Master Thesis Project: Accelerate Auxiliary-Field Quantum Monte Carlo Simulation for Quantum Chemistry

One of the central tasks in Quantum Chemistry is accurately determining the ground state of the electronic Hamiltonian. Among the various computational methods for this problem, Auxiliary-Field Monte Carlo (AFQMC) approach [1,2] has gained increasing attention, due to its balance of accuracy and compuational efficiency.

Despite various algorithmic advances for AFQMC, algorithms to accelerate walker propagation are scarce, which however dominates the overall cost of simulation. This project aims to accelerate the walker propagation step with a novel techique.

[1] *Auxiliary-Field Quantum Monte Carlo for Correlated Electron Systems*. (Forschungszentrum, Zentralbibliothek, Jülich, 2013).

[2] Lee, J., Pham, H. Q. & Reichman, D. R. Twenty Years of Auxiliary-Field Quantum Monte Carlo in Quantum Chemistry: An Overview and Assessment on Main Group Chemistry and Bond-Breaking. *J. Chem. Theory Comput.* **18**, 7024–7042 (2022).

Preferable Qualifications:

- Strong programming skills
- Proficiency in quantum physics or quantum chemistry
- High level of self-motivation

Project Expectation:

- This project is expected to lead to a publication.

Application Materials:

- CV – Please highlight relevant skills, courses or experience. Include a GitHub link if available.
- Academic Transcript

Contact:

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