VariationalMonteCarlo-Helium

Overview

This repository contains a computational study of the helium atom using the Variational Monte Carlo (VMC) method. The project aims to estimate the lowest energy states of helium by applying the principles of quantum mechanics and Monte Carlo integration.

Theoretical Background

The Variational Monte Carlo method is a stochastic technique used to estimate the ground state energies of quantum systems. In this project, we utilize a trial wave function and adjust its parameters to minimize the energy expectation value, which, according to the variational principle, should not be lower than the system's ground state energy.

Features

- **VMC Algorithm Implementation**: Python implementation of the VMC method tailored for the helium atom.
- **Parameter Optimization**: Scripts for optimizing the variational parameters to achieve minimal energy configurations.
- **Data Visualization**: Plots and visual representations of the energy states and convergence behaviors.

Getting Started

To run the simulations and analyze the results, follow these steps:

1. Clone this repository:

```
git clone https://github.com/yourusername/VariationalMonteCarlo-Helium.git
```

2. Navigate to the repository directory:

```
cd VariationalMonteCarlo-Helium
```

3. Install required dependencies:

```
pip install -r requirements.txt
```
4. Run the main script:
```
python vmc_helium.py
```

Results

The main outcomes of this project are:

- Calculation of the energy expectation values for different trial wave functions.
- Optimization of variational parameters to approach the theoretical ground state energy of helium.