FYS-4411: Computational Physics II
Project 2

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   (e) Vary energy using conjugate gradient method, or similar method to find best β. Replace hydrogen-like single particle wave function with 3-21G basis
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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 $E_m in$ 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 α
   (b) Closed form expression Helium Simple
   (c) Introduce importance sampling
    i. Study dependence on δt 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 β. Replace hydrogen-like single particle wave function with 3-21G basis
    i. Study dependence on δt 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