Report 5: Quantum Monte Carlo

Git: https://github.com/simonblaue/MCP-Ex5.git

Simon BLAUE

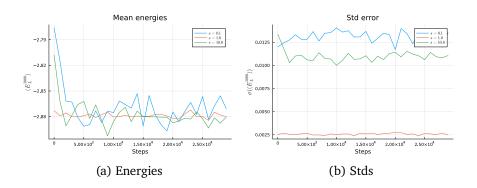
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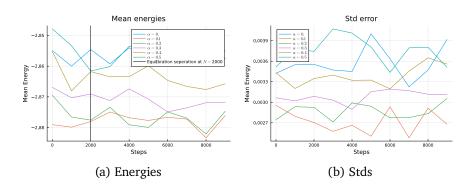
Instructor: Prof. Dr. S. Schumann Tutors: Dr. E. Bothmann, M. Knobbe

1 Variational Monte Carlo simulation of a Helium atom

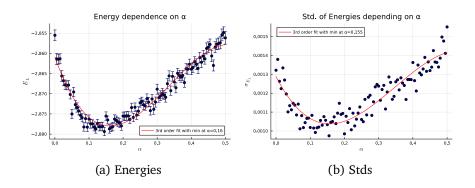
1.1 Investigate stepsize s



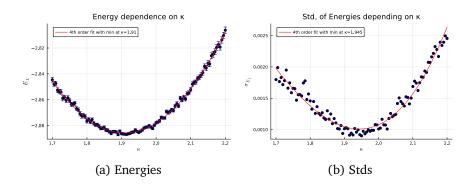
1.2 Approximating equilibration time



1.3 Investigate variational parameter α



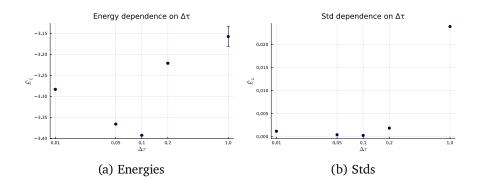
1.4 Investigate variational Parameter κ



1.5 Optimizing parameters α , β and κ

Strange stuff happens, optimizing for minimal energie leads to a lower energie as with given params, but higher std...

2 Variational Monte Carlo with Fokker-Plank support



- 2.1 Quantum force
- 2.2 Investigate variational parameter $\Delta \tau$
- 2.3 Electron density
- 3 Diffusion Monte Carlo simulation of a Helium atom

4 Feynman Path Integral Quantum Mechanics