Dissertation Defense: Improved Trial Wave Functions for Quantum Monte Carlo Calculations of Nuclear Systems and Their Applications

Cody L. Petrie
Advisor: Kevin Schmidt

Arizona State University

June 8, 2018

Outline

Outline

Story: Why do we need to have a good trial wave function? Here are some options to improve the wave function. Here are the results we have gotten including some applications of the wave function.

- Methods to solve the nuclear problem and why we use QMC
  - VMC June 15
  - DMC/AFDMC June 15
- Trial wave function and why it's so important
  - Slater Dets (and Pfaffians) June 15
  - Jastrow and linear correlations June 15
  - Quadratic correlations June 30
    - Results June 30
- Other correlations
  - Exponential correlations June 30
  - Ale's correlations and T^2 fix July 15
- Application to α-clustering July 15
  - Stefano's original results July 15
  - Results with quadratic correlations July 15

Nuclear Many Body Problem

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int \Psi^*(\boldsymbol{R}) H \Psi(\boldsymbol{R}) d\boldsymbol{R}$$

$$H = \sum_{i=1}^{A} \frac{\boldsymbol{p}^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \dots$$

- There are a number of ways to solve this problem.
  - QCD
    - Lattice QCD
  - No-core shell model
  - Coupled-cluster
  - Self consistent Green's function method
  - Quantum Monte Carlo

Should I have a slide for each method or should I have some popup information about each and just describe them here?
Can they be clumped into different styles and talked about together on slides?