Report 5: Quantum Monte Carlo

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

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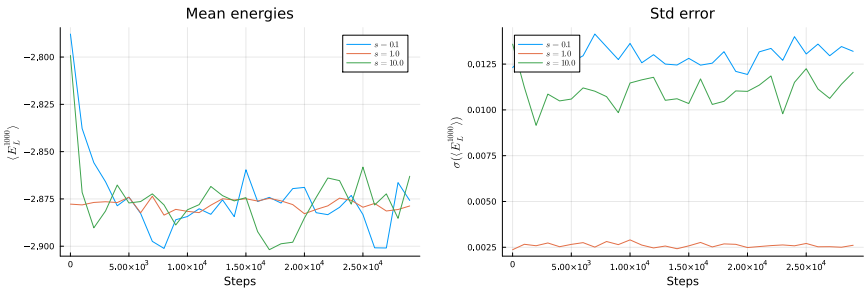
1 Variational Monte Carlo simulation of a Helium atom

1.1 Investigate stepsize s

First we should investiget the step size a, to take the smallest std. error, not influenced by the trial wave function per se. I find, that for $s = 1$ I get an order of magnitude smaller std error compared to $s = 0.1, 10$. Hence I will use $s = 1$ for all other simulations. The results are plotted in Figure 1.

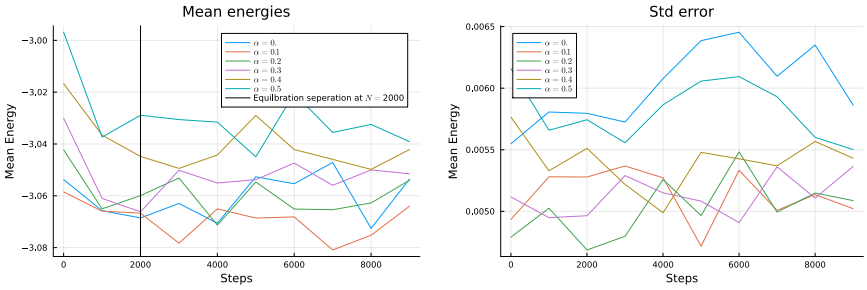


(a) Energies (b) Stds

Figure 1: Finding a good step size s

1.2 Approximating equilibration time

To observe the ground state energy properly, the simulation needs time to equilibrate, as it starts from random initial conditions. To find the equilibration time we vary over a few s values. The results are displayed in Figure 2



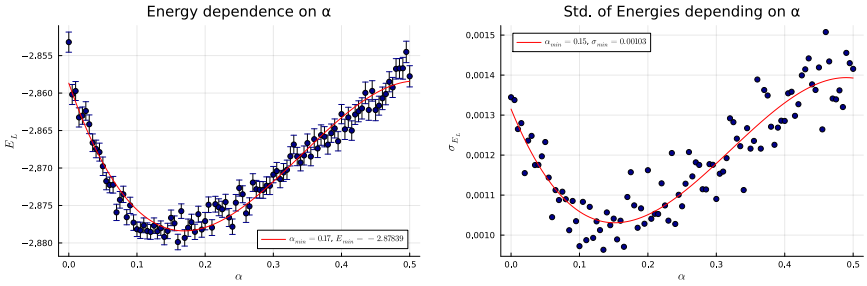
(a) Energies (b) Stds

Figure 2: Found equilibration time with 2000 steps

1.3 Investigate variational parameter α

Now we can stat finding the optimal trial wave function and corresponding minimal energy. For the optimal α I get $\alpha = 0.16$, for the optimal

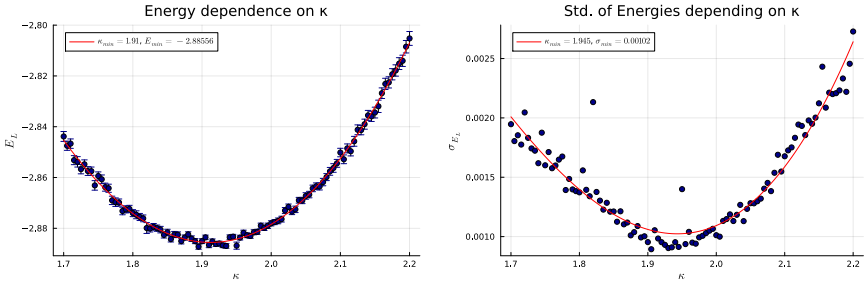
$\kappa = 1.93$ The results are displayed in Figure 3 and Figure 4 respectively. The respective energy minima are quoted in the figures, they are the same in the range of their respective 1-sigma deviation.



(a) Energies (b) Stds

Figure 3: Finding optimal $\alpha = 0.16$

1.4 Investigate variational Parameter κ



(a) Energies (b) Stds

Figure 4: Finding optimal $\kappa = 1.93$

1.5 Optimizing parameters α, β and κ

When running an optimization over all three parameters at the same time I get:

	α	β	κ	E_L
Optimized Run with given	0.18	0.38	1.85	-2.892±0.002
Experimental				-2.90338583(13)

Table 1: Finding the optimal trial wave function parameters.

2 Variational Monte Carlo with Fokker-Plank support

2.1 Quantum force

Given the trial wave function

$$\psi_T = e^{-\kappa r_1} e^{-\kappa r_2} e^{\frac{\beta r_{12}}{1+\alpha r_{12}}}$$

The corresponding quantum force follows

$$\vec{F}(R) = \frac{\nabla \rho}{\rho} = 2\frac{\nabla \psi_T}{\psi_T}.$$

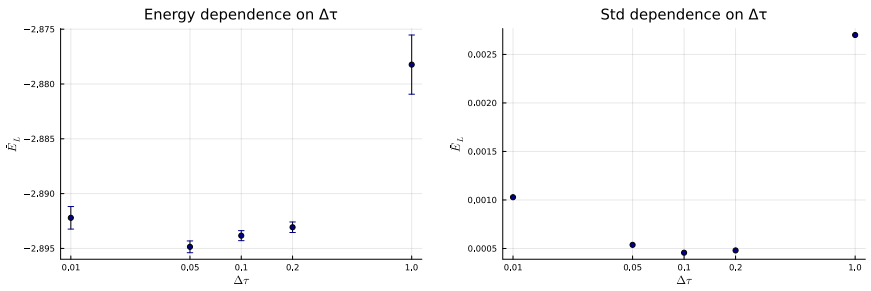
As the trial wave function consist of exp-functions I will only consider $\nabla \Psi_T$ and cancel the Ψ_T terms afterwards.

$$2\nabla\Psi_T = -2\begin{pmatrix} \frac{\kappa}{r_1}\vec{r}_1 + \beta(\frac{u}{r_{12}} - \frac{\alpha}{u^2}) \cdot (\vec{r}_1 - \vec{r}_2) \\ \frac{\kappa}{r_2}\vec{r}_1 - \beta(\frac{u}{r_{12}} - \frac{\alpha}{u^2}) \cdot (\vec{r}_1 - \vec{r}_2) \end{pmatrix} \Psi_T, = \frac{\vec{F}(R)}{\Psi_T}$$

where $u = 1 + \alpha r_{12}$, $r_1 = |\vec{r}_1|$, $r_2 = |\vec{r}_2|$ and $r_{12} = |\vec{r}_1 - \vec{r}_2|$.

2.2 Investigate variational parameter $\Delta\tau$

Investigating the parameter $\Delta\tau$ for four different values revelas thath the best of these is $\Delta\tau = 0.05$ as $E_L = -2.895$. As expected is this result closer to the experimental value than solely using VMC.



(a) Energies (b) Stds

2.3 Electron density

The Electron density, displayed in Figure 6 after equilibration follows a gaussian distribution with mean $\mu = 0.76$. This could be interpreted as the first orbit of the helium atom, where both electrons are located.

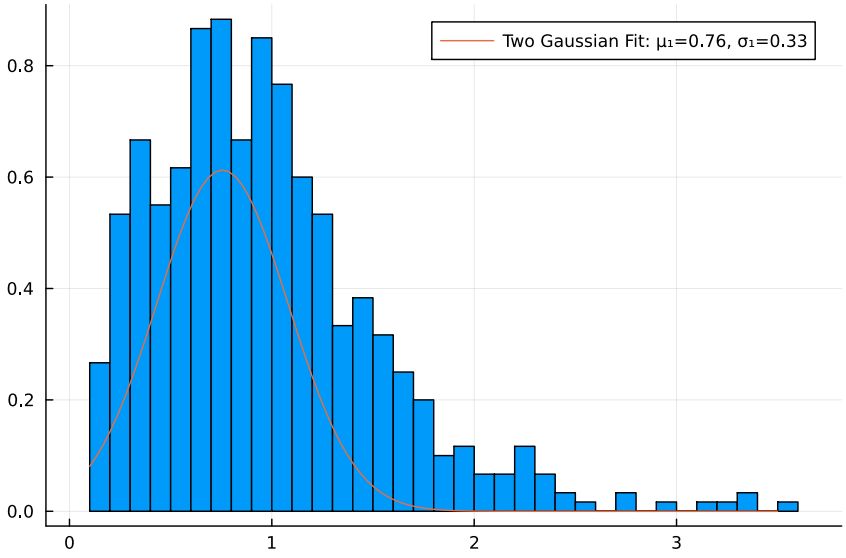


Figure 6: Electron density

3 Diffusion Monte Carlo simulation of a Helium atom

One would use Diffusion Monte Carlo, because it can lead to arbitrary accurate results, given the right loss function. Normaly one uses it after a rough estimate with VMC to get closer to the exact result.
Unfortunately, the Diffusion Monte-Carlo does not converge to the experimental value, as displayed in Figure 7. Also the electron density gives qualitatively not the same as in VMC, as displayed in Figure 8. This indicates a bug, my code can be found under https://github.com/simonblaue/MCP-Ex5.git.

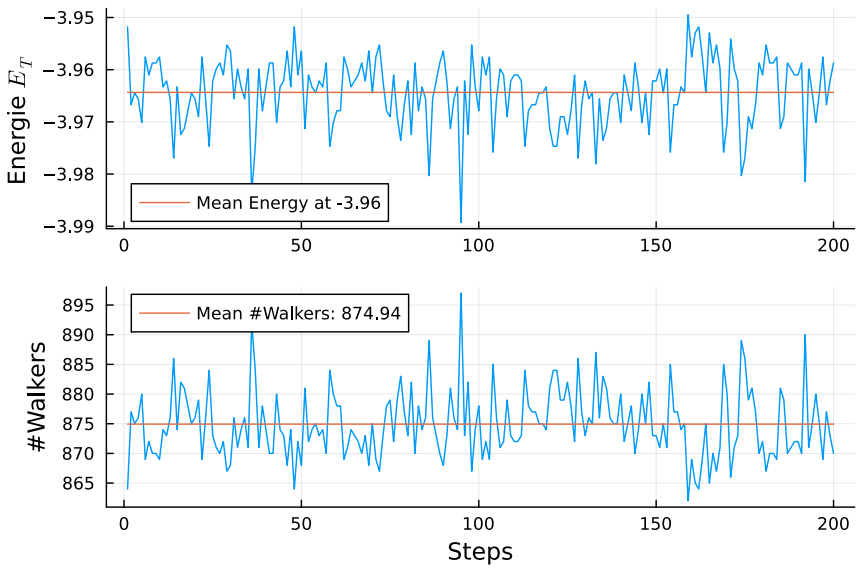


Figure 7: Energy E_T and number of walkers, plotted for every 100th step. In total the simulation run for 20000 steps.

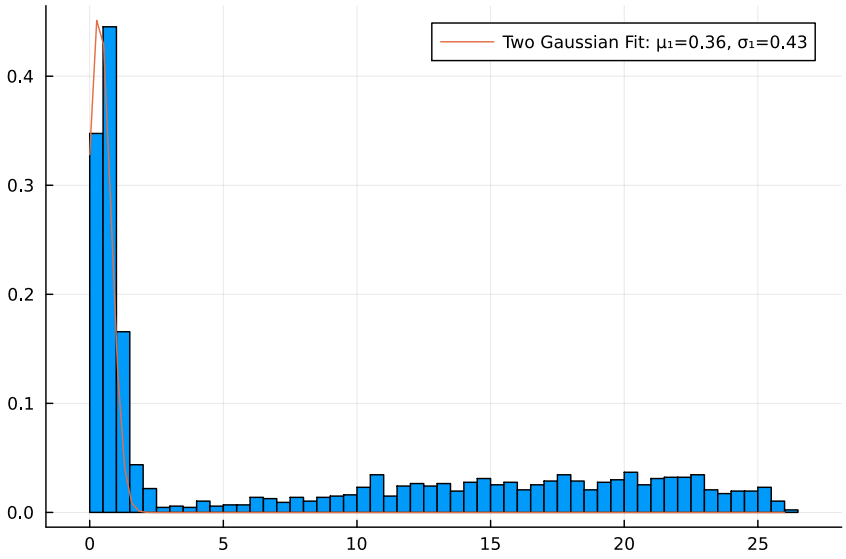


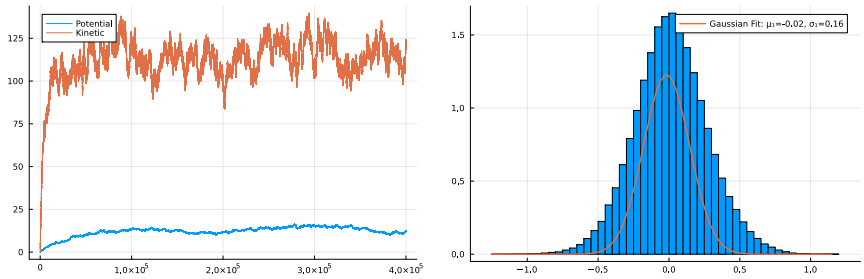
Figure 8: Electron density for DMC

4 Feynman Path Integral Quantum Mechanics

The energy and squared wave function for the 1d oscillator are displayed in Figure 9. The viral theorem does not hold as the kinetic energy dominates. The histogram corresponds to the likelihood of the positions, thus

the probability density and the squared wave function.
The same is true for the 2d case, only now does the kinetic energy not dominate as much as before. The result for 2d is displayed in Figure 10.

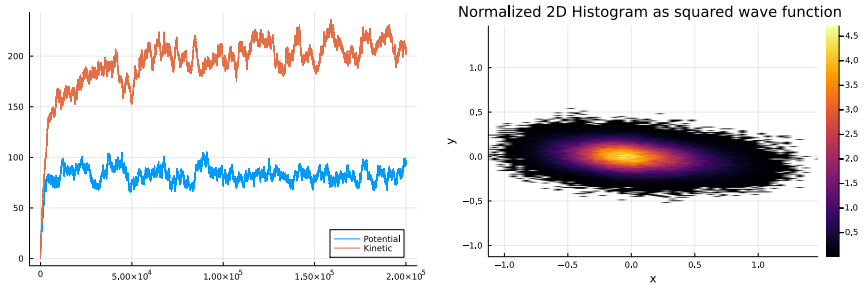
4.1 One dimensional harmonic oscillator



(a) Energies (b) quared wave function

Figure 9: 1D Oszillator

4.2 Two dimensional harmonic oscillator



(a) Energies (b) Squared wave function

Figure 10: 2D Oszillator