HartreeSlaterAnalysis

Overview

This repository is dedicated to exploring and analyzing quantum chemical methods, focusing on the Hartree product and Slater determinants. These foundational techniques are essential for constructing wave functions in multi-electron systems, offering insights into electron interactions and the properties of atoms and molecules.

Contents

- **Hartree Product Analysis**: Detailed exploration of the Hartree product approach, including its mathematical formulation and applications in simplifying the complexity of electron interactions.
- **Slater Determinant Exercises**: Analytical exercises that employ Slater determinants to model wave functions for atoms, showcasing the role of antisymmetry in quantum chemistry.
- **Basis Sets Overview**: Discussion on various basis sets used in quantum chemistry computations, with examples demonstrating their applications and implications on computational efficiency and accuracy.

Learning Outcomes

- Understand the approximation and implications of using the Hartree product in quantum chemistry.
- Gain practical experience with the construction and implications of Slater determinants in describing electron configurations.
- Explore the diversity of basis sets and their role in the accurate depiction of atomic and molecular systems.

Tools and Technologies

- Jupyter Notebooks: Interactive Python notebooks providing step-by-step explanations and live computations.
- Quantum Chemistry Software: Illustrations on how to apply these concepts using popular quantum chemistry software tools.