

Report 5: Quantum Monte Carlo

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

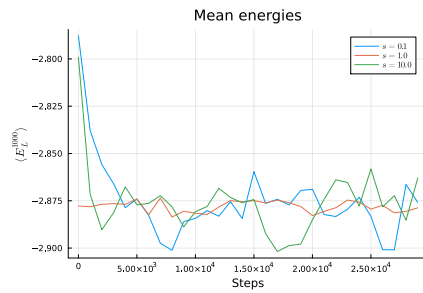
Simon BLAUE

January 19, 2023

Universität Göttingen
Faculty of Physics
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

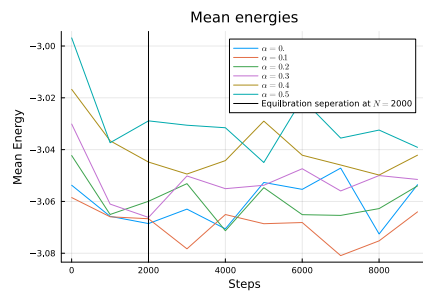


(a) Energies

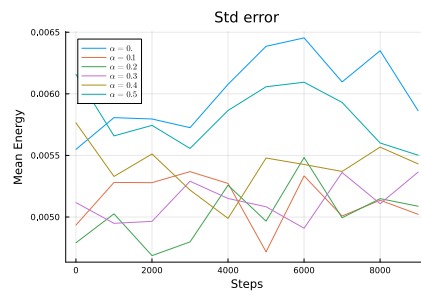


(b) Std

1.2 Approximating equilibration time

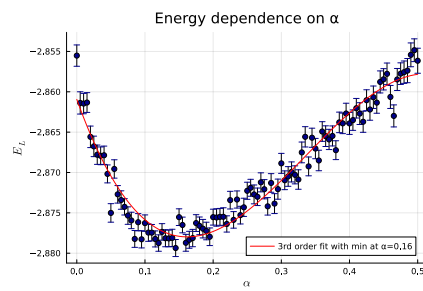


(a) Energies

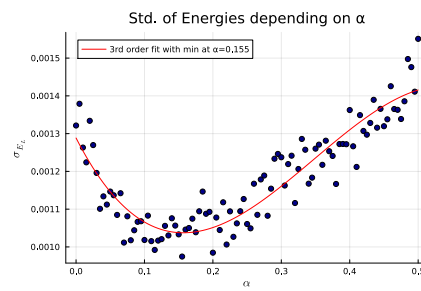


(b) Std

1.3 Investigate variational parameter α

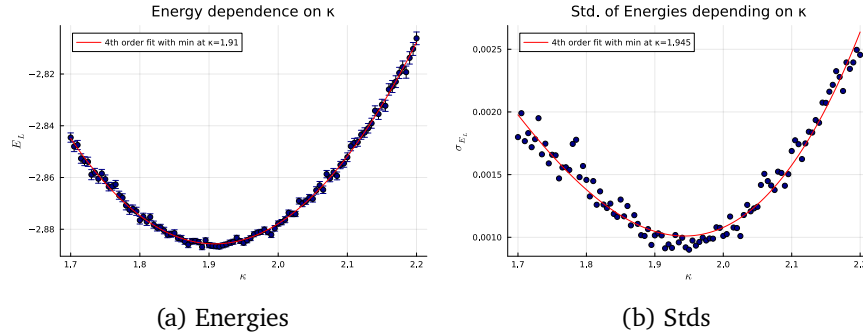


(a) Energies



(b) Std

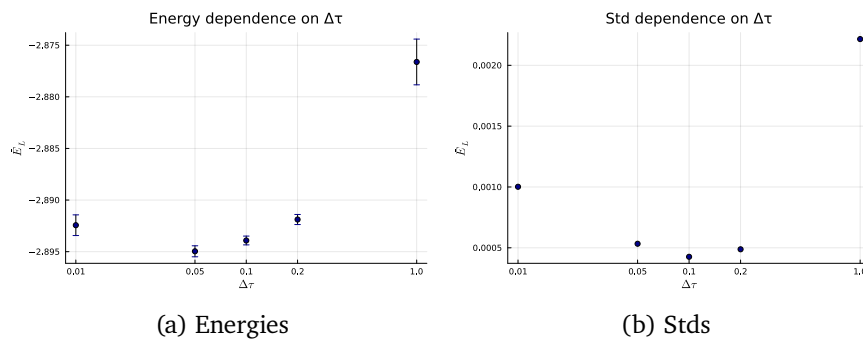
1.4 Investigate variational Parameter κ



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