

# FYS-4411: Computational Physics II

## Project 2

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May 13, 2015

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## 1 Introduction

## 2 Theory

- (a) brute force Metropolis Sampling/simple wavefunction
  - (b) Closed form expression Helium Simple, Cusp conditions
  - (c) Introduce importance sampling and blocking
  - (d) Onebody density, with and without Jastrow
  - (e) Vary energy using conjugate gradient method, or similar method to find best  $\beta$ .  
Replace hydrogen-like single particle wave function with 3-21G basis
- (a) Function to calculate Slater Determinant, spin and derivatives of Jastrow factor
  - (b) Compute one-body stuff
- (a) Compute the expectation value of  $\langle \hat{H} \rangle$  vary  $R$  and  $\beta$
  - (b) Using optimal  $R$  and  $\beta$  calculate average  $r_{12}$
  - (c) Try the wavefunction with subtraction instead
  - (d) Estimate binding energy for  $He_2$  and  $Be_2$

### 3 Results

1. (a) brute force Metropolis Sampling/simple wavefunction
  - i. Energy Minimum
  - ii. Mean  $r_{12}$
  - iii. Variance vs cycles
- (b) Closed form expression Helium Simple
  - i. Compare CPU time vs non-closed form
- (c) Introduce importance sampling and blocking
  - i. Study dependence on  $\delta t$  compare with results without importance sampling
  - ii. blocking as statistical analysis
- (d) Onebody density, with and without Jastrow
  - i. One body density with and without Jastrow, compare with pure hydrogenic wave functions
- (e) Vary energy using conjugate gradient method, or similar method to find best  $\beta$ . Replace hydrogen-like single particle wave function with 3-21G basis
  - i. Study dependence on  $\delta t$  compare with results without importance sampling
  - ii. blocking as statistical analysis
2. (a) Compute ground state energy for Neon and Beryllium: Include Parallized code, blocking, importance sampling, energy minimization using gradient conjugate method, 3-12G basis set
- (b) Compute one body densities
3. (a) Plot  $E_{min}$  as a function of  $\mathbf{R}$
- (b) Compute  $\langle r_{12} \rangle$
- (c) Repeat two previous with subtracting the wavefunctions

### 4 Discussion

1. (a) brute force Metropolis Sampling/simple wavefunction
  - i. Physical interpretation of  $\alpha$
- (b) Closed form expression Helium Simple
- (c) Introduce importance sampling
  - i. Study dependence on  $\delta t$  compare with results without importance sampling
- (d) Onebody density, with and without Jastrow
  - i. Discuss with regards to pure hydrogenic wave functions, importance of correlations introduced by Jastrow factor
- (e) Vary energy using conjugate gradient method, or similar method to find best  $\beta$ . Replace hydrogen-like single particle wave function with 3-21G basis
  - i. Study dependence on  $\delta t$  compare with results without importance sampling

- ii. blocking as statistical analysis
- 2. (a) Discuss the same as 1c for neon and beryllium  
(b) Discuss the same as 1d for neon and beryllium
- 3. (a) Comment on  $\langle r_{12} \rangle$   
(b) Comment on subtracting the wavefunctions

## References