FYS4411 - Project 1

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Abstract

In this work we explore a system of many bosons in a harmonic oscillator trap at temperatures low enough for Bose-Einstein condesation. A variational monte-carlo machinery is implemented as a solution to find the expecation value of the energy as a function of a single variational parameter α. Over this variational parameter the ground-state energies are found by gradient descent both for a non-interactive case and with a repulsive potential. As an additional improvement to the convergence of the algorithm an importance sampling techinque for chosing the proposed next step in the metropolis algorithm is implemented. Lastly we consider the onebody densities for both systems with and without a repulsive interaction and find most particles to be localized for the non-interactive case and distributed according to a bell curve when we introduce interactions.

1 Introduction

The aim of this project is to evaluate the case of a hard sphere trapped Bose gas using Variational Monte Carlo simulations. We want to find the ground state energy for systems containing different number of particles given a trial wave function. As the number of particles grow, so does the complexity of the wave function. What we are looking at is a quantum many-body-problem

$$\imath\hbar\frac{\partial}{\partial x}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

and with a growing exponential complexity in the wave function the more impossible the calculation of the Hamiltonian and the energy becomes. The Variatonal Monte Carlo method allows us to look for the low ground state energy, but we will be using Metropolis-Hastings algorithm and Importance Sampling to make the selection of movements of particles in the system.

Our trail wave function consist of one variational parameter, $\Psi_T(\mathbf{R};\alpha)$. We want to find the optimal value for α that minimizes the energy. For that we use the method of Steepest Descent. For the statistical analysis and error estimates of the numerical data we have used blocking techniques.

All the code in the project can be found in the repository `https://github.com/copperwire/comp_phys_2`

2 Theory

2.1 Ansatz for the wavefunction and the hamiltonian

In this project we study the physics of a dilute many boson system in a Bose Einstein condensate with variational monte carlo methods. The particles are placed in a harmonic oscillator trap described by equation 1 in the project description. We'll start by discussing a hamiltonian in which there is no interaction between particles and being bosons there are no restrictions on the occupancy of a single energy state. But in general the trial wavefunction (or ansatz for the wavefunction) is defined as in equation 1

$$\Psi_T(\{\mathbf{r}\}) = \prod_i g(\alpha, \beta, \mathbf{r}_i) \prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|) \tag{1}$$

Where $g(\alpha, \beta, \mathbf{r}_i)$ is a function proportional to the single particle solution of the harmonic oscillator trap. Which is to say it can be written on the form

$$g(\alpha, \beta, \mathbf{r}_i) = e^{-\alpha(x_i^2 + y_i^2 + \beta z_i^2)} \tag{2}$$

Where α is the variational parameter of interest. Which is to say that minimizing the system energy $\langle \Psi_T(\{\mathbf{r}\}) | \hat{H} | \Psi_T(\{\mathbf{r}\}) \rangle$ by α is the objective of this project.

In equation 1 we also define the correlation wavefunction $f(a, |\mathbf{r}_i - \mathbf{r}_j|)$ is defined as

$$f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} \infty, & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ 0, & |\mathbf{r}_i - \mathbf{r}_j| > a \end{cases} \tag{3}$$

Initially (for tasks a, b, and c) we set the parameter a to equal zero and solve the non-interactive system. As it turns out directly evaluating the inner product to find the expectation for the energy is problematic because for a system with interaction it involves solving a pretty unasvory integral. We then turn to numerical methods as a tool, but we still want avoid directly evaluating the expectation for the hamiltonian for the ensamble. The solution to this problem becomes apparent when you consider the machinery of the VMC scheme.

2.2 Variational Monte Carlo

Monte Carlo simulations are widely used methods in numerical science that employs random walkers. In this project we are taking a closer look at trapped bosons. We are given a trail wave function we assume is as close to the real case as possible, $\Psi_T(\mathbf{R}; \alpha)$ where $\mathbf{R} = (\mathbf{R}_1, ..., \mathbf{R}_N)$ is the position of the different particles. From quantum mechanics we know the probability distribution is given by the wave function.

$$P(\mathbf{R}; \alpha) = \frac{|\Psi_T(\mathbf{R}; \alpha)|^2}{\int |\Psi_T(\mathbf{R}; \alpha)|^2 d\mathbf{R}}$$

Monte Carlo integration allow us to evaluate the integral at hand. The expectation value of the Hamiltonian is given as follows.

$$\langle \widehat{\mathbf{H}} \rangle = \frac{\int d\mathbf{R} \Psi^*(\mathbf{R}) H(\mathbf{R}) \Psi(\mathbf{R})}{\int d\mathbf{R} \Psi^*(\mathbf{R}) \Psi(\mathbf{R})}$$

The variational principle states that the expectation value of the Hamiltonian is an upper-bound for the ground state energy of the Hamiltonian.

$$E_0 \leq \langle H \rangle$$

This is what the Variational Monte Carlo method bases itself on. Given a probability distribution we can evaluate the wave function and look for a local minimum. We define the local energy by

$$\widehat{\mathbf{E}}_L(\mathbf{R}; \alpha) = \frac{1}{\Psi_T(\mathbf{R}; \alpha)} \widehat{\mathbf{H}} \Psi_T(\mathbf{R}; \alpha).$$

Then the expectation value of the local energy is given by

$$\langle \widehat{\mathbf{E}}_L \rangle = \int P(\mathbf{R}) \widehat{\mathbf{E}}_L d\mathbf{R} \approx \frac{1}{N} \sum_{i=1}^{N} \mathbf{E_L}(x_i)$$

where N is the number of Monte Carlo cycles. Now we can calculate the probability distribution and the local energy. And for each cycle we propose a new configuration $\mathbf{R}_p$ for the system and hopefully we come closer to the ground state.

$$\mathbf{R}_p = \mathbf{R} + r * \Delta \mathbf{R}$$

2.3 The Metropolis Algorithm

How we select the new configurations during the simulation is given by the Metropolis Algorithm. Ideally we would have a transition probability matrix which told us how likely it would be for each particle to move in the configuration space. Since we don't we try and model it. We define the following entities:

$P_i^{(n)} \rightarrow$ probability of finding the system in state i at the n'th step.
$j \rightarrow$ possible new step
$A_{i \rightarrow j} \rightarrow$ probability of acceptance.
$T_{j \rightarrow i} \rightarrow$ probability of making the transition

Now we can say that a transition probability matrix can be constructed by $T_{j \rightarrow i} A_{j \rightarrow i}$. The probability of finding the system in state i at step n is

$$P_i^{(n)} = \sum_j \left[P_j^{(n-1)} T_{j \rightarrow i} A_{j \rightarrow i} + P_j^{(n-1)} T_{i \rightarrow j} (1 - A_{i \rightarrow j}) \right]. \tag{4}$$

We want to push the system towards high density regional space of $P_i^{(n)}$. /We want to select states according to the probability distribution. In that way to converge to the desired stationary distribution p_i.

$$P_i^{(n\to\infty)} \to p_i$$

Using this statement and the fact that the sum over all possible transitional probabilities is one we can rewrite the above equation 4.

$$\sum_j [p_j T_{j\to i} A_{j\to i} - p_i T_{i\to j} A_{i\to j}] = 0$$

In order to stop at the configuration where we have reached equilibrium we us the condition of detailed balance, and it gives us

Data: matrix $\mathbf{R}$
Result: float $\mathbf{E}_L$
number of MC-cycles N;
initialize $\mathbf{R}$;
calculate $|\Psi_T(\mathbf{R})|^2$;
for *i in* $[0, N]$ **do**
    $\mathbf{R}_p = \mathbf{R} + r * \Delta\mathbf{R}$;
    calculate $\omega = \frac{|\Psi_T(\mathbf{R}_p)|^2}{|\Psi_T(\mathbf{R})|^2}$;
    if $q \leq \omega$ **then**
        accept new move;
    else
        reject new move;
    end
    update energy, $\mathbf{E}_L$;
end

Algorithm 1: Monte Carlo with Metropolis-Hastings

$$\frac{A_{j\to i}}{A_{i\to j}} = \frac{p_i T_{i\to j}}{p_j T_{j\to i}}.$$

We choose to accept when the acceptance is bigger than 1.

$$A_{j\to i} = \min\left(1, \frac{p_i T_{i\to j}}{p_j T_{j\to i}}\right)$$

What we must calculate is equation 5. And an example of the code is given further down, in Algorithm 1

$$\frac{p_i T_{i\to j}}{p_j T_{j\to i}} = \frac{|\Psi_T(\mathbf{R}_p)|^2}{|\Psi_T(\mathbf{R})|^2} \tag{5}$$

2.4 Importance Sampling

Now we move to an extension of the Metropolis algorithm, the Importance sampling. This method provides us with a better way of suggesting new moves. The expression for the new move, y, is given by the solution of the Langevin equation. It reads

$$y = x + DF(x)\Delta t + \xi\sqrt{\Delta t},$$

where ξ is a gaussian random variable, D is the diffusion coefficient and is $\frac{1}{2}$ and Δt is the time step which take values between $[0.001, 0.01]$. $F(x)$ is the drift force and is given by the gradient of the wave function.

$$F = 2\frac{1}{\Psi_T}\nabla\Psi_T$$

It is the drift force that ensures us we move particles towards regions of configuration space where the trail wave function is large. This method increases the efficiency of our program, since the standard Metropolis can suggest new moves in every direction with same probability. From the solution of the Fokker-Planck equation we get a new transition probability, the Green's function.

$$G(y, x, \Delta t) = \frac{1}{(4\pi D\Delta t)^{3N/2}} \exp(-(y - x - DF(x)\Delta t)^2/4D\Delta t)$$

Now equation 5 from Metropolis algorithm changes to

$$\frac{p_i T_{i\to j}}{p_j T_{j\to i}} = \frac{G(x, y, \Delta t)|\Psi_T(y)|^2}{G(y, x, \Delta t)|\Psi_T(x)|^2},$$

and we must calculate the drift force in order to find new moves and the Green's function to accept/reject these moves.

2.5 Gradient Descent

Like most problems in physics the variational quantum problem is one of optimization. In this project we are optimizing the expectation value of the energy over the parameter α. In the naive implementation we simply span a reasonable range of α [1]. For a multi-parameter variational problem this approach is too computationally expensive to implement in most cases. To remedy this problem iterative gradient methods have been developed to make more intelligent choices for the variational parameters. In this project we have opted to implement a simple gradient descent method. The gradient descent is ordinarily presented as

$$\alpha_{i+1} = \alpha_i - \gamma\frac{\partial\langle E_L(\alpha_i)\rangle}{\partial\alpha_i} \tag{6}$$

[1] an implementation of which can be seen in the file `main_b.cpp`

Where we have opted to update the parameter γ iteratively by the Barzilai-Borwein formula which is a method that uses an iterative approach to the step size γ derived in much the same manner as for quasi-Newton methods[1]. The only constraint we have to enforce is that $0 < \alpha$. In the algorithm we have a simple rule that checks the sign of α and makes a correction if it is out-of-bounds. For $i > 0$ the step size γ_i is then given as:

$$\gamma_i = (\alpha_{i+1} - \alpha_i) \cdot \frac{1}{\langle E_L \rangle_{i+1}^{\alpha} - \langle E_L \rangle_i^{\alpha}} \tag{7}$$

We also introduce the notation $\frac{\partial \langle E_L^i \rangle}{\partial \alpha} = \langle E_L \rangle_i^{\alpha}$ for brevity, and the same notation will be used for the tiral wavefunction ψ_T. The partial derivative itself can be found by the equation[2]

$$\langle E_l \rangle_i^{\alpha} = 2 \left(\langle \frac{\psi^{\alpha}}{\psi} E_L \rangle^i - \langle \frac{\psi^{\alpha}}{\psi} \rangle \langle E_L \rangle^i \right) \tag{8}$$

Wherein the fraction of the partial derivative of the wavefunction by the wavefunction must be derived, which is trivial with the ansatz of the wavefunction.

$$\frac{\psi^{\alpha}}{\psi} = \frac{\psi \prod_i^N (x_i^2 + y_i^2 + \beta z_i^2)}{\psi} \tag{9}$$

$$= \prod_i^N (x_i^2 + y_i^2 + \beta z_i^2) \tag{10}$$

This holds for both the interactive and non-interactive case since the correlation wavefunction, $f(r_i, r_j)$, does not have any dependence on α
In the program the only addition to make is the computation of two additional expecation values[3]. Empirically we've also seen that we can reduce the number of MC-cycles quite drastically and still get a good convergence to the optimal α. In summary gradient descent and other associated methods allows for a radical speedup in estimation of the optimal values of the variational parameters. The implementation of this method can be found in the file `main_f.cpp`.

2.6 Blocking Method

For the statistical analysis and error estimates we have used the technique of blocking. We are looking for the expectation value of the ground state energy of our system. In order to say something about how accurate these results are we want to look at the standard deviation.

[2]The equation was retrieved from the lecture notes
[3]implemented in `vmc.cpp`

If our samples where uncorrelated we could calculate the standard deviation through the following equation

$$\sigma = \sqrt{\frac{1}{n-1}\left(\langle E_L^2\rangle - \langle E_L\rangle^2\right)}.$$

It can be showed that for correlated samples the equation for the standard deviation is

$$\sigma = \sqrt{\frac{1+2\tau/\Delta t}{n-1}\left(\langle E_L^2\rangle - \langle E_L\rangle^2\right)}$$

where τ is the time between one sample and the next uncorrelated sample and Δt is the time between each sample. If we knew what τ was we could simply find our σ, but since we don't we use blocking to find it. The method is simple enough, we divide our samples of data into blocks and calculating the mean of each block. So if we have an amount of samples of $\langle E_L\rangle$, we divide these into M blocks and calculate the mean. By plotting the standard deviation as function of the block size we can keep blocking and blocking until we see that the std. dev. stops increasing, and this is where the blocks are uncorrelated. Now we have an estimate for τ and thus the standard deviation.

2.7 Numerical differentiation

To evaluate the local energy of the system as defined in the project it necessary to compute the second derivative of the trial wavefunction ψ_T. We've chosen to implement the numerical differentiation as a finite difference approximation. Let $\mathbf{R}$ be the row major $N \times D$ matrix where N is the number of particles and D is their dimension. Then the second derivative can be found by the procedure listed as algorithm 2

Since the derivative involves three function calls for each particle the numerical derivative will obviously be quite computationally expensive. It is noted that the differentiation could be substantially optimized from the version included in the code, but is outside the scope of this project.

2.8 One-body densities

The one body density can be defined in terms of an arbitrary position vector $\mathbf{r}_1$ as

$$\rho(\mathbf{r}_1) = \int d\mathbf{r}_2 \ldots d\mathbf{r}_N |\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2 \tag{11}$$

It's a useful size to compute since it relates the number of particles in the simulation to the density by way of equation 12

$$N = \int d\mathbf{r}\rho(\mathbf{r}) \tag{12}$$

It also provides a complete picture of the relative distribution of particles. Which can be used to visually identify the ground state[4].

[4]In the odd case where the computation of $\frac{\partial\langle E_L(\alpha_i)\rangle}{\partial\alpha_i}$ for variational optimization is unavailable or too

Data: matrix $\mathbf{R}$
Result: float $\nabla^2\psi_T(R)$

$\Delta = 0$
$\mathbf{R_p} = \mathbf{R}$
$\mathbf{R_m} = \mathbf{R}$
for i *in* $[0, N-1]$ **do**
    for j *in* $[0, D-1]$ **do**
        $\mathbf{R_p}(i,j) += h$
        $\mathbf{R_m}(i,j) -= h$
        $\Delta = \psi_T(\mathbf{R_p}) + \psi_T(\mathbf{R_m}) - 2\psi_T(\mathbf{R})$
        $\mathbf{R_p}(i,j) -= h$
        $\mathbf{R_m}(i,j) += h$
    end
end
return $\frac{\Delta}{h^2}$

Algorithm 2: Numerical differentiation of the second order of the trial wavefunction on a system $\mathbf{R}$

cumbersome one could ostensibly use very simple ML algorithms to optimize the variational parameter.

3 Results

1a): Local energy

The local energy is derived and presented in appendix B.1

1b): Developing your code and 1d): A better statistical analysis

The results of the simulations are included in the appendix A.1as figures 4 5, 6 and 7. The results were produced with the file `main_b.cpp`[5]. Errors in the expectation value for the energy in the plots are computed with the blocking method[6]. The errors are presented as errorbars in the plots referenced above. The exact answer for the minimum of the expecation value of the energy can be derived from equation 29. The minimum of the local energy has to be where the kinetic and potential energies cancel exactly. In the case of the 3d particle we see the following after imposing units in terms of the characteristic lengths and frequencies of the harmonic oscillator.

$$\min(E_L) \implies \left(\frac{1}{2}\right)[4\alpha^2(x^2+y^2+\beta^2 z^2)] = \frac{1}{2}(x^2+y^2+\beta z^2) \tag{13}$$

$$2\alpha^2 = \frac{1}{2} \tag{14}$$

$$\alpha = 0.5 \tag{15}$$

With α at the minimum we then expect the following values for $\langle E \rangle$

$$\begin{aligned} \text{1D: } E_L|_{\alpha=0.5} &= \sum_i^N \alpha = N\alpha, \\ \text{2D: } E_L|_{\alpha=0.5} &= \sum_i^N 2\alpha = 2N\alpha \\ \text{3D: } E_L|_{\alpha=0.5} &= \sum_i^N 2\alpha + \alpha\beta = 3N\alpha \end{aligned} \tag{16}$$

In general the energy in the non-interactive case at the variational minimum for our trial wavefunction can then be expressed as

$$\min(\langle E[\alpha] \rangle) = 0.5 \cdot N \cdot D \tag{17}$$

Where N is the number of particles and D is their dimension. From the figures referenced in the beginning of this section it is clear that both the numerical and analytic solutions

[5] at commit `b0ff612bc6666335b106af5e22a7a13a13c7cff7`

[6] the blocking implementation is a copy of the code in Ref. [2]

N	α	σ^2	$\langle E_L \rangle$	$\frac{\langle E_L \rangle}{N}$	CPU-time [sek]
10	0.480013	1.73405e-06	21.643	2.1643	12.31
50	0.480127	1.75833e-06	111.066	2.2213	1253.91
100	0.480279	1.75902e-06	228.682	2.2868	9854.01

Table 1: VMC with Metropolis sampling. Calculations done in 3 dimensions with number of cycles $N_{MC} = 10^6$ for an elliptical trap, $\beta = 2.82843$ with interaction, $a = 0.0043$. Step length $t = 0.5$.

have a minimum at that agrees with the analytical solution. The intervals were chosen such that the known optimum for α was included, this information in in general not available and motivated the gradient descent algorithm implemented for task 1.f. From the figures referenced above it is also noted that there is a substantial time difference in the numeric and analytic algorithms.

1e: The repulsive interaction

In Table 1 we see the results for the case of the elliptical trap with a repulsive interaction. We have used the Hamiltonian in Equation 34 to solve this case. The analytic solution of the local energy can be found in Appendix 1. The code that was used to find these results can be found `gaussian_inter_analytic.cpp`[7]. We have used $a = 0.0043$ and $\beta = 2.82843$. We see that the expectation value of the local energy increases slowly as we increase the number of particles. It can seem that this is the case of the variational parameter α as well. As for the CPU-time it increases rapidly. Already for 100 particles we are closing in one 3 hours.

1f: Finding the best parameter

Applying the gradient descent algorithm to tune the variational parameter resulted in satisfying convergence to the optimal value for the variational parameter α. The simulation results are included in figure 1[8]. After the convergence was shown to be satisfactory for the non-interactive case simulations were run for the hamiltonian with interaction [9]. The resulting minimum for the variational parameter is slightly lower than for the non-interactive case with a value of $\alpha_{min} \approx 0.49888\ldots$. These findings are illustrated in figure 2.

[7] at commit `d1c9ec9cc5640e7030b18adbabc802d2414dba75`

[8] The simulations were produced with the file `mainf_f.cpp` at commit `2d03030ec5a711383d582dde23869483d122c6b6`

[9] commit `f285327a7d95349a874aafe16d8ecd5f48c5cef5`

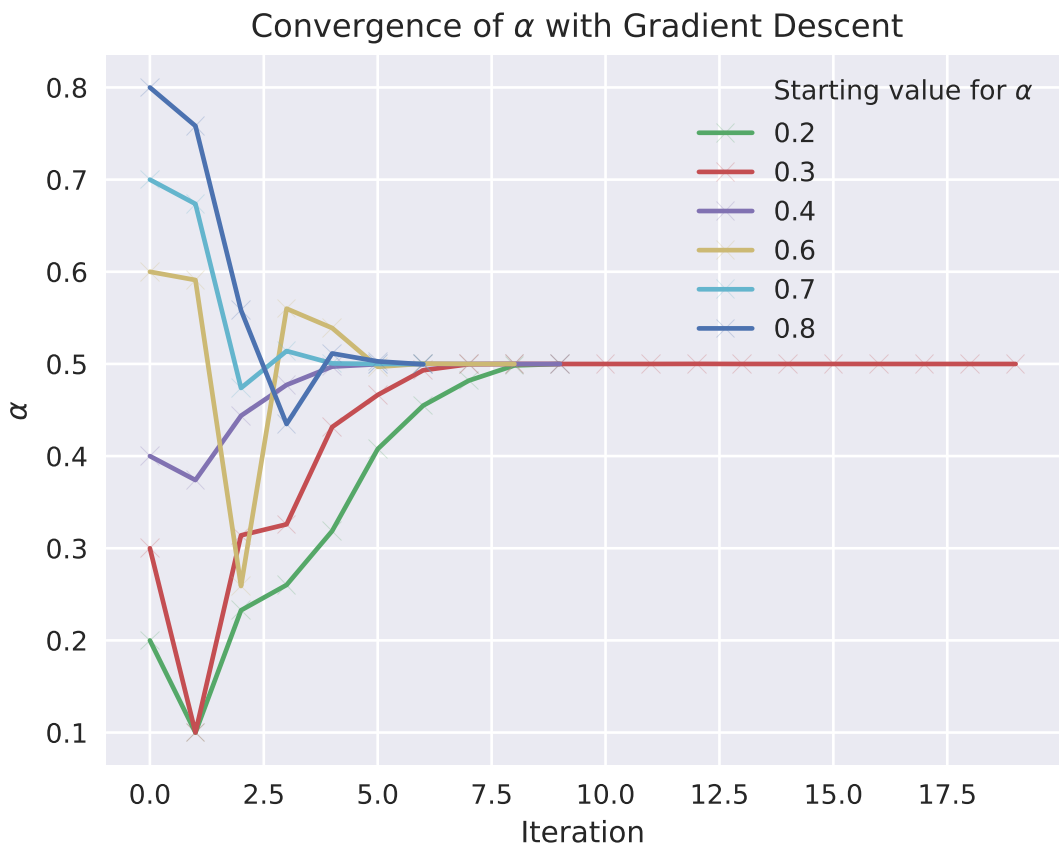


Figure 1: Finding the optimal α with GD. This plot show the number of iterations it took to reach the minimum for the non-interactive spherical trap.

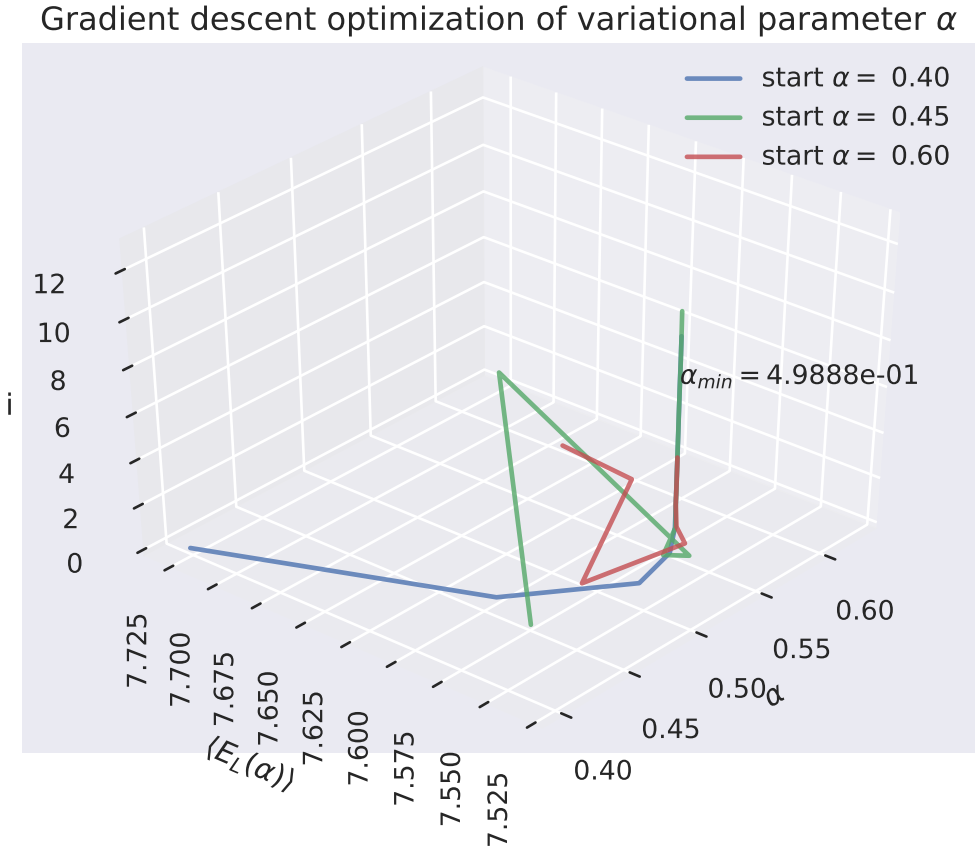


Figure 2: Finding the optimal α with GD. This plot shows the first central moment for the local energy on the y-axis, the variational parameter on the x axis and the GD iteration number on the z-axis for the interactive spherical trap. We observe that the GD algorithm finds a satisfyingly stable minimum with few iterations

1g: Onebody densities

The onebody density was computed by counting particles in equipartitioned bins around the origo. The origo was chosen as a referemce because it is the natural focal point of particles in the harmonic oscillator trap we implemented. The bins were equipartitioned by a set step length trivially determined as $\Delta L = L/n_{bins}$ where L denotes the endpoint of the interval and n_{bins} the total number of bins. Each of those bins were normalized by the total count number and a factor corresponding to the difference in physical space occupied by each bin i.e. 1 for the $1D$ case, r for the $2D$ case and finally r^2 for the $3D$ case. The implementation of the algorithm can be found in `vmc.cpp`. A simulation was run to compute the onebody densities for both the interactive and non-interacitve case for the respective minimas of the variational parameter α. The result of this simulation is shown in figure 3 [10]

[10] at commit `c9c91eaaaadf97f48e5130ab927667038eebcfcc`

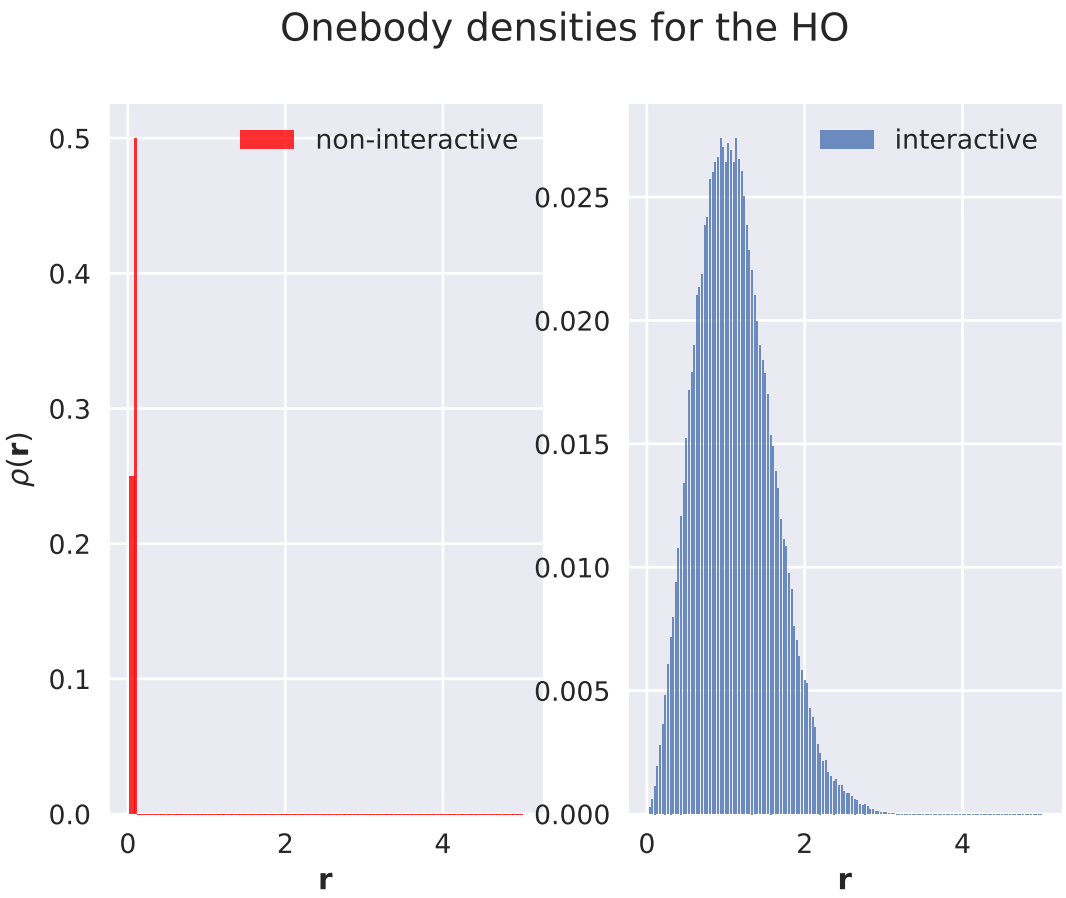


Figure 3: With the optimal parameters for alpha the onebody densities are computed and shown above. We observe that the jastrow factor has a large and pronounced effect on the relative distribution of particles. Additionally we note that for the non-interactive case we expect a density that approximates a delta function as figuratively all bosons will be in the HO ground state.

4 Discussion

5 Non interacting bosons

We've observed that for non-interactive bosons we are able to find an analytical minimum for the local energy, that we've used as a reference to assert that the VMC machinery indeed produces the correct result. As noted in task 1b this information is not in general something that is available to us. Methods like gradient descent ad variations thereof must then be considered. We implemented a GD algorithm that converged fast, and with relatively few MC-cycles, to a stable minimum for α. More complex methods were not considered since we knew the problem to be quadratic, and thus well behaved in that the search space only has one minimum. As and additional metric on the system we computed the one-body desities which shows a delta like behaviour in the non-interactive regime. The physical interpretation of this is that the particles are all very close to eachother and the origio. The authors did not find any demonstrations of the onebody density for bosons in the BEC in a HO trap in the litterature so comparison weren't readily available.

We have also shown that there is, unsurprisingly, a large chunk of time lost by doing numerical estimations of the local energy. While trivial to implement and compute it is only useful as a sanity-check for the analytical solution for many body systems where an analytic derivative is available. Both the numeric and analytic simulations were run with the `-O3` optimization flag.

There is also shown to be experimental indications of the hypothesis [11] that the ground state of the ensamble of bosons also is the one that has the lowest variance in the VMC scheme by presenting the relative error in the measurment of $\langle E_L \rangle$

6 Interacting bosons

In the case of the elliptical trap with interaction we observe the expectation value of the local energy to increases by a small amount as we increase the number of particles in the system. This is consistent with what we see in Fig. 2 in (ref. to paper in Physics by J.L. DuBois). As the density of the gas increases so should the energy. We are able to find an optimal value for α, not without difficulties though. With an analytic solution with many terms something is bound to go wrong. Also with the amount of time it takes to numerically solve the interactive case it is important know the code produces the correct answers. However we are happy with the results.

The onebody densities of the bosons in the ground state was shown to be distributed according to a normal distribution [12]. Which shows a large effect of the jastrow factor on the density, as the shape is nearly delta-function distributed for the non-interactive case.

[11] theory, assumption?

[12] This should probably be rigorously tested, but we didn't

7 Conclusion

Herein lies the conclusions of yonder project, verily I say!

A Figures

A.1 1b)

In the figure title the information about the simulation is noted. NM denotes that a brute force metropolis algorithm was used. The errorbars are computed by a blocking algorithm implemented in `anal_b.py`

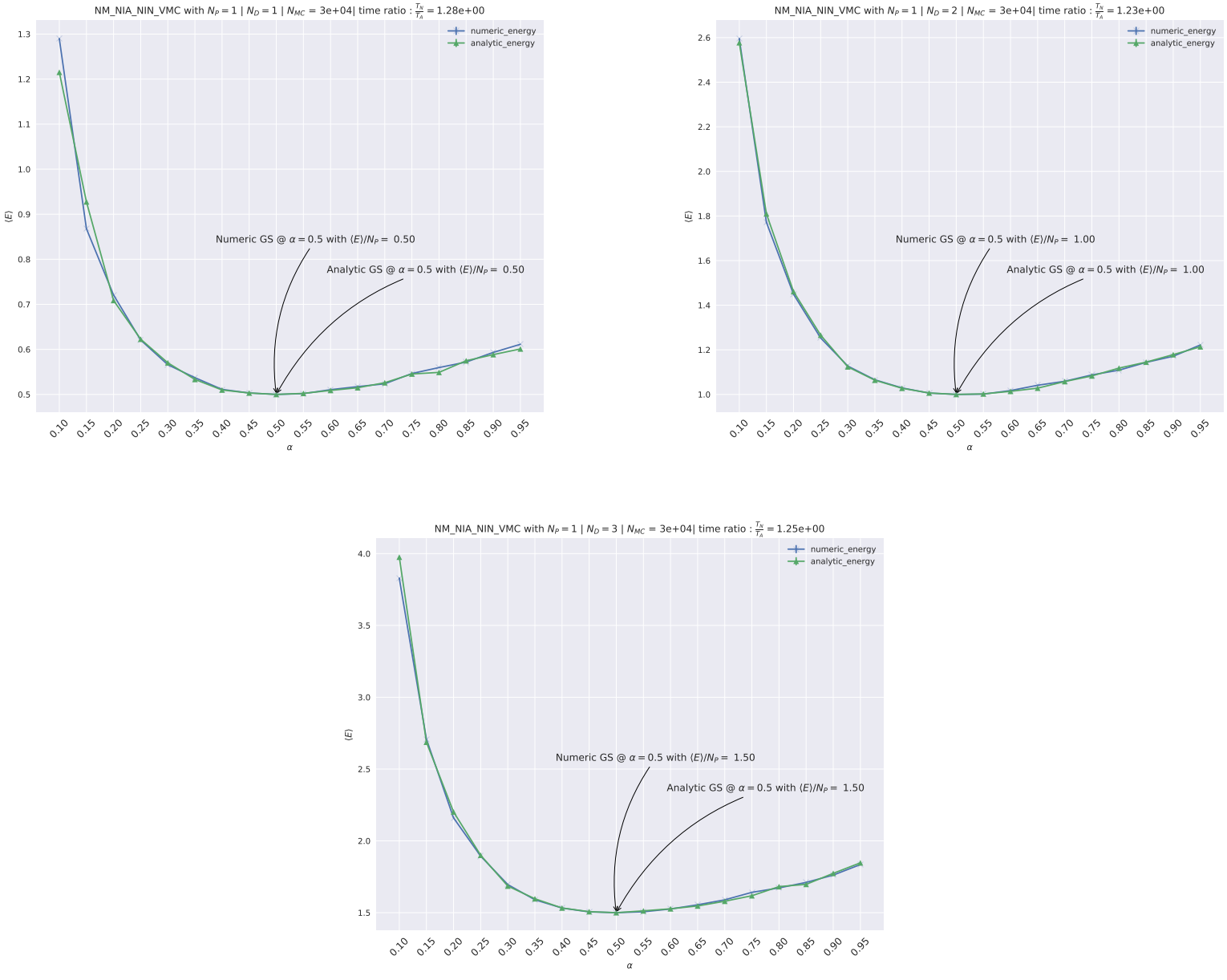


Figure 4: Plots for simulations with 1 particle and 1-3 dimensions. The CPU time difference is noted in the figure captions

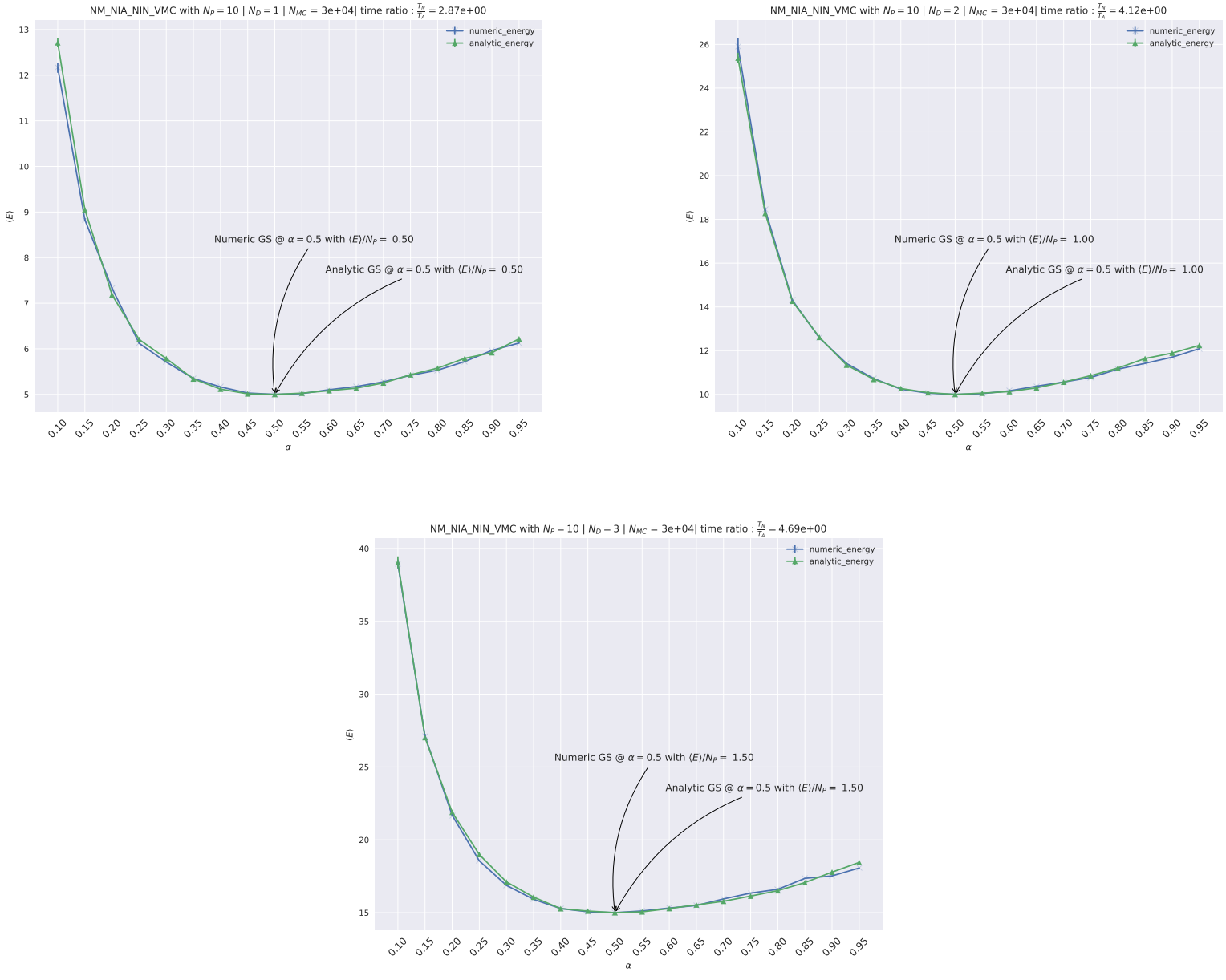


Figure 5: Plots for simulations with 10 particles and 1-3 dimensions. The CPU time difference is noted in the figure captions

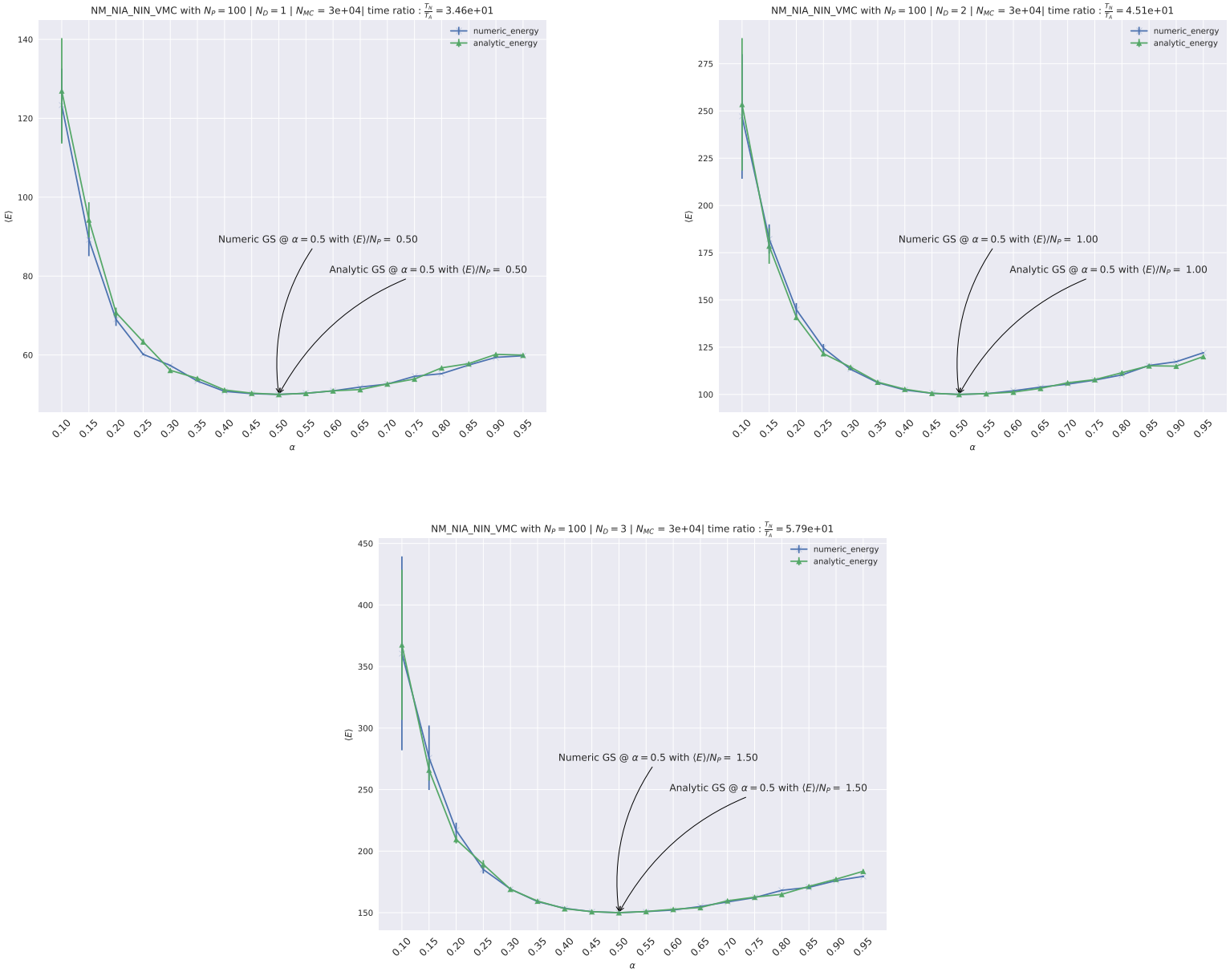
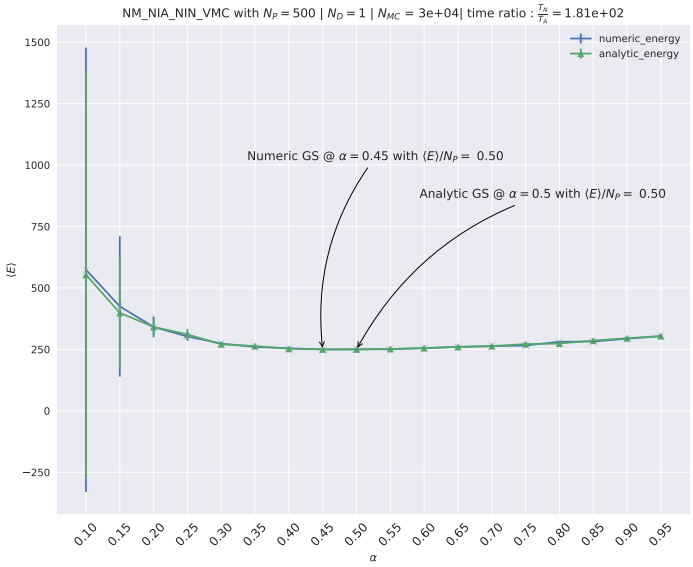
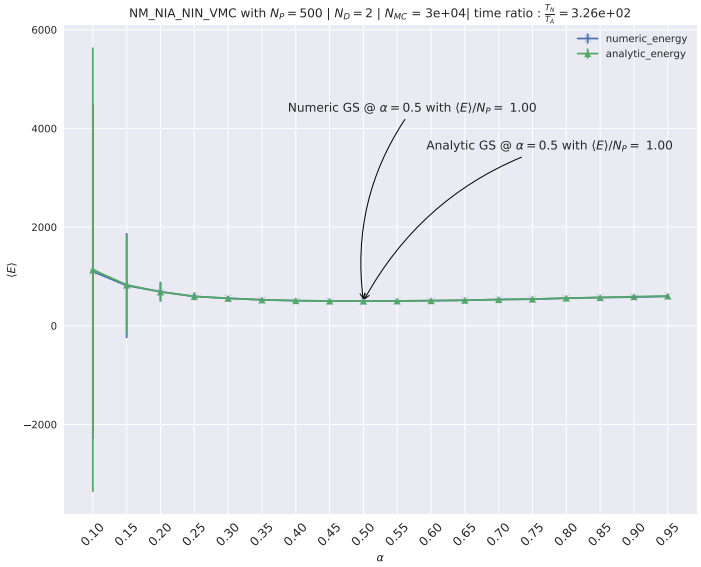


Figure 6: Plots for simulations with 100 particles and 1-3 dimensions. The CPU time difference is noted in the figure captions





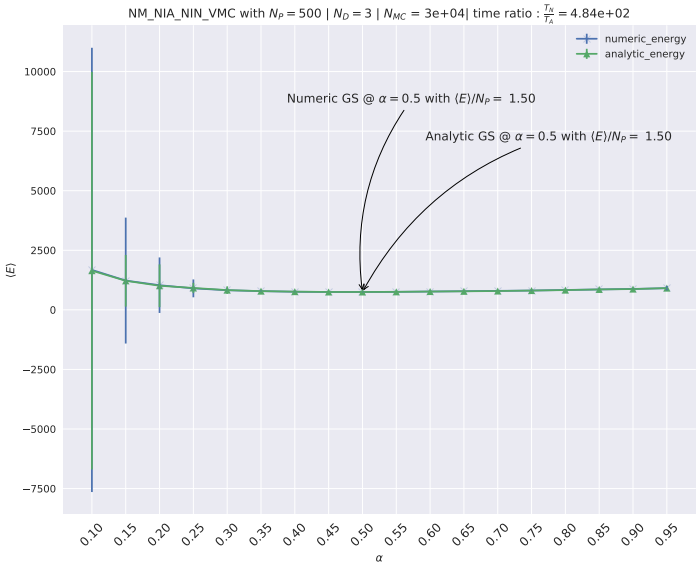


Figure 7: Plots for simulations with 500 particles and 1-3 dimensions. The CPU time difference is noted in the figure captions

B Derivations

B.1 Local energy

The local energy is given by

$$E_L(\mathbf{r}) = \frac{1}{\Psi_T(\mathbf{r})}\hat{H}\Psi_T(\mathbf{r})$$

with trial wave equation

$$\Psi_T(\mathbf{r}) = \prod_i g(\alpha, \beta, \mathbf{r_i}) \prod_{i<j} f(a, |\mathbf{r_i} - \mathbf{r_j}|)$$

The Hamiltonian becomes

$$\hat{H} = \sum_i^N \left(\frac{-\hbar^2}{2m}\nabla_i^2 + V_{ext}(\mathbf{r_i}) \right) + \sum_{i>j}^N V_{int}(\mathbf{r_i}, \mathbf{r_j})$$

where

$$V_{ext}(\mathbf{r_i}) = \begin{cases} \frac{1}{2}m\omega_{ho}^2 r^2 & (S) \\ \frac{1}{2}m[\omega_{ho}^2(x^2+y^2) + \omega_z^2 z^2] & (E) \end{cases}$$

and

$$V_{int}(|\mathbf{r_i} - \mathbf{r_j}|) = \begin{cases} \infty & |\mathbf{r_i} - \mathbf{r_j}| \leq a \\ 0 & |\mathbf{r_i} - \mathbf{r_j}| > a \end{cases}$$

First we solve only the harmonic oscillator (a=0) and we use $\beta = 1$ for one particle in 1D. And for one particle the trial wave equation, Hamiltonian and local energy becomes

$$\Psi_T(\mathbf{r}) = g(\alpha, x) = e^{-\alpha x_i^2}, \tag{18}$$

$$\hat{H} = \left(\frac{-\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega_{ho}^2 x^2 \right) \tag{19}$$

$$E_L = \frac{1}{e^{-\alpha x^2}} \left(\frac{-\hbar^2}{2m}\nabla^2(e^{-\alpha x^2}) + \frac{1}{2}m\omega_{ho}^2 x^2 (e^{-\alpha x^2}) \right) \tag{20}$$

We then need to compute the laplacian of the trial wave-function.

$$\nabla^2(e^{-\alpha x^2}) = \frac{d^2 e^{-\alpha x^2}}{dx^2} \tag{21}$$

$$= \frac{d}{dx}\left(\frac{de^{-\alpha x^2}}{dx}\right) \tag{22}$$

$$= \frac{d}{dx}(-2\alpha x \cdot e^{-\alpha x^2}) \tag{23}$$

$$= (4\alpha^2 x^2 - 2\alpha)e^{-\alpha x^2} \tag{24}$$

Finally, the local energy becomes

$$E_L = \frac{e^{-\alpha x^2}}{e^{-\alpha x^2}}\left(\frac{-\hbar^2}{2m}(4\alpha^2 x^2 - 2\alpha) + \frac{1}{2}m\omega_{ho}^2 x^2\right) \tag{25}$$

$$E_L = \frac{-\hbar^2}{2m}(4\alpha^2 x^2 - 2\alpha) + \frac{1}{2}m\omega_{ho}^2 x^2 \tag{26}$$

Solving the same problem for one particle in 2D and 3D we get something similar,

$$E_L = (\frac{-\hbar^2}{2m})4\alpha^2(x^2 + y^2) - 4\alpha + \frac{1}{2}m\omega_{ho}^2(x^2 + y^2), \tag{27}$$

$$E_L = (\frac{-\hbar^2}{2m})4\alpha^2(x^2 + y^2 + z^2) - 6\alpha + \frac{1}{2}m\omega_{ho}^2(x^2 + y^2 + z^2) \tag{28}$$

We can now easily see that the local energy energy for N number of particles in 1D, 2D and 3D becomes

$$\begin{aligned}
&\text{1D: } E_L = \sum_i^N (\frac{-\hbar^2}{2m})[4\alpha^2(x^2) - 2\alpha] + \frac{1}{2}m\omega_{ho}^2(x^2), \\
&\text{2D: } E_L = \sum_i^N (\frac{-\hbar^2}{2m})[4\alpha^2(x^2 + y^2) - 4\alpha] + \frac{1}{2}m\omega_{ho}^2(x^2 + y^2) \\
&\text{3D: } E_L = \sum_i^N (\frac{-\hbar^2}{2m})[4\alpha^2(x^2 + y^2 + \beta^2 z^2) - 4\alpha - 2\alpha\beta] + \frac{1}{2}m\omega_{ho}^2(x^2 + y^2 + \beta z^2)
\end{aligned} \tag{29}$$

since the energy is simply the sum of the derivatives of each particle.
Now we can try to solve the complete problem. The trial wave function is now

$$\Psi_T(\mathbf{r}) = \prod_i g(\alpha, \beta, \mathbf{r_i}) \prod_{i<j} f(a, |\mathbf{r_i} - \mathbf{r_j}|)$$

and first we rewrite it using

$$g(\alpha, \beta, \mathbf{r_i}) = \exp -\alpha(x_i^2 + y_i^2 + \beta z_i^2) = \phi(\mathbf{r_i})$$

and

$$f(r_{ij}) \exp\left(\sum_{i<j} u(r_{ij})\right)$$

getting

$$\Psi_T(\mathbf{r}) = \prod_i \phi(r_i) \exp\left(\sum_{i<j} u(r_{ij})\right).$$

The local energy for this problem becomes:

$$E_L = \frac{1}{\Psi_T(\boldsymbol{r})}\left(\sum_i^N \left(\frac{\hbar^2}{2m}\nabla_i^2 \Psi_T(\mathbf{r}) + \frac{1}{2} m\omega_{ho}^2 r^2 \Psi_T(\mathbf{r})\right) + \sum_{i<j}^N V_{int}(\mathbf{r_i}, \mathbf{r_j})\Psi_T(\mathbf{r})\right). \quad (30)$$

The difficulty in (30) is solving the derivatives of the wave equation given the complexity of the exponential. We begin with the first derivative.

$$\nabla_i^2 \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij})\right) = \nabla_i \cdot \nabla_i \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij})\right)$$

The first derivative of particle k:

$$\nabla_k \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij})\right) = \nabla_k \left(\prod_i \phi(\mathbf{r_i})\right) \exp\left(\sum_{i<j} u(r_{ij})\right) + \nabla_k \left(\exp\left(\sum_{i<j} u(r_{ij})\right)\right) \prod_i \phi(r_i)$$

$$\begin{aligned}
\nabla_k \left(\prod_i \phi(\mathbf{r_i}) \right) &= \nabla_k (\phi(r_1)(\phi(r_2)...(\phi(r_k)..(\phi(r_N)) \\
&= \nabla_k \left(e^{-\alpha(x_1^2+y_1^2+z_1^2)} e^{-\alpha(x_2^2+y_2^2+z_2^2)} ... e^{-\alpha(x_k^2+y_k^2+z_k^2)} ... e^{-\alpha(x_N^2+y_N^2+z_N^2)} \right) \\
&= \nabla_k \phi(r_k) \left[\prod_{i \neq k} \phi(\mathbf{r_i}) \right] \\
\nabla_k \exp \left(\sum_{i<j} u(r_{ij}) \right) &= \nabla_k \exp(u(r_{12}) + u(r_{13}) + ... + u(r_{23}) + ... + u(r_{kj}) + .. + u(r_{N-1,N})) \\
&= \exp \left(\sum_{i<j} u(r_{ij}) \right) \sum_{i \neq k} \nabla_k u(r_{kj})
\end{aligned}$$

And the first derivative of the trial wave equation is

$$\nabla_k \Psi_T(\mathbf{r}) = \nabla_k \phi(r_k) \left[\prod_{i \neq k} \phi(\mathbf{r_i}) \right] \exp \left(\sum_{i<j} u(r_{ij}) \right) + \prod_i \phi(\mathbf{r_i}) \exp \left(\sum_{i<j} u(r_{ij}) \right) \sum_{j \neq k} \nabla_k u(r_{kj}).$$

Now we find the second derivative of the wave function.

$$\frac{1}{\Psi_T(\mathbf{r})}\nabla_k^2\Psi_T(\mathbf{r}) = \frac{1}{\nabla_k \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij})\right)} \left(\nabla_k \left(\nabla_k \phi(r_k) \left[\prod_{i\neq k} \phi(\mathbf{r_i}) \right] \right) \cdot \exp\left(\sum_{i<j} u(r_{ij}) \right) \right.$$

$$+ \nabla_k \phi(r_k) \left[\prod_{i\neq k} \phi(\mathbf{r_i}) \right] \cdot \nabla_k \left(\exp\left(\sum_{i<j} u(r_{ij}) \right) \right)$$

$$+ \nabla_k \left(\prod_i \phi(\mathbf{r_i}) \right) \cdot \exp\left(\sum_{i<j} u(r_{ij}) \right) \sum_{j\neq k} \nabla_k u(r_{kj})$$

$$+ \prod_i \phi(\mathbf{r_i}) \cdot \nabla_k \left(\exp\left(\sum_{i<j} u(r_{ij}) \right) \right) \sum_{j\neq k} \nabla_k u(r_{kj})$$

$$\left. + \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij}) \right) \cdot \nabla_k \left(\sum_{j\neq k} \nabla_k u(r_{kj}) \right) \right)$$

Solving these equations separately makes it easier.

$$\frac{\nabla_k^2 \phi(r_k) \left[\prod_{i\neq k} \phi(\mathbf{r_i}) \right] \cdot \exp\left(\sum_{i<j} u(r_{ij}) \right)}{\nabla_k \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij}) \right)} = \frac{\nabla_k^2 \phi(r_k)}{\phi(r_k)}$$

$$\frac{\nabla_k \phi(r_k) \left[\prod_{i\neq k} \phi(\mathbf{r_i}) \right] \cdot \nabla_k \left(\exp\left(\sum_{i<j} u(r_{ij}) \right) \right)}{\nabla_k \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij}) \right)} = \frac{\nabla_k \phi(r_k)}{\phi(r_k)} \sum_{j\neq k} \nabla_k u(r_{kj})$$

$$\frac{\nabla_k \left(\prod_i \phi(\mathbf{r_i}) \right) \cdot \exp\left(\sum_{i<j} u(r_{ij}) \right) \sum_{j\neq k} \nabla_k u(r_{kj})}{\nabla_k \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij}) \right)} = \frac{\nabla_k \phi(r_k)}{\phi(r_k)} \sum_{j\neq k} \nabla_k u(r_{kj})$$

$$\frac{\prod_i \phi(\mathbf{r_i}) \cdot \nabla_k \left(\exp\left(\sum_{i<j} u(r_{ij}) \right) \right) \sum_{j\neq k} \nabla_k u(r_{kj})}{\nabla_k \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij}) \right)} = \sum_{i\neq k} \nabla_k u(r_{ki}) \sum_{j\neq k} \nabla_k u(r_{kj})$$

$$\frac{\prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij})\right) \cdot \nabla_k \left(\sum_{j\neq k} \nabla_k u(r_{kj})\right)}{\nabla_k \prod_i \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij})\right)} = \sum_{j\neq k} \nabla_k^2 u(r_{kj})$$

Putting them together again we get the following

$$\frac{1}{\Psi_T(\mathbf{r})}\nabla_k^2 \Psi_T(\mathbf{r}) = \frac{\nabla_k^2\phi(r_k)}{\phi(r_k)} + 2\frac{\nabla_k\phi(r_k)}{\phi(r_k)} \sum_{j\neq k} \nabla_k u(r_{kj}) + \sum_{i\neq k} \nabla_k u(r_{ki}) \sum_{j\neq k} \nabla_k u(r_{kj}) + \sum_{j\neq k} \nabla_k^2 u(r_{kj}) \tag{31}$$

We solve the first and second derivatives of $u(r_{kj})$.

$$\nabla_k u(r_{kj}) = \left(\vec{i}\frac{\partial}{\partial x_k} + \vec{j}\frac{\partial}{\partial y_k} + \vec{k}\frac{\partial}{\partial z_k}\right) u(r_{kj}) \tag{32}$$

From Rottmann p. 128 we have that

$$\begin{aligned}
\frac{\partial u(r_{kj})}{\partial x_k}\,\vec{i} &= \frac{\partial u(r_{kj})}{\partial r_{kj}}\frac{\partial r_{kj}}{\partial x_k}\,\vec{i} \\
&= u'(r_{kj})\frac{\partial\sqrt{|x_k - x_j|^2 + |y_k - y_j|^2 + |z_k - z_j|^2}}{\partial x_k}\vec{i} \\
&= u'(r_{kj})\frac{1}{2}2|x_k - x_j|\frac{1}{r_{kj}}\vec{i} \\
&= \frac{u'(r_{kj})|x_k - x_j|}{r_{kj}}\vec{i} \\
\frac{\partial u(r_{kj})}{\partial y_k}\,\vec{j} &= \frac{u'(r_{kj})|y_k - y_j|}{r_{kj}}\vec{j} \\
\frac{\partial u(r_{kj})}{\partial z_k}\,\vec{k} &= \frac{u'(r_{kj})|z_k - z_j|}{r_{kj}}\vec{k}
\end{aligned}$$

where we have used the fact that $r_{kj} = \sqrt{|x_k - x_j|^2 + |y_k - y_j|^2 + |z_k - z_j|^2}$. Now equation (32) becomes

$$\begin{aligned}
\nabla_k u(r_{kj}) &= u'(r_{kj})\frac{(|x_k - x_j|\vec{i} + |y_k - y_j|\vec{j} + |z_k - z_j|\vec{k})}{r_{kj}} \\
&= u'(r_{kj})\frac{(\boldsymbol{r_k} - \boldsymbol{r_j})}{r_{kj}}.
\end{aligned}$$

And for the second derivative have that

$$\nabla_k^2 u(r_{kj}) = \left(\frac{\partial^2}{\partial x_k^2} + \frac{\partial^2}{\partial y_k^2} + \frac{\partial^2}{\partial z_k^2}\right) u(r_{kj}) \tag{33}$$

and use Rottmann p. 128 again and see that

$$\begin{aligned}
\frac{\partial^2 u(r_{kj})}{\partial x_{kj}^2} &= \frac{\partial^2 u(r_{kj})}{\partial r_{kj}^2}\left(\frac{\partial r_{kj}}{\partial x_{kj}}\right)^2 + \frac{\partial u(r_{kj})}{\partial r_{kj}}\frac{\partial^2 r_{kj}}{\partial x_{kj}^2} \\
&= u''(r_{kj})\frac{(x_k - x_j)^2}{r_{kj}^2} + u'(r_{kj})\frac{\partial^2 r_{kj}}{\partial x_{kj}^2} \\
\frac{\partial^2 r_{kj}}{\partial x_{kj}^2} &= \frac{\partial^2 \sqrt{|x_k - x_j|^2 + |y_k - y_j|^2 + |z_k - z_j|^2}}{\partial x_{kj}^2} \\
&= \frac{\partial \frac{x_k - x_j}{\sqrt{|x_k - x_j|^2 + |y_k - y_j|^2 + |z_k - z_j|^2}}}{\partial x_{kj}} \\
&= \frac{r_{kj} - \frac{1}{2}(x_k - x_j)\cdot\frac{2(x_k - x_j)}{r_{kj}}}{r_{kj}^2} \\
&= \frac{1}{r_{kj}} - \frac{(x_k - x_j)^2}{r_{kj}^3}.
\end{aligned}$$

These equations put together and solving with respect to y and z we get

$$\begin{aligned}
\frac{\partial^2 u(r_{kj})}{\partial x_{kj}^2} &= u''(r_{kj})\frac{(x_k - x_j)^2}{r_{kj}^2} + u'(r_{kj})\left(\frac{1}{r_{kj}} - \frac{(x_k - x_j)^2}{r_{kj}^3}\right), \\
\frac{\partial^2 u(r_{kj})}{\partial y_{kj}^2} &= u''(r_{kj})\frac{(y_k - y_j)^2}{r_{kj}^2} + u'(r_{kj})\left(\frac{1}{r_{kj}} - \frac{(y_k - y_j)^2}{r_{kj}^3}\right), \\
\frac{\partial^2 u(r_{kj})}{\partial z_{kj}^2} &= u''(r_{kj})\frac{(z_k - z_j)^2}{r_{kj}^2} + u'(r_{kj})\left(\frac{1}{r_{kj}} - \frac{(z_k - z_j)^2}{r_{kj}^3}\right).
\end{aligned}$$

Now we can add them all together and equation (33) becomes

$$\begin{aligned}
\nabla_k^2 u(r_{kj}) &= \frac{u''(r_{kj})}{r_{kj}^2}((x_k - x_j)^2 + (y_k - y_j)^2 + (z_k - z_j)^2) \\
&\quad + u'(r_{kj})\left(\frac{3}{r_{kj}} - \frac{(x_k - x_j)^2 + (y_k - y_j)^2 + (z_k - z_j)^2}{r_{kj}^3}\right) \\
&= \frac{u''(r_{kj})r_{kj}^2}{r_{kj}^2} + u'(r_{kj})\left(\frac{3}{r_{kj}} - \frac{r_{kj}^2}{r_{kj}^3}\right) \\
&= u''(r_{kj}) + u'(r_{kj})\frac{2}{r_{kj}}
\end{aligned}$$

Now we can write out the complete second derivative, equation (31)

$$\frac{1}{\Psi_T(\mathbf{r})}\nabla_k^2\Psi_T(\mathbf{r}) = \frac{\nabla_k^2\phi(r_k)}{\phi(r_k)} + 2\frac{\nabla_k\phi(r_k)}{\phi(r_k)}\sum_{j\neq k}\frac{(\boldsymbol{r_k}-\boldsymbol{r_j})}{r_{kj}}u'(r_{kj}) + \sum_{ij\neq k}\frac{(\boldsymbol{r_k}-\boldsymbol{r_i})}{r_{ki}}\frac{(\boldsymbol{r_k}-\boldsymbol{r_j})}{r_{kj}}u'(r_{ki})u'(r_{kj}) + \sum_{j\neq k}\left(u''(r_{kj}) + \frac{2}{r_{kj}}u'(r_{kj})\right).$$

For the full analytical solution of the interacting problem we solve each term by it self.

$$\begin{aligned}\frac{1}{\phi(r_k)}\nabla_k^2\phi(r_k) &= \frac{\nabla_k^2\ exp(-\alpha(x_k^2+y_k^2+\beta z_k^2))}{exp(-\alpha(x_k^2+y_k^2+\beta z_k^2))}\\ &= ((2\alpha(2\alpha x_k^2-1)) + (2\alpha(2\alpha y_k^2-1)) + (2\alpha\beta(2\alpha\beta z_k^2-1)))\cdot\frac{\phi(r_k)}{\phi(r_k)}\\ &= -4\alpha^2 - 2\alpha\beta + 4\alpha^2(x_k^2+y_k^2+\beta z_k^2)\end{aligned}$$

$$\begin{aligned}\frac{1}{\phi(r_k)}\nabla_k\phi(r_k) &= \frac{\nabla_k\ exp(-\alpha(x_k^2+y_k^2+\beta z_k^2))}{exp(-\alpha(x_k^2+y_k^2+\beta z_k^2))}\\ &= (2\alpha x_k\vec{i} + 2\alpha y_k\vec{j} + 2\alpha\beta z_k\vec{k})\cdot\frac{\phi(r_k)}{\phi(r_k)}\\ &= (2\alpha x_k\vec{i} + 2\alpha y_k\vec{j} + 2\alpha\beta z_k\vec{k})\end{aligned}$$

Wolfram alpha gives to solution the first and second derivatives of function $u(r_{kj})$.

$$\begin{aligned}u'(r_{kj}) &= \frac{d(\ln f(r_{kj}))}{dr_{kj}}\\ &= \frac{d\ \ln\left(1-\frac{a}{(r_k-r_j)}\right)}{dr_{kj}}\\ &= -\frac{a}{ar_{kj}-r_{kj}^2}\end{aligned}$$

$$\begin{aligned}u''(r_{kj}) &= \frac{d^2(\ln f(r_{kj}))}{dr_{kj}^2}\\ &= \frac{a(a-2r_{kj})}{r_{kj}^2(a-r_{kj})^2}\end{aligned}$$

Putting all of this together we end up with the following expression for the second derivative of the wave equation divided by it self:

$$\frac{1}{\Psi_T(\mathbf{r})}\nabla_k^2\Psi_T(\mathbf{r}) = -4\alpha^2 - 2\alpha\beta + 4\alpha^2(x_k^2 + y_k^2 + \beta z_k^2)$$
$$+ 2((2\alpha x_k\vec{i} + 2\alpha y_k\vec{j} + 2\alpha\beta z_k\vec{k}))\sum_{j\neq k}\left(\frac{(x_k - x_j)\vec{i} + (y_k - y_j)\vec{j} + (z_k - z_j)\vec{k}}{r_{kj}}\left(\frac{-a}{ar_{kj} - r_{kj}^2}\right)\right)$$
$$+ \sum_{j\neq k}\left(\frac{(x_k - x_i)\vec{i} + (y_k - y_i)\vec{j} + (z_k - z_i)\vec{k}}{r_{ki}}\right)\left(\frac{(x_k - x_j)\vec{i} + (y_k - y_j)\vec{j} + (z_k - z_j)\vec{k}}{r_{kj}}\right)$$
$$* \left(\frac{-a}{ar_{ki} - r_{ki}^2}\right)\left(\frac{-a}{ar_{kj} - r_{kj}^2}\right)$$
$$+ \sum_{j\neq k}\left(\frac{a(a - 2r_{kj})}{r_{kj}^2(a - r_{kj})^2} + \frac{2}{r_{kj}} - \frac{a}{ar_{kj} - r_{kj}^2}\right)$$

B.2 Drift force

As for the drift force we simply write down the solutions for one particle in 1D, 2D and 3D as they are just the first derivative of the wave function,

$$F = \frac{2\nabla\Psi_T}{\Psi_T}.$$

And are easily solved;

$$F = -4\alpha x,$$

$$F = -4\alpha(x + y),$$

$$F = -4\alpha(x + y + \beta z).$$

For N-particles we must solve $\nabla_k\Psi_T$. In 1D this is

$$\nabla_k\Psi_T = -2\alpha x_k\prod_{k\neq i}^{N} e^{-\alpha x_i^2},$$

$$F_k = -4\alpha x_k\frac{\prod_{k\neq i}^{N} e^{-\alpha x_i^2}}{\prod_i^N e^{-\alpha x_i^2}} = -4\alpha x_k\frac{1}{e^{-\alpha x_k^2}},$$

$$F = \sum_i^N -4\alpha x_i\frac{1}{e^{-\alpha x_i^2}}.$$

And for 2D and 3D;

$$F = \sum_{i}^{N} -4\alpha(x_i + y_i)\frac{1}{e^{-\alpha(x_i^2+y_i^2)}},$$

$$F = \sum_{i}^{N} -4\alpha(x_i + y_i + \beta z_i)\frac{1}{e^{-\alpha(x_i^2+y_i^2+\beta z_i^2)}}.$$

Finally we can solve for N-particles with interaction.
We have already solved the first derivative of the wave equation when we dealt with the local energy problem.

$$\nabla_k \Psi_T(\mathbf{r}) = \nabla_k \phi(r_k) \left[\prod_{i\neq k} \phi(\mathbf{r_i})\right] \exp\left(\sum_{i<j} u(r_{ij})\right) + \prod_{i} \phi(\mathbf{r_i}) \exp\left(\sum_{i<j} u(r_{ij})\right) \sum_{j\neq k} \nabla_k u(r_{kj})$$

$$\begin{aligned}
\nabla_k \phi(r_k) &= \frac{\partial}{\partial x_k} e^{(-\alpha(x_k^2+y_k^2+\beta z_k^2))}\vec{i} \\
&+ \frac{\partial}{\partial y_k} e^{(-\alpha(x_k^2+y_k^2+\beta z_k^2))}\vec{j} \\
&+ \frac{\partial}{\partial z_k} e^{(-\alpha(x_k^2+y_k^2+\beta z_k^2))}\vec{k} \\
&= (-2\alpha x_k \vec{i} - 2\alpha y_k \vec{j} - 2\alpha\beta z_k \vec{k}) e^{(-\alpha(x_k^2+y_k^2+\beta z_k^2))} \\
\nabla_k u(r_{kj}) &= u'(r_{kj}) \frac{(\mathbf{r_k} - \mathbf{r_j})}{r_{kj}} \\
&= -\frac{a(\vec{r_k} - \vec{r_j})}{a r_{kj}^2 - r_{kj})^3}
\end{aligned}$$

$$\nabla_k \Psi_T(\mathbf{r}) = (-2\alpha x_k \vec{i} - 2\alpha y_k \vec{j} - 2\alpha\beta z_k \vec{k}) \Psi_T(\mathbf{r}) + \sum_{j\neq k} \left(-\frac{a(\vec{r_k} - \vec{r_j})}{a r_{kj}^2 - r_{kj})^3}\right) \Psi_T(\mathbf{r})$$

$$F = (-4\alpha x_k \vec{i} - 4\alpha y_k \vec{j} - 4\alpha\beta z_k \vec{k}) + \sum_{j\neq k} \left(-\frac{a(\vec{r_k} - \vec{r_j})}{a r_{kj}^2 - r_{kj})^3}\right)$$

For the elliptical trap we are given an external potential that turns the Hamiltonian to the following

$$\hat{H} = \sum_{i}^{N} \left(\frac{-\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m[\omega_{ho}^2 (x^2 + y^2) + \omega_z^2 z^2] \right) + \sum_{i<j}^{N} V_{int}(\mathbf{r_i}, \mathbf{r_j}).$$

Using that $\omega_{ho} = \omega_\perp$ and $\omega_z = \lambda \omega_{ho}$ we see easily that we can rewrite this to

$$\hat{H} = \sum_{i}^{N} \left(\frac{-\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m\omega_{ho}^2 (x^2 + y^2 + \lambda^2 z^2) \right) + \sum_{i<j}^{N} V_{int}(\mathbf{r_i}, \mathbf{r_j}), \tag{34}$$

which is simply the Hamiltonian for the spherical trap with interaction and $\beta = \gamma = \lambda^2$.

References

[1] Yuan Ya-Xiang Sun, Wenyu. *Optimization Theory and Methods*. springer, 2006.

[2] M Hjorth-Jensen. Computational physics 2: Computational quantum mechanics. `https://github.com/CompPhysics/ComputationalPhysics2`, 2018.