Monte Carlo Techniques

Quantum Monte Carlo (QMC) methods solve the Schrödinger Equation by casting it as an integral and evaluating it through stochastic sampling.

\[ \hat{H} \psi = E \psi \]

Application of QMC

Description of the physical properties of the microscopic systems with a finite number of particles: nuclei, atoms and molecules, isolated or confined inside of molecular complexes.

Parallellism

Quantum Monte Carlo:
- Computationally expensive
- Well suited to parallelization (Higher sampling implies higher statistic)

Parallellization in CPU or in GPU?

GPU vs CPU

• CPU:
  - Up to 8 processors
  - Optimized for sequential serial processing

• GPU:
  - Up to hundreds of light processors
  - Specialized for highly parallel computation

Some Examples

H atom Ground State Calculation with QMC Variational

Morse Potential Calculation with QMC Path Integral

Future Work:

- QMC Variational for Many electrons atoms
- Diffusion Monte Carlo (DMC) for fermionic systems

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References