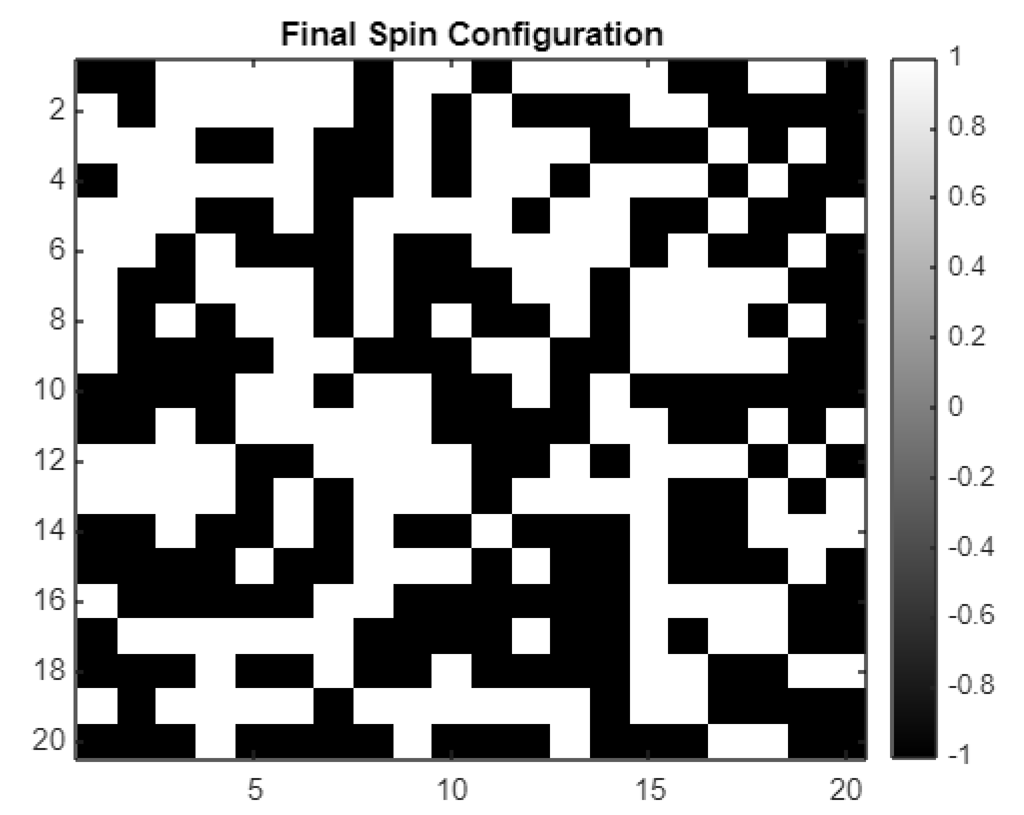
  The total energy of the system is given by the Hamiltonian:

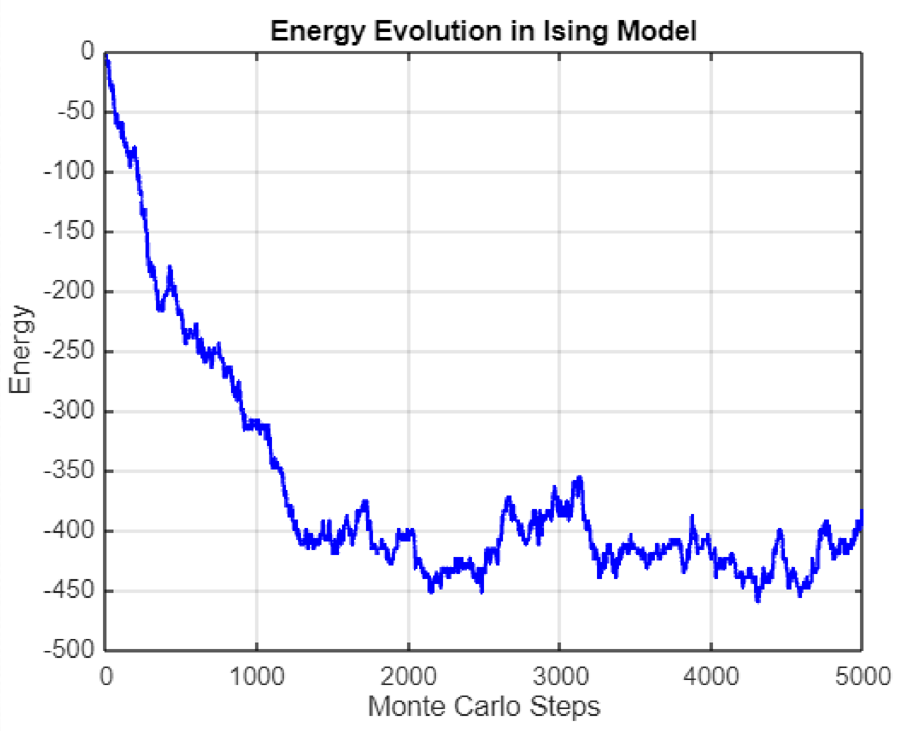
$$H = -J \sum_{\langle i,j \rangle} S_i S_j$$

- **Monte Carlo Algorithm (Metropolis-Hastings) :** Select a **random site** and compute the energy change due to flipping the spin.

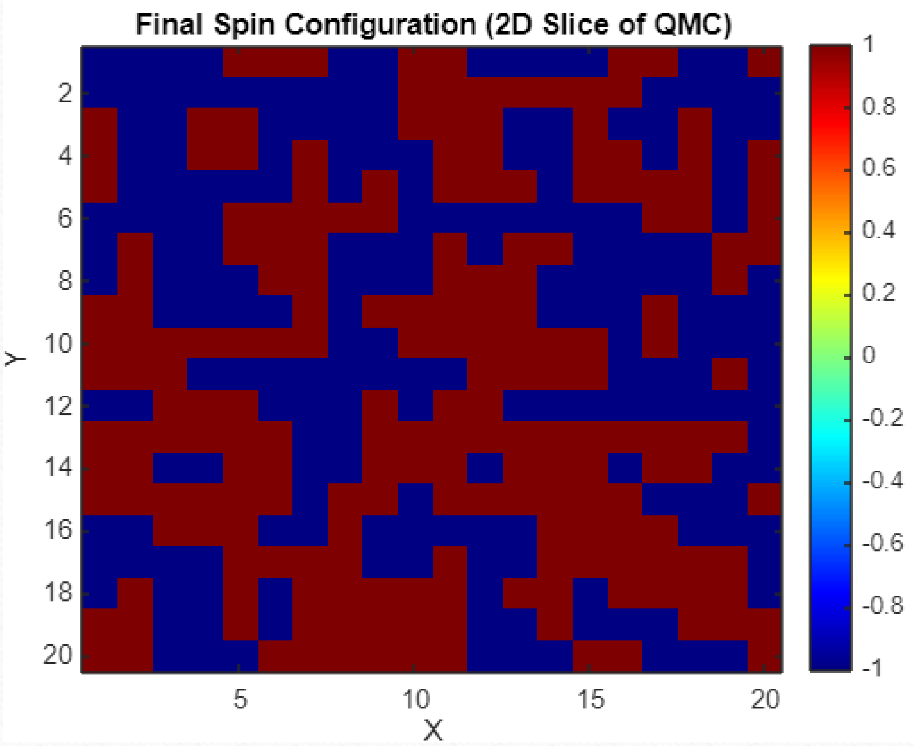
  Accept the flip **if energy decreases H>0 ;** or with probability : $P = e^{-\Delta H / k_B T}$
- Repeat the process over many Monte Carlo steps
- A **heatmap of spin flips** reveals the most unstable regions of the lattice.
- Regions with **high flip activity** correspond to electrons that contribute significantly to energy relaxation.

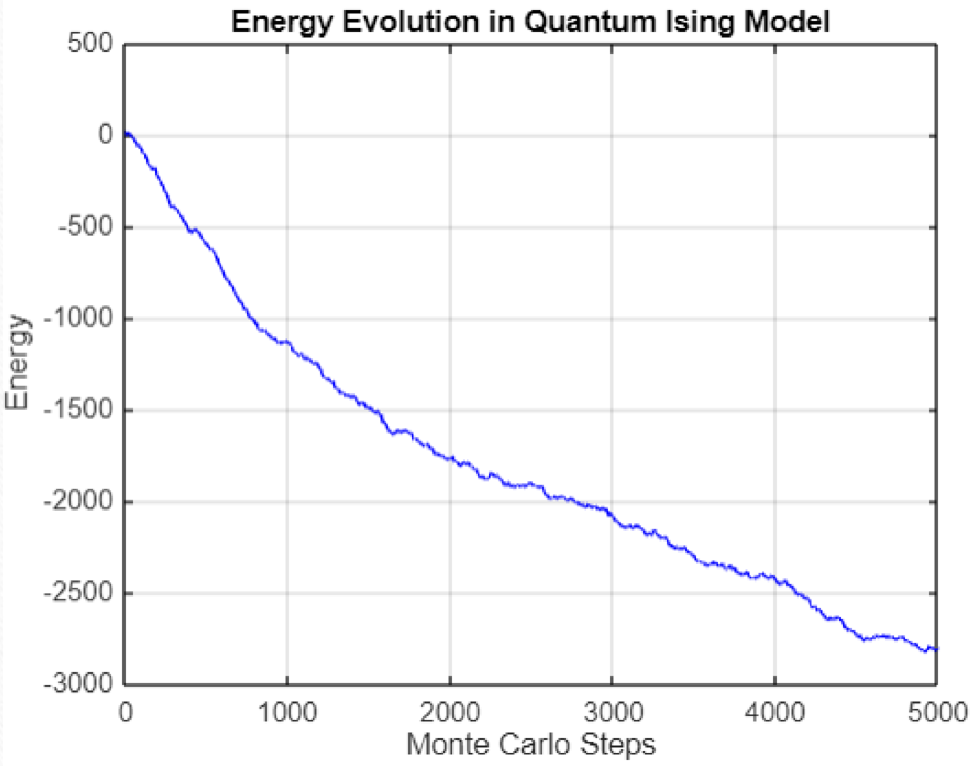
2D Ising model using Monte carlo



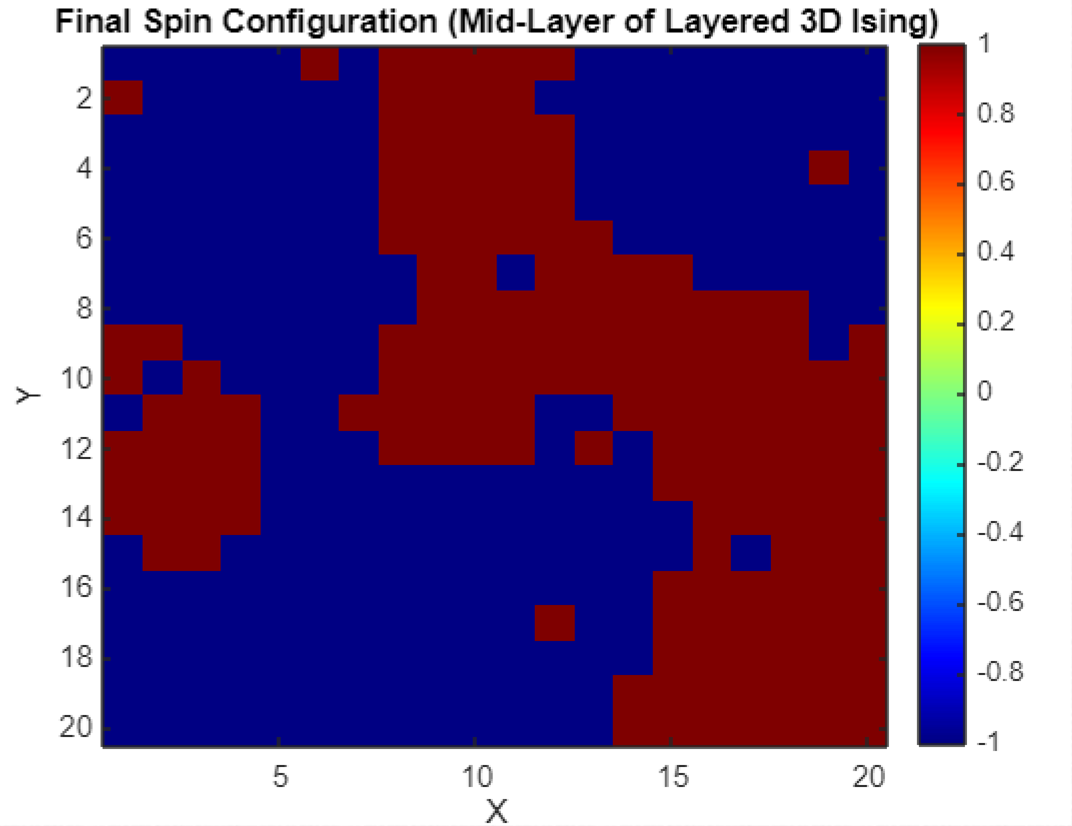


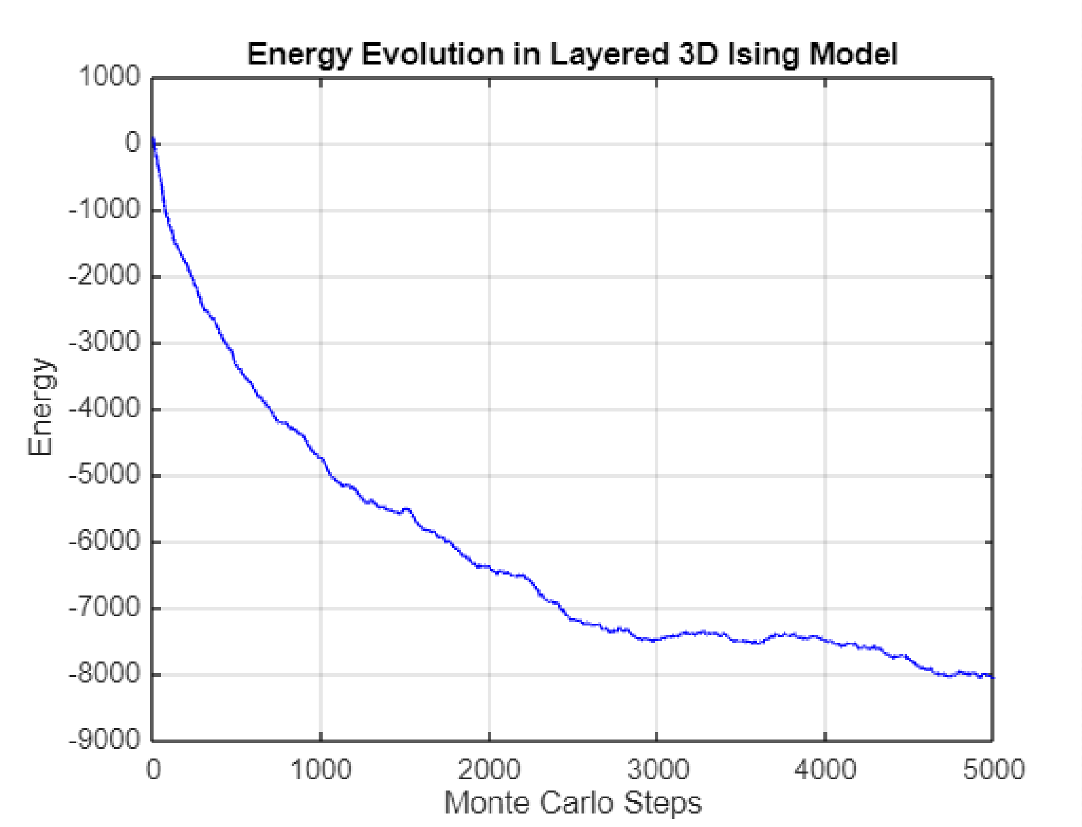
2D Ising model using Quantum monte carlo



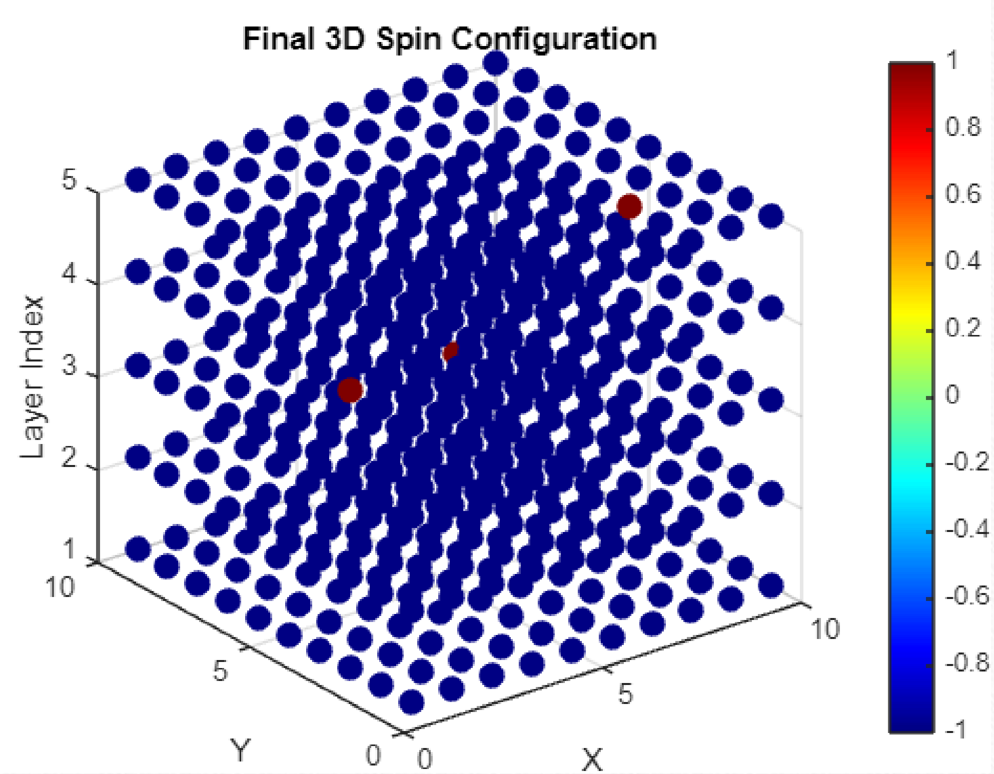


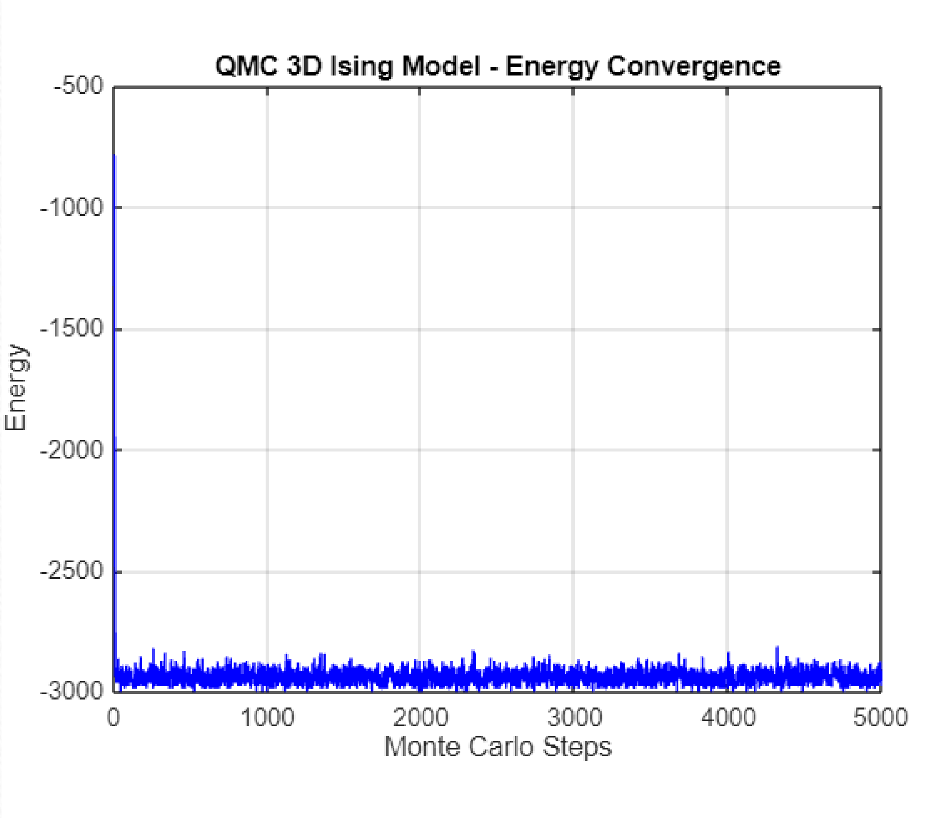
2D stacked 3D lattice Ising model for MC





3D ising model using QMC with Markov chain





Differences of the dimensional analysis

Feature	2D Classical Ising Model	2D Quantum Ising Model	3D Classical Ising Model	3D Quantum Ising Model
Lattice Type	2D square grid	2D square grid with Trotter layers	3D cubic lattice	3D cubic lattice with quantum fluctuations
Algorithm Used	Metropolis-Hastings (MC)	Metropolis-Hastings + Suzuki-Trotter (QMC)	Metropolis-Hastings (MC)	Metropolis-Hastings + Suzuki-Trotter (QMC)
Energy Function	$H = -J \sum S_i S_j$	$H = -J \sum S_i S_j - \Gamma \sum S_i^x$	$H = -J \sum S_i S_j$	$H = -J \sum S_i S_j - \Gamma \sum S_i^x$
Energy Conversion Rate	Fast stabilization	Slower due to quantum fluctuations	Slower than 2D due to more interactions	Slowest due to both quantum effects and 3D interactions
Final Energy	Relatively low (stable)	Lower due to quantum tunneling	Higher due to 3D interactions	Lowest due to both tunneling and 3D stability