Variational Quantum Monte Carlo Simulations

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In the case of quantum mechanical systems, the exact solution is hardly known. To find the approximate ground state energy, this paper will use variational Monte Carlo integration. This paper will consider 3 kinds of quantum systems, the Harmonic Oscillator, Hydrogen atom and the Helium atom. In the simulations the metropolis algorithm was used to sample different distributions according to the wave function. The steepest descent method was used as a minimization algorithm to find the optimal value of the ground state energy given variational parameters α. and in the case of helium also a second parameter β. For Helium with 1 parameter trail wave function, the energy was found to be $E = -2.8799 \pm 0.0004$ and $E = -2.8852 \pm 0.0003$ for 2 parameters. These values were compared to the experimental value of $E = -2.9037$ a.u. It was found that having a better trail wave function and more variational parameters, gives results closer to the values in literature.

1 Introduction

The variational Monte Carlo method is widely used in the describing quantum mechanical systems. One often deals with such systems where no analytical solution can be found. Except for basic systems in the field of quantum mechanics such as spin particles (toy models), harmonic oscillator and the hydrogen atom, there exists no analytical solution. It is the task to develop approximately analytical models in order to obtain numerical data with minimum uncertainty. In this paper we start off with a theoretical background and discuss the three particular systems. For such systems we introduce the concept of trial wave function which turns out to be important when using the Monte Carlo method. In addition to the theory, the computational method will be outlined. The Metropolis algorithm is explained as well as data blocking and energy minimization. The results and plots will analysed in the results and discussion section. At the end a conclusion will be drawn and an answer to the research question will be given.

2 Theory

A theoretical background of three physical models is first introduced. Before studying the models in depth, a brief review of the variational method will be given. In the next section the usage of Both Monte Carlo method and Importance sampling are explained. At last, The ground state energies of the physical models will be calculated.

2.1 Variational calculus Schrödinger equation

Consider an interacting system containing many subsystems (particles). The Schrödinger equation For such system with many degrees of freedom can be solved by Variational calculus. To do so, one construct a trial wave function $\psi_T(\mathbf{r}, \alpha_1, ..., \alpha_n)$. where $\mathbf{r}$ is the displacement vector and $\alpha_1, ..., \alpha_n$ are the variational parameters. Once the wave function is known, the expected value can be calculated from the Schrödinger equation:

$$\langle E \rangle = \frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}. \tag{1}$$

By varying the parameters, this procedure can be repeated to obtain an expression with a minimum deviation.

From Eq. 1 it is clear that finding the expected value for the energy in say, the ground state cannot be calculated analytically. For this, Computational physics methods are essential to simulate the problem.

2.2 Monte Carlo and importance sampling

In order to solve integrals numerically, a sum over a certain interval must be computed. When the interval is uniformly distributed, the Monte Carlo integral is defined as

$$I = \int_a^b dx f(x) \approx \frac{(b-a)}{N} \sum_{i=1}^{N} f(x_i) \tag{2}$$

where x_i's are uniformly distributed. By way of definition, the variance can be calculated using the expression obtained from the integral

$$\sigma^2 = \frac{(b-a)}{N} \sum_{i=1}^{N} f^2(x_i) - \left[\frac{(b-a)}{N} \sum_{i=1}^{N} f(x_i) \right]^2. \tag{3}$$

Similarly, the error can be found as following

$$\sigma_n = \frac{\sigma}{\sqrt{N}}. \tag{4}$$

The error can be reduced by increasing the number of trials. however, such process is not efficient since increasing the number of trials results in lower computational performance. Another way of reducing the uncertainty is by decreasing the variation of the Monte Carlo method using Importance sampling.

Importance sampling is based on defining an interval of sampling which contributes more to the problem. This is done by choosing an estimator close to the shape of the actual function. Consider a probability density function $g(x)$ defined on a close interval. The relation between a PDF and a function obtained from the Monte Carlo method is

$$\frac{g(x)}{f(x)} \approx c \tag{5}$$

where c is a positive constant. Note that such a density function must meet the following criteria:

- $g(x)$ is defined everywhere positive on the interval $[a, b]$.
- the sum over the interval $[a, b]$ equals one.

Returning to the formal definition of the Monte Carlo integration, Eq. 2 can be rewritten in the following way

$$\int_a^b dx f(x) \to \int_a^b dx \frac{f(x)}{g(x)} g(x) = c \int_a^b g(x) dx. \tag{6}$$

observe that the error reduces significantly when defining an appropriate $g(x)$ resulting in $c \to 1$.

2.3 Local energy

The expression for the energy can now be reformulated in terms of the theory developed in the previous sections

$$E = \int d\mathbf{r} \sigma(\mathbf{r}) E_{loc}(\mathbf{r}). \tag{7}$$

This expression for the energy contains two parts, the local energy

$$E_{loc} = \frac{H\Psi(r,\alpha)}{\Psi(r,\alpha)} \tag{8}$$

and the distribution function

$$\sigma(\mathbf{r}) = \frac{|\psi_T(R)|^2}{\int dR' |\psi_T(R')|^2}. \tag{9}$$

The next task is to determine such trial function. The following sections deal with this problem. For certain physical system, a trial wave function will be used and numerical data will be studied.

2.4 Harmonic oscillator

The reason for considering this system in particular, is due to the fact it is one of few for which one can find an analytical solution. Reformulating the Hamiltonian in dimensionless units gives:

$$H = -\frac{d^2}{dx^2} + \frac{1}{2}x^2. \tag{10}$$

An educated guess for the trial wave function will be

$$\psi_T = e^{-\alpha x^2}. \tag{11}$$

The exact solution for the harmonic oscillator scales with e^{x^2}. Similarly, we find for the dimensionless local energy

$$E_{loc} = \alpha + x^2 \left(\frac{1}{2} - 2\alpha^2 \right). \tag{12}$$

2.5 Hydrogen atom

For simplicity, the notion of centre of mass will be used in the Hamiltonian. This results in in effective potential as a result of the motion of the proton and electron to relative to one another. The second simplification will be the setting all constant equal to one, to obtain a dimensionless expression

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r}. \tag{13}$$

Note that r is the relative distance as mentioned earlier. The transformation resulted in filtering out unnecessary degrees of freedom, which left the model into a one dimensional problem. The ground state energy for this H has the solution

$$\psi(r) = e^{-r}. \tag{14}$$

Thus, the trial wave function is chosen to be

$$\psi_T(r,\alpha) = e^{-\alpha r}. \tag{15}$$

In a similar way, the local energy can be found:

$$E_{loc} = -\frac{1}{r} - \frac{1}{2}\alpha \left(\alpha - \frac{2}{r} \right). \tag{16}$$

2.6 Helium atom

The complexity of the system increases significantly when an additional electron is provided to the physical model. This is the case for a Helium atom, where a one dimensional problem seems to be impossible to maintain. This is due to the repulsion potential between both electrons. The position of the nucleus is assumed to be at rest while both electron are distances r_1 and r_2 away from the nucleus. The dimensionless Hamiltonian reads

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_1^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}. \tag{17}$$

As for the trial wave function, the following expression is used for the ground state energy[2]

$$\psi_T(r_1, r_2) = e^{-2r_1}e^{-2r_2}e^{\frac{r_{12}}{2(l+\alpha r_{12})}}. \tag{18}$$

For this given function, the expression for the local energy

$$E_{loc}(r_1, r_2) = -4 + (\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2) \times (\mathbf{r_1} - \mathbf{r_2})\beta(r_{12}, \alpha) \tag{19}$$

where

$$\begin{aligned}\beta(r_{12}, \alpha) = &\frac{1}{r_{12}(l + \alpha r_{12})^2} \\ &- \frac{1}{r_{12}(l + \alpha r_{12})^3} \\ &- \frac{1}{4(l + \alpha r_{12})^4} - \frac{1}{r_{12}}.\end{aligned} \tag{20}$$

2.6.1 2 parameter Helium Atom

The correctness of the variational Monte Carlo integration can be seen as how well the trail wave function overlaps the real wave function. To get as close as possible with the variational method one needs to implement the trail wave function wisely. This paper will also try to investigate the effect of having 2 variational parameters. The trail wave function will look very similar to the one above.

$$\Psi_T(\alpha, \beta, \boldsymbol{r_1}, \boldsymbol{r_2}) = e^{-\beta(r_1 + r_2)}e^{\frac{r_{12}}{2(1+\alpha r_{12})}} \tag{21}$$

The 2 in equation 18 has been replaced with β. The local energy has the following form [2]

$$E_{loc2} = E_{loc1} + \frac{1}{2(1 + \alpha r_{12})^2}\left\{\frac{\beta(r_1 + r_2}{r_{12}}(1 - \frac{\boldsymbol{r_2 r_2}}{r_1 r_2})\right.$$

$$\left. - \frac{1}{2(1 + \alpha r_{12})^2} - \frac{2}{r_{12}} + \frac{2\alpha}{1 + \alpha r_{12}}\right\} \tag{22}$$

Where E_{loc1} is as follows:

$$E_{loc1} = (\beta - 2)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{r_{12}} - \beta^2 \tag{23}$$

3 Computational method

3.1 Metropolis algorithm

As known from importance sampling, one wants to find an appropriate density function $g(x)$. However, the complicity of finding increases rapidly with the system's dimensionality. For one dimensional models, it is still possible to construct a good working function which is used in the various Monte Carlo method. The inverse of a function is the the hard to task find obtain analytically. Therefore, The Metropolis algorithm proves to be handy in this case. Consider a finite set of walkers

$$X = \{x_i \mid i \in \mathbb{N}\}. \tag{24}$$

Define a new trial point in the neighbourhood of the original point with an interval h. thus, the new point lies in the interval $[x_i - \frac{h}{2}, x_i + \frac{h}{2}]$. The acceptance ratio can then be calculated

$$\alpha = \frac{f(trial)}{f(x_i)} = A\frac{p(trial)}{p(x_i)}. \tag{25}$$

The next step is choose a point, say u from a uniform distribution and examine it. If $u \leq a$ then the move is accepted, therefore: $x_i = x_{trial}$. Otherwise the move will not be accepted and $x_i = x_i$.

Repeating this process will ultimately result in the density function one requires. Obviously, taking more points in account results in higher accuracy. As for the step size however, if it exceeds the upper limit, the points might be out of the desired region of definition. similarly, if the size step is too small, a significant larger amount of steps is needed.

3.2 Minimization algorithm

At this final stage, a general solution can be found whenever the energy is minimized. There have been many attempts for this procedure both analytically and numerically. If one chooses to proceed with numerical methods, a derivative of such variables are correlated with high uncertainties. Instead, consider the trial wave function first take the natural logarithm of it and differentiate with respect to α

$$\frac{\partial E}{\partial \alpha} = 2\left(\left\langle E_L \frac{\partial \ln(\psi_T)}{\partial \alpha}\right\rangle - E\left\langle \frac{\partial \ln(\psi_T)}{\partial \alpha}\right\rangle\right). \tag{26}$$

This results in a new value for α obtained form the exact definition

$$\alpha_n = \alpha - \gamma\left(\frac{\partial E}{\partial \alpha}\right) \tag{27}$$

where γ is the learning rate and can be set to a certain value. This process will repeat itself till the conditions are met.

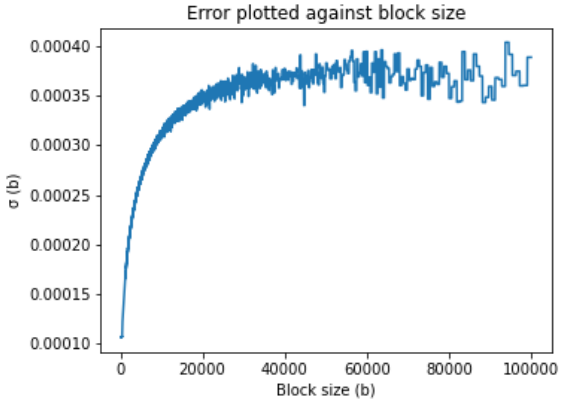

Figure 1: *Error of $\langle E \rangle$ of Helium with $\alpha = 0.14$ plotted against different block sizes b. At roughly around block size $b = 40000$ the error becomes constant.*

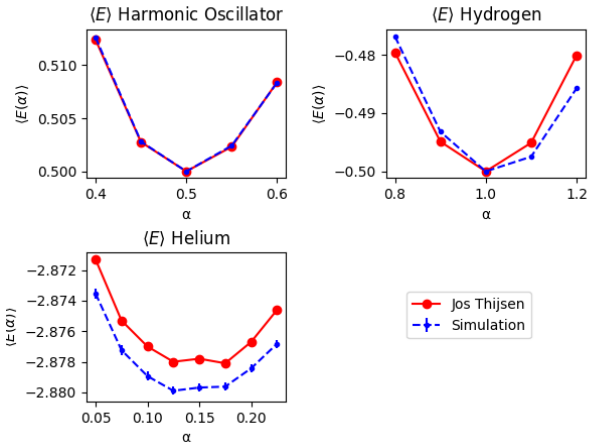

Figure 2: *A comparison of $\langle E \rangle$ of the ground state for a Harmonic Oscillator, Hydrogen atom and Helium atom. $\langle E \rangle$ was calculated using monte carlo integration for diffrent values of alpha, those values are then compared to the values of Jos Thijsen. For all systems $N_{tries} = 30000$ and $N_{walker} = 400$.*

3.3 Data blocking Error

Because the data obtained from the metropolis algorithm is correlated, the error can not be computed as is usual. For that, the data needs to be made uncorrelated first. This is done by block averaging the data. Suppose, one gets a time series $(A_1, A_2..)$, this is divided into blocks of size b and the average of that block is then calculated.

$$a_i = \frac{1}{b} \sum_{(i-1)*b+1}^{i*b} A_i \tag{28}$$

Where a_i is the block averaged version. If the blocksize is chosen large enough the data will have become uncorrelated and the error can be computed in the following way:

$$\sigma_A(b) = \sqrt{\frac{1}{N_b - 1}(\langle a^2 \rangle - \langle a \rangle^2)} \tag{29}$$

Where N_b is the number of blocks. To obtain the correct blocksize so the data will be uncorrelated, the error has to be plotted against the blocksize, this is shown in FIg 1. From there it can be seen that at a certain blocksize the error remains rougly constant, in the case of the Helium atom with $\alpha = 0.14$, with $N_{tries} = 30000$ and $N_{walkers} = 400$, the error becomes constant at around $b = 40000$. This blocksize has been chosen for all further simulations.

4 Results and Discussion

In the following section the Results will be presented and discussed. First the correctness of the simulations will be checked by comparing the values obtained to the literature. A broader picture will be presented to have more insight on the problem. Next the results of the proper minimization of the expectation value $\langle E \rangle$ of the ground state will be presented for the different systems. And lastly the performance will be discussed.

4.1 Correctness Check

Before the proper minimization of the ground state energy, the computational methods described in the previous section has to be checked whether it was implemented correctly. To do this the results of the variational simulation will be compared to the literature. More specifically the values of the book of Jos Thijsen [1].

The accuracy of the results partially depend on the overall acceptance rate of the metropolis algorithm, it should not be too high or low. Therefore the metropolis algorithm was tuned accordingly for each system to have an overall acceptance rate of around 0.5 by varying the size of the displacement of the walkers.

The results for the expectation value $\langle E \rangle$ of the ground state, for the different systems are compared in Fig 2 and in Fig 3 the variance of $\langle E \rangle$ are compared.

From Fig 2, the minimum energy for the harmonic oscillator and hydrogen atom is at $\alpha = 0.5$ and $\alpha = 1$ corresponding to $\langle E \rangle = 0.5$ and $\langle E \rangle = -0.5$ respectively. Indeed these values are precisely the energy eigenvalues of the systems, because the exact solution, lies in the variational space. This can be further backed up in Fig 3, where it is seen that the variance of $\langle E \rangle$ becomes exactly zero when the trail wave function is the exact solution.
On the other hand for the Helium atom the exact solution is unknown. Therefore, even though $\langle E \rangle$ becomes

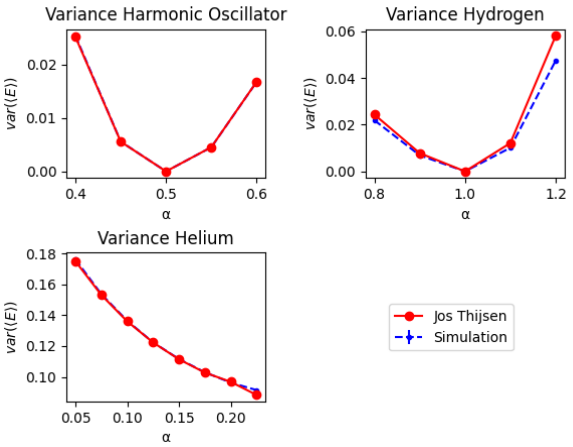

Figure 3: *A comparison of the variance for a Harmonic Oscillator, Hydrogen atom and Helium atom between the values obtained in the simulations and that of Jos Thijsen.*

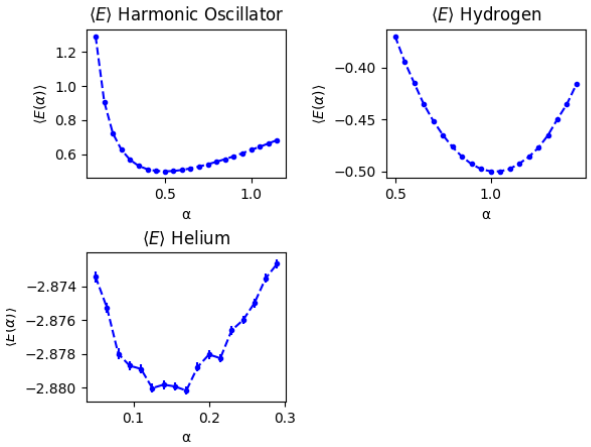

Figure 4: *The $\langle E \rangle$ of the ground state for a Harmonic Oscillator, Hydrogen atom and Helium atom, for a broader range of α. For all systems $N_{tries} = 30000$ and $N_{walker} = 400$.*

minimal at $\alpha \approx 0.15$, the variance does not. This is because the trail wave function that was used is not an eigenfunction of the system.
It can be noted that the overlap between the values obtained from the simulation and the values from Jos thijsen is quite large. Especially the variance is almost identical. This indicates that the implementation of the monte carlo integration is done correctly.
It is interesting that for the Helium atom all the values found from the simulations are lower than the values from Jos Thijsen, seeing how the variance are identical.

4.2 A broader picture

To get more insight, a wider range of α was used to calculate and plot the expectation values of the energy. This is illustrated in Fig 4. For the Harmonic Oscillator the energy is calculated for α ranging from 0.1 to 1.2 in steps of 0.05. For the Hydrogen atom α ranges from 0.5 to 1.5 in steps of 0.05. Finally the Helium atom is plotted for α between 0.05 and 0.3 in steps of 0.015.

With the help of Fig 4, the minimization can be preformed better, since the initial value for the optimization algorithm can be set according to the findings here.

4.3 Minimization Ground State Energy

The optimization was performed for the 3 systems. It uses the gradient of the energy with respect to the varying parameter to find the optimal value for the ground state energy. A thing to note is that the results of this optimization are highly depended on the learning rate of the algorithm together with the tolerance for stopping the algorithm. Having the learning rate too high might mean that it will overshoot in finding the minimum and will have trouble converging. On the other hand having a learning rate that is too small, the convergence will take too long. In addition to this the initial starting value off course is important, but with the results obtained earlier we can make an educated guess on where to start. The tolerance for all the simulations was set to $toll = 0.001$.

4.3.1 Harmonic Oscillator and Hydrogen

For a smooth convergence, a learning rate of $\gamma = 0.3$ was used for both the Harmonic oscillator and the Hydrogen atom. Both of their initial value of the variation parameter was chosen as $\alpha_{init} = 1.2$. The minimization of the harmonic oscillator is shown in Fig 5 and the Hydrogen atom in Fig 6.

For the Harmonics Oscillator system the initial value was $\alpha_{init} = 1.2$. It took 12 iterations to obtain the optimal value of $\alpha = 0.5008$, this corresponds with a ground state energy of $\langle E \rangle = 0.5000 \pm 2.7e^{-6}$. Likewise for the Hydrogen atom the initial value was $\alpha_{init} = 1.2$. It took 13 iterations to obtain the optimal value of $\alpha = 1.0013$, this corresponds with a ground state energy of $\langle E \rangle = -0.5001 \pm 2e^{-5}$, with a variance of $var = 1.2e^{-5}$.

It it interesting to note that the minimization of the energy resembles the curvature that is seen in Fig 4 coming from the right side. For the harmonic oscillator the graph is more linear on the right side and for the Hydrogen atom it is more quadratic. Indeed, this is seen again in the top half of Fig 5 for the Harmonic Oscillator and in Fig 6 for the Hydrogen atom. Together with the values obtained above it means that the minimization process is done correctly.

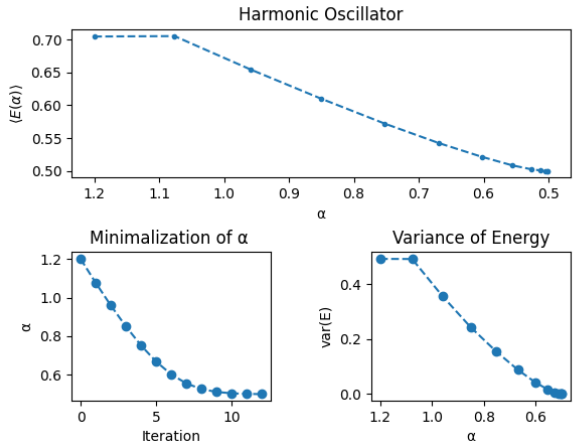

Figure 5: *The optimization of the parameter alpha to obtain the ground state of the Harmonic Oscillator system. The starting value was $\alpha_{init} = 1.2$. It took 12 iterations to obtain the optimal value of $\alpha = 0.5008$, this corresponds with a ground state energy of $\langle E \rangle = 0.5000 \pm 2.7e^{-6}$.*

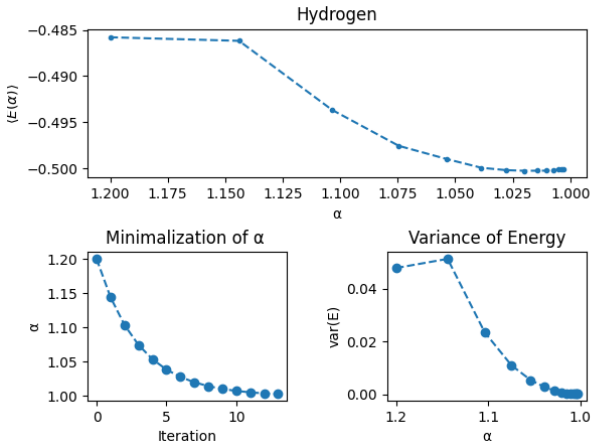

Figure 6: *The optimization of the parameter alpha to obtain the ground state of the Hydrogen atom system. The starting value was $\alpha_{init} = 1.2$. It took 13 iterations to obtain the optimal value of $\alpha = 1.0013$, this corresponds with a ground state energy of $\langle E \rangle = -0.5001 \pm 2e^{-5}$, with a variance of $var = 1.2e^{-5}$.*

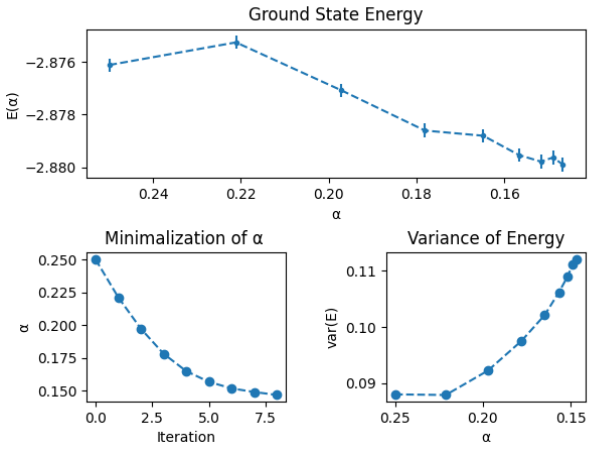

Figure 7: *The optimization of the parameter alpha to obtain the ground state of the Helium atom. The starting value was $\alpha_{init} = 0.25$. It took 8 iterations to obtain the optimal value of $\alpha = 0.1464$, this corresponds with a ground state energy of $\langle E \rangle = -2.8799 \pm 0.0004$.*

4.3.2 Helium

For the Helium atom one can take an educated guess judging from the results above. Therefore the starting point of the varying parameter will be $\alpha_{init} = 0.25$, as per usual the number of tries and walkers is taken as $N_{tries} = 30000$ and $N_{walker} = 400$ respectively. Here the learning rate was set to $\gamma = 0.5$. Figure 7 shows the optimization process.

It took the algorithm 8 iterations to obtain a value of $\alpha = 0.1466$ with a tolerance of 0.001. The energy corresponding to this value is $\langle E \rangle = -2.8799 \pm 0.0004$ and a variance of $var(E) = 0.1123$. The results do agree with our previous results where the minimum of the energy in Fig 2 was around $\alpha \approx 0.15$. Comparing the energy found to the experimental value of $E = -2.9037$ a.u. [1], there is a 0.82% deviation taking account the worst case scenario where the error is the largest. There is quite a nice overlap between the findings and the experimental value, this is mainly because of the quality of the trail wave function used.

To improve the results even more, a trail wave function with 2 parameters α and β was also used to obtain an optimal ground state. Especially in this case the learning rate and the initial value are important. It turned out when having the learning rate too high, and the initial value of β too far from the optimum together with the initial value of α being too close to 0, the algorithm would overshoot the α to the negative causing the exponent of the wave function to explode. An example is shown in Fig 8, where the initial values are taken to be $\alpha_{init} = 0.3$ and $\beta_{init} = 3$ with learning rate of $\gamma = 0.5$. Both parameters initially shoot down because of β, therefore α needs to gradually go back up to find the optimum. It it still possible to have any

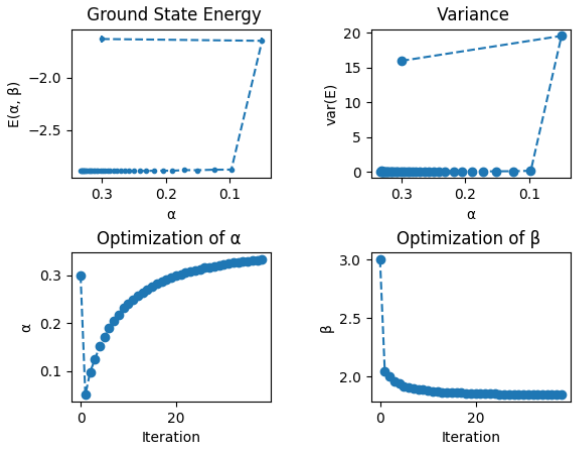

Figure 8: *Example of overshooting when optimizing for parameters. With initial values of $\alpha = 0.3$ and $\beta = 3$. To speed up the results the number of walkers and tries was lowered to $N_{tries} = 10000$ and $N_{walker} = 50$ respectively.*

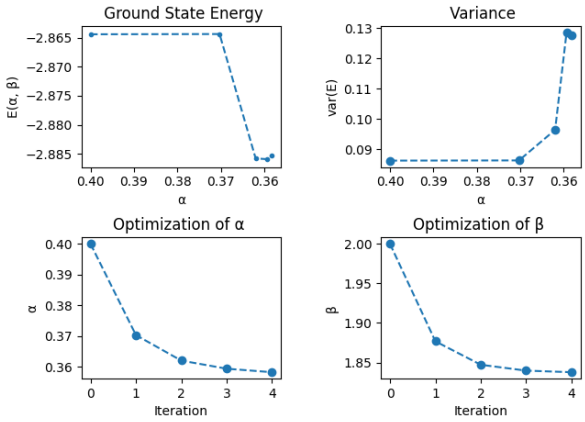

Figure 9: *The optimization of variational parameters with initial values of $\alpha = 0.4$ and $\beta = 2$. The optimal values were found to be $\alpha = 0.3582$, $\beta = 1.8376$. The corresponding energy $\langle E \rangle = -2.8852 \pm 0.0003$. With $N_{tries} = 30000$ and $N_{walker} = 400$.*

initial value, but then the learning rate needs to be low enough causing the algorithm to take too many iterations.

Because of this the learning rate was set to 0.4, with initial values of $\alpha_{init} = 0.4$ and $\beta_{init} = 2$. The optimal values were found to be $\alpha = 0.3582$, $\beta = 1.8376$. The corresponding energy $\langle E \rangle = -2.8852 \pm 0.0003$ with a variance of $var(E) = 0.1276$. It took 4 iterations with the process shown in Fig 9 .

Comparing the results with the experimental value of $E = -2.9037$ a.u. , there is a deviation 0.64%. Therefore there is indeed an improvement of the results by introducing a second variational parameter β. From this line of thought one might improve on the results even more by introducing more parameters to vary. But off course this will have an impact of the run time of the simulation.

4.4 Performance

The performance of the code is an important aspect for the simulation. Where it was applicable, for loops were avoided, for example in the metropolis algorithm the numpy library was used efficiently. However, the number of tries to take and the number of walkers to place give an indication how well the result will be. In principle one can just place a single walker for the metropolis algorithm, but the chances that it will get stuck are quite high. Therefore a multitude of walkers are used. But this has the effect that the run time will be quite slow. The run time for the Helium simulation with 8 values of alpha for different number of walkers is shown in Table below

Table 1: *Run time of the Helium system simulation, for 8 values of α, $N_{tries} = 30000$ and for different number of walkers*

Number of walkers	Time elapsed (s)
10	39.16
50	53.10
100	78.21
200	115.26
400	191.39

These values are however for prefixed values of α, meaning the calculations of the code is done only 8 timed for these α. When performing a minimization, the number of iterations can become quite high if the precision is necessary. The number of calculations the code has to do can become quite large, and therefore the simulations in this paper were limited to a precision of only 0.001 to ensure a reasonable run time.

5 Conclusion

The Monte Carlo simulation was implemented and checked for correctness by comparing it to the book from Jos Thijsen [1]. The expectation energy $\langle E \rangle$ of the ground state was calculated with Monte Carlo Integration for varying parameter α and with that also the variance of that energy. It was found that for all 3 systems of Harmonic Oscillator, Hydrogen atom and Helium atom, there was a great overlap in the values obtained in this paper and to that of Jos Thijsen. For the Variance there even was almost a 1 to 1 correspondence in the values.
From the simulations it was found that the minimal $\langle E \rangle$ of the ground state for the Harmonic oscillator and Hydrogen atom is at $\alpha = 0.5$ and $\alpha = 1$ corresponding

to $\langle E \rangle = 0.5$ and $\langle E \rangle = -0.5$ respectively. With both of the variances being $var = 0$ for these systems because at these values for α the trail wave function used becomes the exact solution of the system.
For Helium atom there is no exact solution, which was noticed as a finite variance at the minimum energy.

The proper minimization was also performed for these 3 systems, using the steepest descent method. For the Harmonics Oscillator system the initial value was $\alpha = 1.2$. It took 12 iterations to obtain the optimal value of $\alpha = 0.5008$, this corresponds with a ground state energy of $E = 0.5000 \pm 2.7e^{-6}$. Likewise for the Hydrogen atom the initial value was $\alpha = 1.2$. It took 13 iterations to obtain the optimal value of $\alpha = 1.0013$, this corresponds with a ground state energy of $E = -0.5001 \pm 2e^{-5}$, with a variance of $var = 1.2e^{-5}$. Both of these values correspond the the results earlier and that of Jos Thijsen.

For Helium 2 minimization were performed, for 1 and 2 variational parameters in the trail wave function. For only 1 parameter α, starting at $\alpha = 0.25$ it took the algorithm 8 iterations to obtain a value of $\alpha = 0.1466$ with a tolerance of 0.001. The energy corresponding to this value is $E = -2.8799 \pm 0.0004$ and a variance of $var(E) = 0.1123$. For 2 parameters with initial values of $\alpha = 0.4$ and $\beta = 2$. The optimal values were found to be $\alpha = 0.3582$, $\beta = 1.8376$. The corresponding energy $E = -2.8852 \pm 0.0003$ with a variance of $var(E) = 0.1276$ which took 4 iterations. It was found that indeed with more parameters to vary, one can obtain a more precise value for the Helium atom since there is no exact solution.

Bibliography

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