Project 1 - FYS 4411
Bosons trapped in HO potentials

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Abstract

The ground state energy of a Bose-Einstein condensate trapped in an elliptical harmonic oscillator trap is studied using Variational Monte Carlo methods. We consider non-interacting bosons, and also interacting bosons using the hard-shell model. The study is done in 1, 2 and 3 dimensions for up to 500 particles in the non-interacting case and up to 100 in the interacting one. In this context, to choose moves, we implement the Brute Force Metropolis and Importance Sampling methods. In the non-interacting system, the variational method can be solved analytically to find optimal $\alpha = 0.5$. In the interacting case the optimal parameter α is computed through the gradient descent method (e.g. $\alpha(N = 10) = 0.50018 \pm 0.00001$ with a corresponding energy of (24.1917 ± 0.0002), natural units adopted). The one-body density of interacting and non bosons in spherical and elliptical traps is also discussed.
All programs used can be found on the GIT page: `https://github.com/mathisre/FYS4411---Project-1-VMC`.

1 Introduction

The purpose of this project is to study the ground state energy of a Bose-Einstein gas trapped with a spheric or elliptic trap for a different number of particles. A Bose-Einstein gas is a state of matter in which dilute gases of bosons undergo a phase transition when they are cooled to low temperature ($T \to 0$ K). As a result the majority of bosons condense into the system ground state. This gives rise to new quantum phenomena such as super conductivity, super fluidity and quantum turbulence [1]. BEC in dilute gases such as the ones formed of alkali atoms in magnetic traps are described by the Gross-Pitaevskii equation.

In this paper, two cases are studied: one in which bosons don't interact with each other and one in which they interact as if they have hard shells. In the first case the trial many-particle wavefunction proposed is reduced to the product of each single-particle wavefunction which is a gaussian characterised by a variational parameter α. With no interaction, the ground state can be solved exactly. In the case of boson-boson interaction modeled by the hard shell model, a correlation wavefunction term is multiplied in. The potentials used to trap the particles are spherical and elliptical harmonic oscillators.

The ground state energy is computed through Variational Monte Carlo methods, where to propose and accept moves "Brute force" Metropolis and Importance Sampling are implemented. The second one is a much better alternative since it proposes better moves that are more likely to be accepted and thus we waste less computation time on moves that will not be accepted.

In the case considered the kinetic energy can be solved exactly. Therefore there is no need to do a numeric calculation of the second derivative of the many-particle wavefunction. The result is a significant speedup which will be shown.

The variational method allows us to find the an upper limit to the ground state energy which depends on a variational parameter. Therefore the variational parameter α which minimizes the energy is the one that will give the best estimate for the ground state. The gradient descent method is applied to find the optimal

α for both interacting and non case. The non-interacting case is used to prove the efficiency of the method since the best variational parameter can be easily computed.

Eventually the one body density with and without the Jastrow factor is studied by considering the best optimal parameters found through gradient descent method.

The results are presented with an appropriate statistical error computed through blocking method which takes into account correlations between data.

The code is object oriented in order to achieve the best flexibility possible. In principle it should be straightforward to (let us say) change the initial configurations of particles or to study systems of fermions.

2 System description

We consider a gas of N bosons in spherical and elliptical harmonic oscillator potentials. The interaction between bosons in modeled by the hard-shell model. The Hamiltonian of the system is

$$H = \sum_{i=1}^{N} \left[-\frac{1}{2}\frac{\hbar^2}{m}\nabla_i^2 + V_{ext}(\mathbf{r}_i) \right] + \sum_{i \neq k} V_{int}(r_{ik}),$$

where $\Psi_T(\mathbf{R})$ is the trial wavefunction, $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$, $V_{ext}(\mathbf{r})$ is the harmonic oscillator potential given by

$$V_{ext}(\mathbf{r}) = \begin{cases} \frac{1}{2}m\omega_{ho}^2 r^2 & \text{Spherical} \\ \frac{1}{2}m\left[\omega_{ho}^2\left(x^2+y^2\right) + \omega_z^2 z^2\right] & \text{Elliptical} \end{cases}$$

and $V_{int}(r_{ik})$ is the hard-shell interaction potential

$$V_{int}(r_{ik}) = \begin{cases} 0, & r_{ik} > a \\ \infty, & r_{ik} < a. \end{cases}$$

$r_{ik} = |\mathbf{r}_i - \mathbf{r}_k|$ is the distance between particle i and k. a is the size of the interaction between particles.

In our case the trial wavefunction is dependent on the variational parameter α. It is given by

$$\Psi_T(\mathbf{R}, \alpha) = \prod_i \phi(\mathbf{r}_i, \alpha) \prod_{j<i} f(a, r_{ij}), \tag{1}$$

where $\phi\mathbf{r}_i)$ is the macroscopic wavefunction given by

$$\phi(\mathbf{r}_i) = \exp\left(-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\right) \tag{2}$$

and $f(a, r_{ij})$ is the correlation wavefunction that monitors the interaction between particle i and j given by

$$f(a, r_{ij}) = \begin{cases} 0, & r_{ij} > a \\ \left(1 - \frac{a}{r_{ij}}\right), & r_{ij} < a. \end{cases}$$

By setting $u(r_{ij}) = \ln(f(a, r_{ij}))$, we can rewrite the wavefunction eq. (1) as

$$\Psi_T(\mathbf{R}, \alpha) = \prod_i \phi(\mathbf{r}_i, \alpha) \exp\left(\sum_{j<i} u(r_{ij})\right)$$

During the whole project, we will use natural units $\hbar = m = \omega_{ho} = 1$.

3 Methods

To compute the ground state energy of the gas of bosons considered, we use the variational method from quantum mechanics which gives an upper bound for the ground state energy E_{gs} given a trial wavefunction (in our case $\Psi_T = \Psi(\mathbf{R}, \alpha)$):

$$E_{gs} \leq \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} = \frac{\int \Psi_T^*(\mathbf{R}, \alpha) H \Psi_T(\mathbf{R}, \alpha) d\mathbf{R}}{\int \Psi_T^*(\mathbf{R}, \alpha) \Psi_T(\mathbf{R}, \alpha) d\mathbf{R}}.$$

this integral is impossible to evaluate with methods such as Gaussian quadrature in a resonable amount of time. In such a situation, Monte Carlo methods are needed.

Let us consider the trial wavefunction (eq. (1)) and define the probability density function (PDF)

$$P(\mathbf{R}, \alpha) = \frac{|\Psi_T|^2}{\int d\mathbf{R} |\Psi_T|^2} \tag{3}$$

and define the local energy as

$$E_L = \frac{1}{\Psi_T} H \Psi_T. \tag{4}$$

By using eq. (3) and eq. (4), we have

$$E_{gs} \leq \frac{\int d\mathbf{R} \Psi_T^* H \Psi_T}{\int d\mathbf{R} |\Psi_T|^2} = \int d\mathbf{R}\ P(\mathbf{R}, \alpha) E_L(\mathbf{R}, \alpha) \simeq \frac{1}{N_{MC}} \sum_{i=1}^{N} P(\mathbf{R}_i, \alpha) E_L(\mathbf{R}_i, \alpha)$$

where N_{MC} is the number of Monte Carlo steps.

In our case we can use MC methods to compute the mean local energy for different alphas and then see what alphas return the minimum energy. An automated version of this is to use numeric methods that finds function minimums based on the calculations from the MC cycles. For instance conjugate gradient and gradient descent are good iterative methods. This project will use the gradient descent method. Then the outline is to do some MC cycles to calculate quantities needed for the numeric minimum finder per iteration. Eventually the numeric method will find a minimum and return an optimal α. Then we can do MC sampling with many more steps on the system with the optimal parameters. This is called the variational Monte Carlo [2] (VMC) method.

3.1 Sampling methods

We use MC methods to measure system quantities such as energy. The basic recipe is to choose one particle at random, and propose a step for that particle. Then according to some rule we wish to either accept or decline the move. This project will use two methods to propose and accept moves: standard Metropolis and Metropolis-Hastings.

3.1.1 Metropolis sampling

The standard Metropolis algorithm (also referred to in this text as Brute Force Metropolis) follows the basic recipe for choosing new positions given by

$$x_{k+1} = x_k + Lr,$$

where L is a step length and r is a uniformly distributed random variable $\in [0, 1]$. We accept moves that are deemed likely by the ratio of the absolute square wavefunctions before and after the move. We choose a new random number r, and if

$$r \leq \frac{|\Psi_T(\mathbf{r}_{k+1})|^2}{|\Psi_T(\mathbf{r}_k)|^2}, \tag{5}$$

then we accept the move. If not we decline it.

3.1.2 Importance sampling

The issue with brute force Metropolis sampling is that the algorithm proposes a lot of moves that get rejected. These rejected moves are wasted computation time and as such, it becomes desirable to use an algorithm that proposes moves that are more likely to be accepted. For this we will use the Importance Sampling method. The Fokker-Planck equation is

$$\frac{\partial P}{\partial t} = D\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} - F\right)P,$$

where P is the probability density function of the system, D is the diffusion coefficient and F is the drift force. This equation governs the time evolution of the probability density function for a diffusing system under random forces. In the bosonic system the probability density function is the wavefunction itself and we call F the quantum force. $D = 1/2$ comes from the half factor in the kinetic energy.

The solution of the Fokker-Planck equation is

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

The gradient with respect to the $k-$th particle coordinate is found in Eq. 9. Dividing by the wavefunction gives

$$\frac{\nabla_k\Psi_T(\mathbf{r})}{\Psi_T(\mathbf{r})} = \frac{\nabla\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \sum_{j\neq k}\boldsymbol{\nabla}_k u_{kj}.$$

Finally the quantum force acting on particle i is

$$\mathbf{F}_i = \frac{2\nabla\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \sum_{i\neq k}\boldsymbol{\nabla}_k u_{ik} = -2\alpha\mathbf{r}_i + \sum_{i\neq k}\frac{a}{r_{ik}^2(r_{ik}-a)}(\mathbf{r}_i - \mathbf{r}_k).$$

The new move is given by

$$x_{k+1} = x_k + DF\Delta t + r\sqrt{\Delta t},$$

where Δt is some time step parameter that can be tuned.

Now that we have changed the proposal of moves we need to alter the method of accepting such moves. We move then to the Metropolis-Hastings algorithm. The probability of diffusion can be solved from the Fokker-Planck equation through a Green function

$$G(x_{k+1}, x_k, \Delta t) = \frac{1}{(2\pi\Delta t)^{3N/2}}\exp\left[-\frac{(x_{k+1} - x_k - \Delta t F(x_k))^2}{2\Delta t}\right].$$

The new moves are now accepted following the rule

$$r \leq \frac{G(x_k, x_{k+1}, \Delta t)|\Psi_T(x_{k+1})|^2}{G(x_{k+1}, x_k, \Delta t)|\Psi_T(x_k)|^2}, \tag{6}$$

where r is a Gaussian distributed random number

3.2 Analysis of Hamiltonian

In this section we compute the expression for the Hamiltonian for our trial wave function in both interacting and non cases. The local energy is dependent on the second derivative of the wavefunction. The second derivative is a numerically costly process going as n^2 flops. Since there is an explicit expression for the trial wavefunction the analytic second derivative can be found. This greatly speeds up the program.

3.2.1 Non-interacting bosons

In the case of no interaction the wavefunction is given without the correlation term as

$$\Psi_T(\mathbf{R}) = \prod_i \phi(\mathbf{r}_i) = \prod_i \exp\left[-\alpha\left(x_i^2 + y_i^2 + z_i^2\right)\right].$$

In this case the Hamiltonian is set with $V_{int} = 0$. The local energy is then

$$E_L = \frac{H\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} = \frac{1}{\Psi_T(\mathbf{R})}\sum_i^N \left(-\frac{1}{2}\nabla^2 + \frac{1}{2}\omega^2 r_i^2\right)\Psi_T(\mathbf{R}).$$

For convenience we introduce the quantities $\mathbf{r}_i^\beta = \mathbf{x}_i + \mathbf{y}_i + \beta\mathbf{z}_i$ and $r_{i\beta}^2 = x_i^2 + y_i^2 + \beta^2 z_i^2$. The laplacian of the wavefunction is

$$\nabla_i^2\Psi_T(\mathbf{R}) = [4\alpha^2\mathbf{r}_{k\beta}^2 - 2((\mathcal{D}-1)\alpha + \alpha\beta)]\Psi_T(\mathbf{r})$$

where d is the dimension of the particles. With the spherical traps ($\beta = \omega_z = 1$), the local energy is

$$E_L = \sum_k^N \left[-2\alpha^2 r_k^2 + d\alpha + \frac{1}{2}\omega^2 r_k^2\right]$$

At this point, we look at the mean local energy and impose the result $\langle x_i^2\rangle = \frac{1}{2\omega}$. The dimensionality gives the number of elements in r^2, $\langle r^2\rangle = \frac{d}{2\omega}$. The result is

$$\langle E_L\rangle = \sum_i^N \left[r_i^2\left(\frac{1}{2}\omega^2 - 2\alpha^2\right) + \alpha d\right] = Nd\left(\frac{1}{4} - \frac{\alpha^2}{\omega} + \alpha\right) \tag{7}$$

Taking the derivative with respect to α and setting it to zero gives the optimal α parameter:

$$\frac{\partial E_L}{\partial\alpha} = Nd\left(-\frac{2\alpha}{\omega} + 1\right) = 0 \Rightarrow \alpha = \frac{1}{2\omega}$$

In the case of $\omega = 1$ we get $\alpha = 1/2$. Putting the result into eq. (7) gives

$$\langle E_L\rangle = \frac{Nd}{2} \tag{8}$$

3.2.2 Interacting bosons

In the interacting case, the trial wavefunction is

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

The derivative with respect to the k'th particle coordinate is

$$\nabla_k\Psi_T(\mathbf{r}) = \nabla\phi(\mathbf{r}_k)\prod_{i\neq k}\phi(\mathbf{r}_i)\exp\left(\sum_{i<j}u(r_{ij})\right) + \prod_i\phi(\mathbf{r}_i)\sum_{j\neq k}\nabla_k u(r_{ij})\exp\left(\sum_{i<j}u(r_{ij})\right). \tag{9}$$

The second derivative is

$$\nabla_k^2\Psi_T(\mathbf{r}) = \nabla_k^2\phi(\mathbf{r}_k)\prod_{i\neq k}\phi(\mathbf{r}_i)\exp\left(\sum_{i<j}u(r_{ij})\right) + \nabla_k\phi(\mathbf{r}_k)\prod_{i\neq k}\phi(\mathbf{r}_i)\sum_{j\neq k}\nabla_k u(r_{ij})\exp\left(\sum_{i<j}u(r_{ij})\right)$$
$$+ \nabla_k\phi(\mathbf{r}_k)\prod_{i\neq k}\phi(\mathbf{r}_i)\sum_{j\neq k}\nabla_k u(r_{ij})\exp\left(\sum_{i<j}u(r_{ij})\right) + \prod_i\phi(\mathbf{r}_i)\sum_{j\neq k}\nabla_k^2 u(r_{ij})\exp\left(\sum_{i<j}u(r_{ij})\right)$$
$$+ \prod_i\phi(\mathbf{r}_i)\left(\sum_{j\neq k}\nabla_k u(r_{ij})\right)^2\exp\left(\sum_{i<j}u(r_{ij})\right)$$

The quantity we are interested in is the second derivative divided by the trial wavefunction which is

$$\frac{\nabla_k^2\Psi_T(\mathbf{r})}{\Psi_T(\mathbf{r})} = \frac{\nabla_k^2\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \frac{2\nabla_k\phi(\mathbf{r}_k)\sum_{j\neq k}\nabla_k u(r_{ij})}{\phi(\mathbf{r}_k)} + \sum_{j\neq k}\nabla_k^2 u(r_{ij}) + \left(\sum_{j\neq k}\nabla_k u(r_{ij})\right)^2. \tag{10}$$

At this point, we let the gradient to act on $u(r_{ij})$ in eq. (10). By changing variables, we get

$$\sum_{j\neq k}\nabla_k u(r_{ij}) = \sum_{j\neq k}u'(r_{ij})\nabla_k r_{ij} = \sum_{j\neq k}u'(r_{ij})\sum_k\frac{\mathbf{r}_i-\mathbf{r}_j}{|\mathbf{r}_i-\mathbf{r}_j|}\Big(\underbrace{\frac{\partial\mathbf{r}_i}{\partial\mathbf{r}_k}}_{\delta_{ik}} - \underbrace{\frac{\partial\mathbf{r}_j}{\partial\mathbf{r}_k}}_{\delta_{jk}}\Big) = \sum_{j\neq k}u'(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{|\mathbf{r}_k-\mathbf{r}_j|}$$

and

$$\sum_{j\neq k}\nabla_k^2 u(r_{ij}) = \sum_{j\neq k}\nabla_k\left(u'(r_{ij})\frac{\mathbf{r}_k-\mathbf{r}_j}{|\mathbf{r}_k-\mathbf{r}_j|}\right) =$$
$$= \sum_{j\neq k}\sum_k\left(u''(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{|\mathbf{r}_k-\mathbf{r}_j|}\frac{\mathbf{r}_k-\mathbf{r}_j}{|\mathbf{r}_k-\mathbf{r}_j|} + \frac{\nabla\cdot(\mathbf{r}_k-\mathbf{r}_j)r_{kj} - (\mathbf{r}_k-\mathbf{r}_j)\frac{(\mathbf{r}_k-\mathbf{r}_j)}{|\mathbf{r}_k-\mathbf{r}_j|}(1-\delta_{kj})}{r_{kj}^2}u'(r_{ij})\right) =$$
$$= \sum_{j\neq k}u''(r_{kj}) + \frac{3r_{kj}-r_{kj}}{r_{kj}^2}u'(r_{kj}) = \sum_{j\neq k}u''(r_{kj}) + \frac{2}{r_{kj}}u'(r_{kj}).$$

Therefore eq. (10) becomes

$$\frac{\nabla_k^2\Psi_T(\mathbf{r})}{\Psi_T(\mathbf{r})} = \frac{\nabla_k^2\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + \frac{2\nabla_k\phi(\mathbf{r}_k)\sum_{j\neq k}u'(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{|\mathbf{r}_k-\mathbf{r}_j|}}{\phi(\mathbf{r}_k)} + \sum_{j\neq k}\left(u''(r_{kj}) + \frac{2}{r_{kj}}u'(r_{kj})\right) + \sum_{j,i\neq k}u'(r_{kj})u'(r_{ki})\frac{\mathbf{r}_k-\mathbf{r}_j}{|\mathbf{r}_k-\mathbf{r}_j|}\frac{\mathbf{r}_k-\mathbf{r}_i}{|\mathbf{r}_k-\mathbf{r}_i|}. \tag{11}$$

In eq. (11), we can distinguish two terms: the first one $(\nabla_k^2\phi(\mathbf{r})_k/\phi(\mathbf{r})_k)$, which is independent on the interaction and it the one that we found above when we were deriving the kinetic energy for the non-interacting case, and another formed with the other terms of the double derivative that are dependent on the interaction. We already know that in the case of non-interacting bosons the second term will be zero. We can use the expressions for $\phi(\mathbf{r}_i)$ in eq. (2) and $u(r_{ij})$ in eq. (2) to obtain [1]

[1] In the derivation we take into account the presence of β for the elliptic trap.

$$\frac{\nabla_k^2\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} = 4\alpha\mathbf{r}_k^\beta - 2((\mathcal{D}-1)\alpha+\alpha\beta)$$
$$\frac{2\nabla_k\phi(\mathbf{r}_k)\sum_{j\neq k}u'(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{|\mathbf{r}_k-\mathbf{r}_j|}}{\phi(\mathbf{r}_k)} = -4\alpha\Big(\sum_{j\neq k}\frac{\mathbf{r}_k^\beta\cdot(\mathbf{r}_k-\mathbf{r}_j)}{r_{kj}}\frac{a}{r_{kj}-a}\Big)$$
$$\sum_{j\neq k}\Big(u''(r_{kj})+\frac{2}{r_{kj}}u'(r_{kj})\Big) = \sum_{j\neq k}\frac{-a}{(r_{kj}-a)^2(r_{kj})^2}$$
$$\sum_{j,i\neq k}u'(r_{kj})u'(r_{ki})\frac{\mathbf{r}_k-\mathbf{r}_j}{|\mathbf{r}_k-\mathbf{r}_j|}\frac{\mathbf{r}_k-\mathbf{r}_i}{|\mathbf{r}_k-\mathbf{r}_i|} = \Big(\sum_{j\neq k}\frac{a}{r_{kj}(r_{kj}-a)}\Big)^2.$$

where $\mathcal{D}$ is the number of dimensions and $\mathbf{r}_k^\beta = (x_k\hat{x}_k + y_k\hat{y}_k + \beta z_k\hat{z}_k)$.
Therefore the analytical second derivative is

$$\frac{\nabla_k^2\Psi_T(\mathbf{r})}{\Psi_T(\mathbf{r})} = 4\alpha\mathbf{r}_k^\beta - 2((\mathcal{D}-1)\alpha+\alpha\beta) - 4\alpha\Big(\sum_{j\neq k}\frac{\mathbf{r}_k^\beta\cdot(\mathbf{r}_k-\mathbf{r}_j)}{r_{kj}}\frac{a}{r_{kj}-a}\Big) + \sum_{j\neq k}\frac{-a}{(r_{kj}-a)^2(r_{kj})^2} + \\ + \Big(\sum_{j\neq k}\frac{a}{r_{kj}(r_{kj}-a)}\Big)^2.$$

By defining

$$E_k^{one\ body} = -2\alpha\mathbf{r}_k^\beta + ((\mathcal{D}-1)\alpha+\alpha\beta)$$
$$E_k^{interacting} = 2\alpha\Big(\sum_{j\neq k}\frac{\mathbf{r}_k^\beta\cdot(\mathbf{r}_k-\mathbf{r}_j)}{r_{kj}}\frac{a}{r_{kj}-a}\Big) + \frac{1}{2}\sum_{j\neq k}\frac{a}{(r_{kj}-a)^2(r_{kj})^2} - \frac{1}{2}\Big(\sum_{j\neq k}\frac{a}{r_{kj}(r_{kj}-a)}\Big)^2,$$

the local energy is

$$E_L = \sum_{k=1}^{N}\Big(E_k^{\text{one body}} + E_k^{\text{interacting}} + V_{ext}(\mathbf{r}_k)\Big)$$

Elliptic trap In the interacting case we consider an elliptic trap. Let us introduce lengths in unit of $a_{ho} = (1-2)\times 10^4$ Å (characteristic dimension of a typical trap of ^{87}Rb), $r \to r/a_{ho}$ and energy in units of $\hbar\omega_{ho}$. The Hamiltonian can be rearranged as

$$H = \sum_{k=1}^{N}\Big(-\frac{\hbar^2}{2m}\nabla_k^2 + \frac{1}{2}m[\omega_{ho}^2(x_k^2+y_k^2)+\omega_z^2z_k^2]\Big) + \sum_{k<i}^{N}V_{int}(\mathbf{r}_k,\mathbf{r}_i)$$
$$= \sum_{k=1}^{N}\frac{\hbar\omega_{ho}}{2}\Big(-\frac{\hbar}{m\omega_{ho}}\nabla_k^2 + \frac{\omega_{ho}m}{\hbar}\Big[x_k^2+y_k^2+\frac{\omega_z^2}{\omega_{ho}^2}z_k^2\Big]\Big) + \sum_{k<i}^{N}V_{int}(\mathbf{r}_k,\mathbf{r}_i)$$
$$= \sum_{k=1}^{N}\frac{\hbar\omega_{ho}}{2}\Big(-a_{ho}\nabla_k^2 + a_{ho}\hbar\Big[x_k^2+y_k^2+\frac{\omega_z^2}{\omega_{ho}^2}z_k^2\Big]\Big) + \sum_{k<i}^{N}V_{int}(\mathbf{r}_k,\mathbf{r}_i).$$

where we use $a_{ho} = \sqrt{\hbar/(m\omega_{ho)}}$ [3]. Now, by using the units proposed at the beginning of this paragraph and by setting $\gamma = \omega_z/\omega_{ho}$, we get

$$H = \sum_{k=1}^{N}\frac{1}{2}\Big(-\nabla_k^2 + x_k^2 + y_k^2 + \gamma^2z_k^2\Big) + \sum_{k<i}^{N}V_{int}(\mathbf{r}_k,\mathbf{r}_i). \tag{12}$$

From eq. (12), we can find the local energy:

$$E_L = \sum_{k=1}^{N} \left(E_k^{\text{one body}} + E_k^{\text{interacting}} + \frac{1}{2}(x_k^2 + y_k^2 + \gamma^2 z_k^2) \right).$$

3.3 Gradient descent

Sometimes referred to as steepest descent, the gradient descent method is an iterative method used to find local minima of functions. The basic idea is to choose an initial $\mathbf{x}$ and find a new $\mathbf{x}$ following

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \lambda_k \nabla f(\mathbf{x}_k),$$

where λ_n is some factor, preferably small. If the derivative is negative, then x will increase. If the derivative is positive, x will decrease. At the minimum the derivative will be zero and thus the method will converge. There are many gradient descent methods which differ by choice of λ_n. The ideal method is to have some algorithm such that λ approaches zero when the function approaches the minimum. This project will use constant λ. The simple algorithm can be implemented as

```
while (iter < maxIterations && energyDerivative < tolerance){
   x -= lambda*gradF(x)
}
```

An issue with the gradient descent method is that it can only find local minimum without knowing whether it is the global one or not. This can be bypassed by running the algorithm multiple times with different initial guesses. If they converge to the same minimum, it is a good indication that the function only has one local(global) minimum.

3.4 One-body density

The onebody density $\rho(r)$ describes the probability of finding a boson at a distance r away from the origin. It is an important measure of the system since it is something that can be measured by real experiments. For instance the charge distribution can be computed from the one-body density. Hence we can compare our results with the experiments to check the validity of our simulations. It is defined as

$$\rho(r_1) = \int d\mathbf{r}_2 ... d\mathbf{r}_N |\Psi_T(\mathbf{r})|^2,$$

where r_1 is the coordinates of the first particle. We can replace this with r because the particles are indistinguishable. In practice $\rho(r)$ can be calculated by Monte Carlo integration. For every particle we calculate r and place them into bins in a histogram. We do this for every MC cycle and normalize by the number of particles and number of MC cycles. We want to sample the system properties that do not depend on the initial properties. Therefore we begin sampling the radius histogram after the equilibration time has passed.

3.5 Statistical analysis - blocking method

It is important to have an estimate for the error of our results, without it they are useless. The simple way of getting an error estimate is to take the standard deviation of our data. The issue with that method is that the standard deviation does not take the correlation of the data into account and, in this project, in fact, data are correlated. It is simple to see that because the energy is a time series: the energy does change discontinuously, in Monte Carlo steps, but the change is typically small compared to the total energy and thus it can be classified as a time series.

An excellent tool for analyzing time series correlation is the blocking method [4]. The basic idea is to start with a correlated dataset and turn it into an uncorrelated dataset which we take the standard deviation of. The method works in this way: suppose that our initial dataset is

$$\mathbf{X}_0 = (X_1, X_2, ..., X_N) \quad \text{where } X_1 = (\mathbf{X_0})_1,$$

we average $X_1$and X_2 and place it into $(\mathbf{X}_1)_1$. Then we do the same for X_3 and X_4 and place it in $(\mathbf{X}_1)_2$ and so on. This is one blocking iteration. Our new array is less correlated because the elements are further from each other than in the original time series.

By following the calculations of [4], the variance of the data set after blocking k times is

$$V(\bar{\mathbf{X}}_k) = \frac{\sigma_k^2}{n_k} + \frac{2}{n_k}\sum_{h=1}^{n_k-1}\left(1 - \frac{h}{n_k}\right)\gamma_k(h) = \frac{\sigma_k^2}{n_k} + \epsilon_k,$$

where $\bar{\mathbf{X}}_k$ is the mean of $\mathbf{X}_k$, σ_k is the standard deviation in $\mathbf{X}_k$, n_k is the number of elements in $\mathbf{X}_k$ and γ_k is the autocovariance of $\mathbf{X}_k$. We call ϵ_k the truncation error. It can be shown [4] that ϵ_k tends to zero as we keep on blocking. The result is that the error of the mean is just the standard deviation of the data set. This error should better reflect the error of our results than the simple standard deviation and it should also be larger since it takes into account correlations.

The blocking method is specifically useful for large data sets since the computation cost is of the order of $O(n)$ whereas other methods are $O(n^2)$ or worse. Indeed, when we are dealing with data sets sizes of the order of $10^5 - 10^6$, there is a large speed difference between $O(n)$ and $O(n^2)$.

4 Results and discussions

4.0.1 Standard deviation vs blocking error

An example result of the mean energy using the standard deviation of the error in the non-interacting case with 10 3-dimensional particles with $\alpha = 0.4$ is $E = 15.3691 \pm 0.0009$. This error is unrealistically small. By applying blocking, we get an error of ± 0.02. It is obvious that the blocking error gives a better estimate since it takes into account the time-series correlation of the dataset. Therefore all errors presented in this project will be calculated by applying the blocking method to our data sets.

4.1 No boson-boson interaction

We gather data using two methods: brute force Metropolis and Importance Sampling algorithms.

4.1.1 Brute force Metropolis

As discussed in 3.2, in both interacting and non cases, we have an analytical expression for the local energy. Nevertheless at the beginning of the developing of the program, it is useful to benchmark the computation with a different approach. With such a spirit we used a numerical derivative to compute the kinetic energy. This approach is much slower than the analytical evaluation: the time required to perform numerical derivative is at least twice than the one spent for the analytical one as it is possible to see from Tab. 1. In this first part of the project, we use the brute force Metropolis algorithm as method to choose new moves (eq. (5)). From Tab. 2 we can state that our code is successful in computing the local energy with both numerical and analytical derivative. The accuracy of the analytical energy is perfect as we would aspect. We note that also the accuracy of the numerical energy is really good which is quite surpring by considering that the formula of the double derivative is obviously an approximation. The length step used in all this computations is determined in a really roughly way by trial and errors. In our case we find $L = 1$ to be an appropriate value for our aims.

From Tab. 2 we note also the drawback of this brute force Metropolis which is the relative low acceptance rate (about ~ 74 %): this means that we lose an important amount of time by proposing moves which get rejected. To avoid this issue, the Importance Sampling is implemented.

Table 1: Computation time used to calculate ground state energy in the one dimensional case using 10^6 MC cycles and the brute force Metropolis algorithm. The results presented include the time used by the analytic and numeric solutions to the second derivative.

N	$\mathcal{D}$	**Time [s] (analytical)**	**Time [s] (numerical)**
1	1	2.9	5.8
10	1	4.7	13.4
100	1	42.6	118.9
500	1	756.6	$\gg 1500$
1	3	3.7	6.0
10	3	8.9	31.1
100	3	79.6	565.6
500	3	932.4	$\gg 1500$

Table 2: Energy of the many-particle boson system in three dimensions compared with the analytical and numerical results obtained using Metropolis algorithm. The exact energy is calculated from eq. (8). Note the relative low acceptance ratio.

N	**d**	**Exact energy**	**Analytical energy**	**Numerical energy**	**Acceptance ratio**
1	3	1.5	1.5 ± 0.0	$1.5 \pm 3 \times 10^{-7}$	0.74
10	3	15	15 ± 0	15 ± 0	0.74
100	3	150	150 ± 0	150 ± 0	0.74
500	3	750	750 ± 0	750 ± 0	0.74

4.1.2 Importance Sampling

We implement the Importance Sampling with the acceptance rule shown previously in eq. (6). To check whether our implementation is correct we compare the local energy obtained with different variational parameter α with the Brute Force Metropolis and the Importance Sampling method. From Tab. 3 we don't note relevant differences between the two sets of data except the error which is usually more in the importance sampling case. These sets of data are also plotted in Fig. (1) where the length of the vertical lines represents the uncertainty on the data. As we expect from the theory, the minimum of the local energy with respect to α is clearly in 0.5 where all the methods flow into perfectly. This shown once again the goodness of the procedures adopted.

All the data mentioned above are obtained by using a $\Delta t = 0.01$. We decide to perform a further analysis on the value of Δt since the use of the value 0.01 was completely due to trial and errors experiments. Therefore we compute the local energy for $\alpha = 0.4$ with several values of Δt from 1 to 10^{-5}. We find the best interval with three consideration: the smoothness of the local energy during time (MC cycles), the acceptance rate of the moves and the uncertainty. The first one can be evalueted from Fig. (2), where we note how the function local energy becomes flatter as the time step decrease or in another way the noise is less. Here good choices of time steps seem $0.1, 0.01, 0.001, 0.0001$. The last one is excluded because the method moves the particle so close that the configuration doesn't really change from the initial one i.e. it is totally biased by how the random decides to put the particles at the beginning and thus it is not to be trusted. The acceptance ratio can be evaluated in Tab. (4). Brute force MC sampling accepted around 73-74% of the moves proposed by the algorithm, by adding the importance sampling the acceptance rate is boosted to $97 - 98\%$. On the other hand, at the lowest step, the system accepts all the moves since the particles are moved too close to the

previous positions as explained above. Whereas the opposite happens to the largest steps. From the table but better from Fig. (3), we can note how the uncertainties tend to increase as Δt is lowered, a consequence of the increasing correlation of data, with the exception of the lowest value which, however, we tend to exclude from the motives already explained. From these considerations, $\Delta t \in [0.01, 0.1]$. From our purposes, we stick with the choice made before of $\Delta t = 0.01$.

Table 3: Local energy using analytic and numeric solutions to the second derivative for the 10 particle case in three dimensions with Brute force Metropolis and Importance Sampling. The results are produced using 10^6 MC cycles.

	Brute Force Metropolis		**Importance Sampling**	
α	**Analytic**	**Numeric**	**Analytic**	**Numeric**
0.40	15.37 ± 0.02	15.40 ± 0.02	15.40 ± 0.04	15.43 ± 0.05
0.45	15.09 ± 0.01	15.08 ± 0.01	15.06 ± 0.02	15.09 ± 0.02
0.50	15.00 ± 0.0	15.00 ± 0.0	15.00 ± 0.0	15.00 ± 0.0
0.55	15.06 ± 0.01	15.06 ± 0.01	15.06 ± 0.01	15.07 ± 0.01
0.60	15.26 ± 0.01	15.25 ± 0.01	15.27 ± 0.02	15.23 ± 0.03

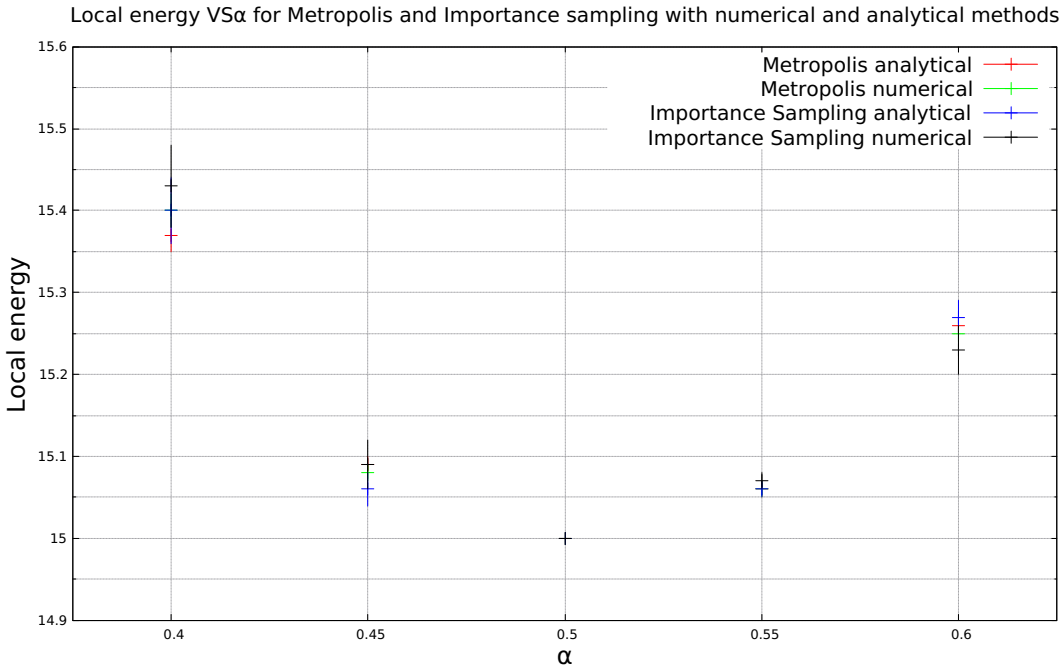

Figure 1: Plot of the local energies from Tab. 3 as function of α for Metropolis and Importance Sampling ($\Delta t = 0.01$) with numerical and analytical evaluation of energy. 10 particles in $3D$ are used.

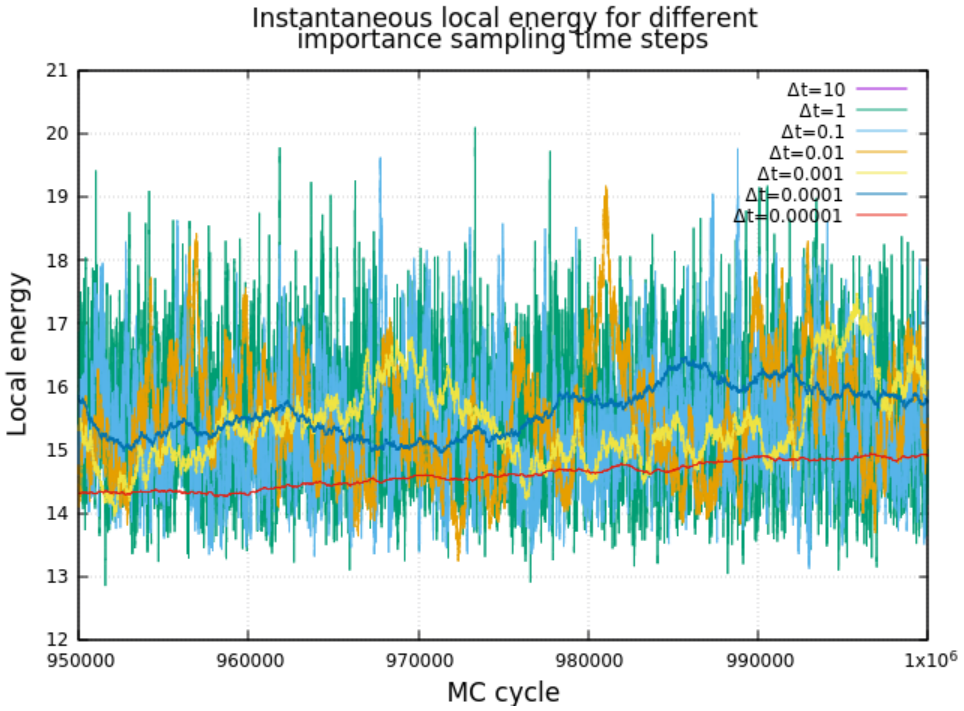

Figure 2: Variations in instantaneous local energy for various importance sampling Δt with $\alpha = 0.4$. The energy curve fluctuations are really big for $\Delta t \geq 0.1$

Table 4: In the table the values of local energy and acceptance rate are reported as functions of different Δt. 10 particle case in three dimensions are considered with 10^6 MC cycles and $\alpha = 0.4$.

Δt	**Mean local energy**	**Acceptance ratio**
10	15.14 ± 0.04	0.00014
1	15.36 ± 0.006	0.68
0.1	15.37 ± 0.01	0.986
0.01	15.40 ± 0.04	0.990
0.001	15.44 ± 0.08	0.994
0.0001	15.3 ± 0.1	0.9997
0.00001	14.38 ± 0.04	1

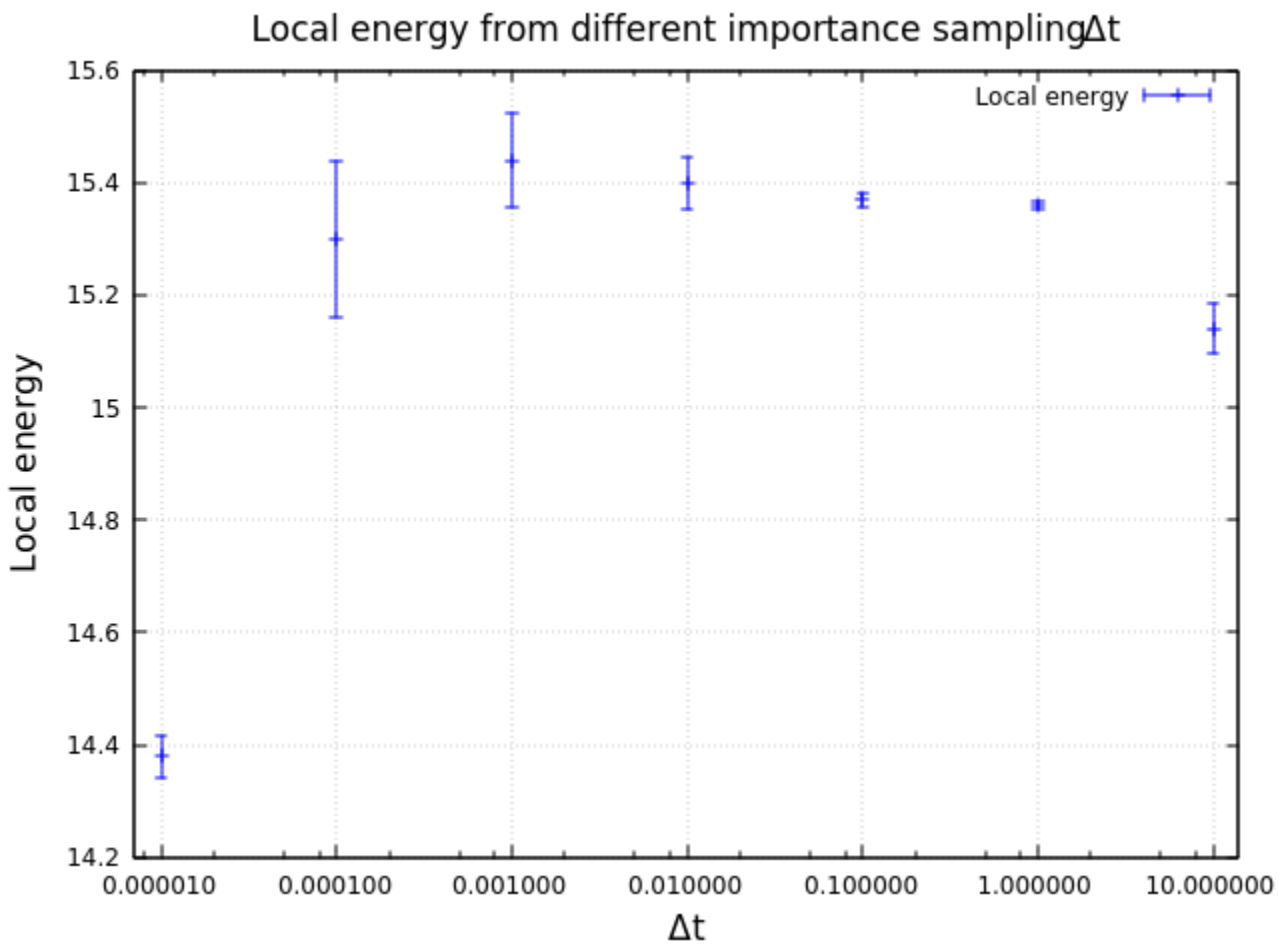

Figure 3: Mean local energy computed from sets of 10^6 MC cycles using various importance sampling Δt with $\alpha = 0.4$ for 10 particles in $3D$.

4.2 Interacting bosons

In this section we turn on the interaction between bosons and we trap them in an elliptic harmonic potential. The energy of the systems of interacting particles in 3 dimensions is computed and presented in table 5 together with benchmark energies retrieved from Pederiva and Isacchini's article [5].

As we can see, our results follow the behaviour shown by the benchmark even though for the majority of cases our results are not compatible with them (Fig. (4)). We note that for 10 particles we overestimate the results whereas for the other sets of particles we underestimate them. We do not know why it happens, but we can state that if we would have a variational parameter also in the expression of the Jastrow factor, we would probably be able to find better results. Nevertheless, by looking at the plot in Fig. (5) we can already safely say that the optimal parameter α would be in an interval around $\alpha = 0.5$ which will be better inspected with the Gradient Descent method in next section.

Table 5: Energies of interacting particles. Benchmark results taken from [5].

N	**10**		**50**		**100**	
α	**Benchmark**	**Result**	**Benchmark**	**Result**	**Benchmark**	**Result**
0.2	34.9	35.3 ± 0.3	175	174 ± 1	353	343.2 ± 2.1
0.3	24.7	27.7 ± 0.1	138	136.4 ± 0.6	278	279.0 ± 3.3
0.4	24.2	24.84 ± 0.04	125	123.3 ± 0.3	253	248.4 ± 0.7
0.5	24.2	$24.1915 \pm 2 \times 10^{-4}$	122	119.81 ± 0.04	247	241.30 ± 0.02
0.6	24.6	24.55 ± 0.04	125	121.2 ± 0.1	252	246.4 ± 0.7
0.7	24.5	25.6 ± 0.1	129	127.1 ± 0.3	263	253.7 ± 0.9
0.8	–	26.8 ± 0.1	–	134.5 ± 0.3	–	271 ± 2

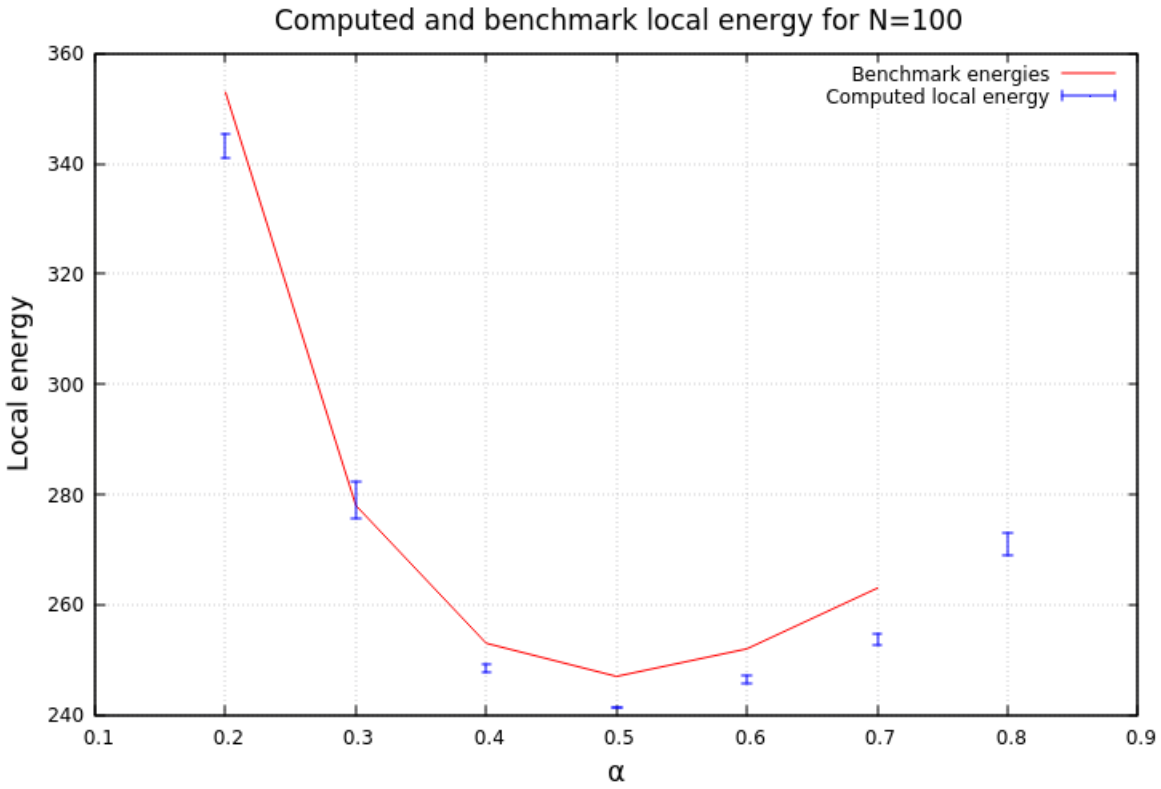

Figure 4: Plot of the N=100 data from Tab. 5. The figure shows that the computed energies follow the tendency of the benchmarks, but they underestimate them.

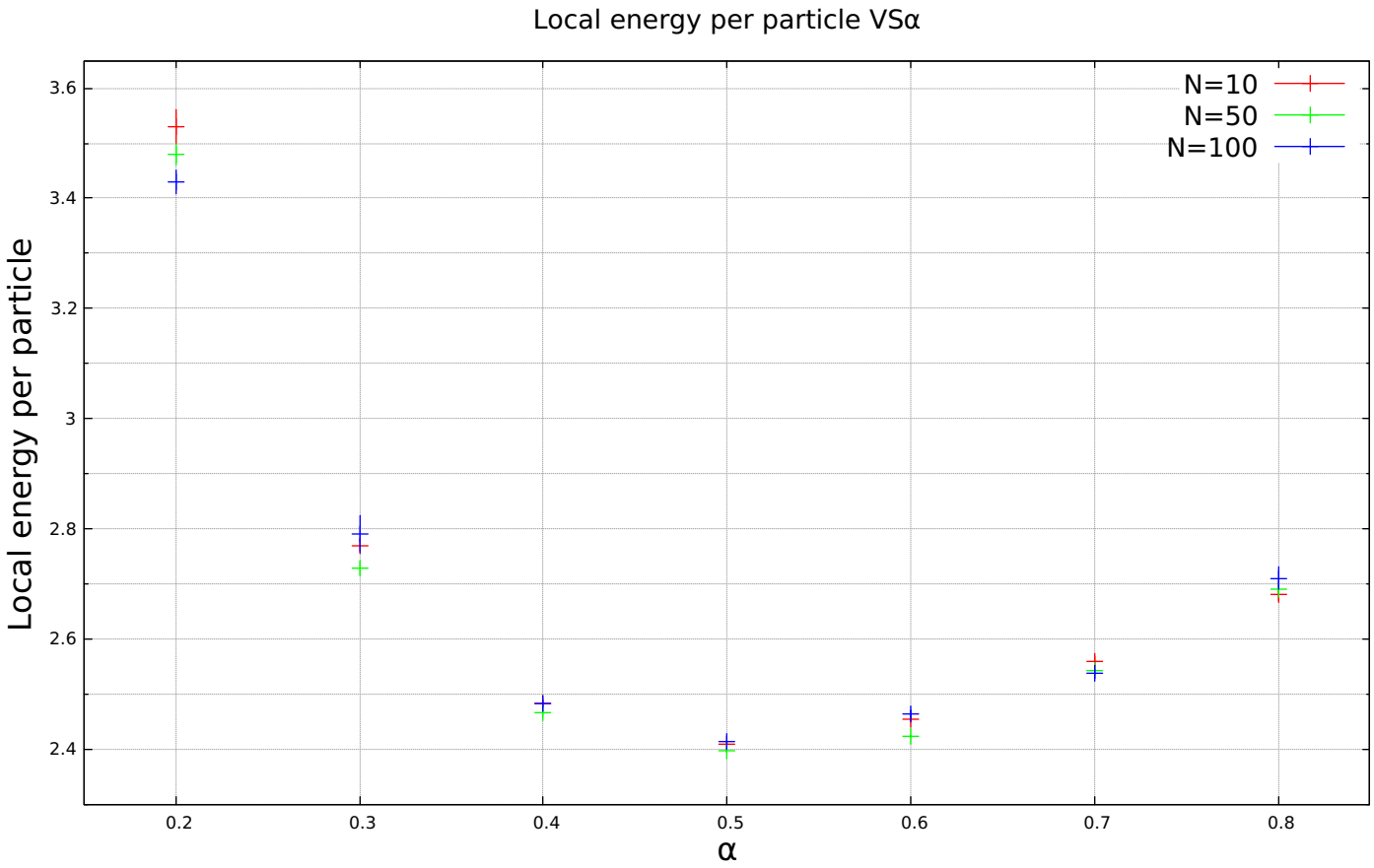

Figure 5: Local energy per particle for different α's. The figure shows that the energy per particle for the most part is independent of the particle number. This breaks down at $\alpha = 0.2$.

4.3 Finding the optimal α using gradient descent

The gradient descent method is applied to the interacting bosons to find the energy minimum. The results are presented in Fig. (6). Each data point is made using 10^5 MC cycles. The initial guesses used for all the systems are $\alpha = 0.40$ and $\alpha = 0.60$. The location of the minimum can be found by taking the mean value of the α values after the method has converged. We are therefore interested in the region in Fig. (6b) where the blue and red dots overlap. By looking at the data this region can be set to $[0.50014, 0.500175]$. The mean α for the red dots is $\alpha = 0.50018 \pm (1.6 \times 10^{-5})$ and for the blue dots is $\alpha = 0.50018 \pm (1.3 \times 10^{-5})$. By combining the data, the final answer becomes $\alpha_{optimal} = 0.50018 \pm (1 \times 10^{-5})$.

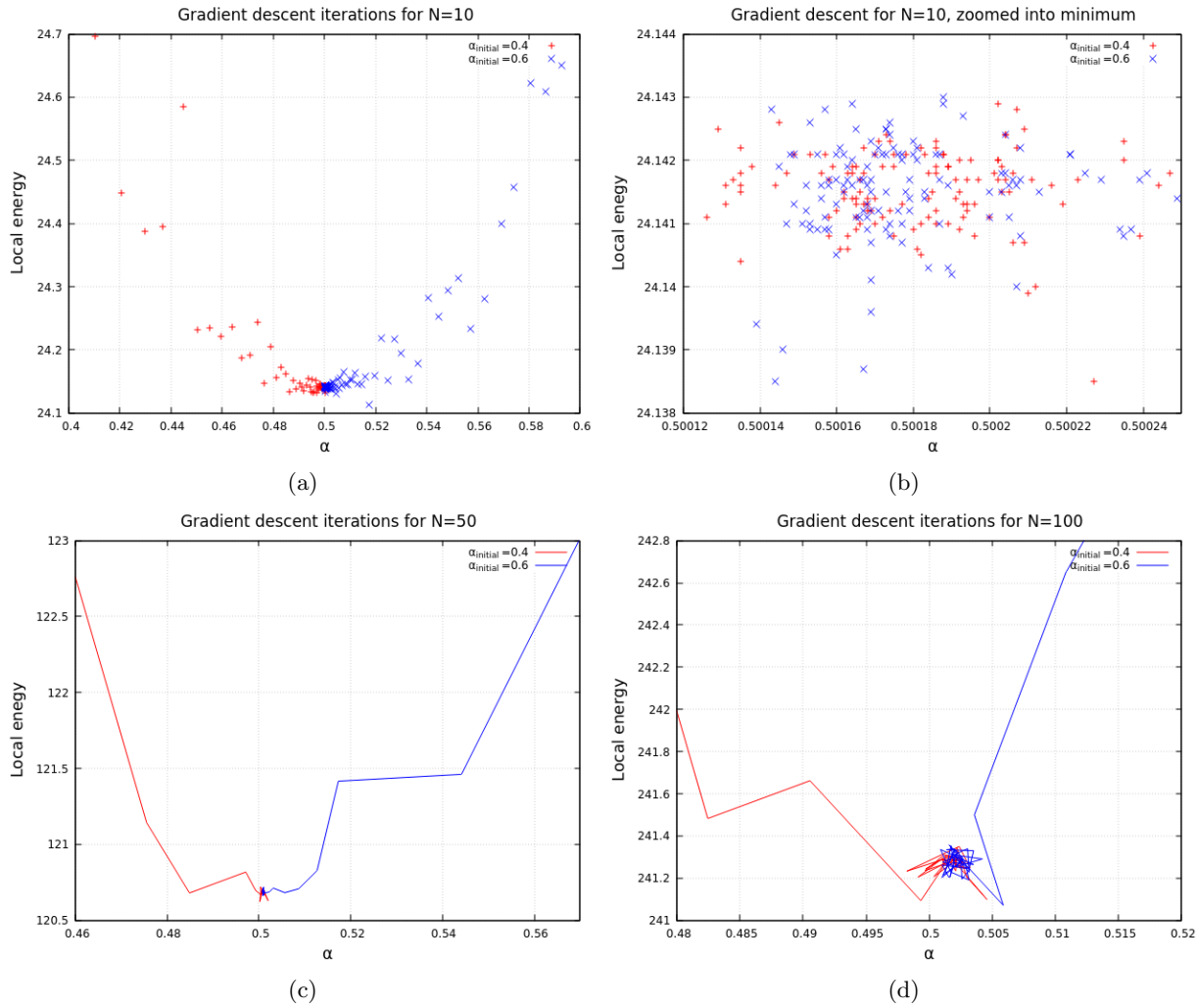

Figure 6: Gradient descent results from (a,b) 10, (c) 50, (d) 100 interacting bosons in an elliptical harmonic oscillator trap with $\beta = 2.82843$. The results were made using $\lambda = 0.001$. Fewer data points were used for the higher number of particles because of the large amount of time used to calculate the points.

The same method can be applied to the 50 and 100 particle case. The data are presented in Fig. (6c) and Fig. (6d). 50 iterations are used in the 50 particle case and 30 iterations for the 100 particle case (for each initial α). A good estimate for the optimal α is found by using the same procedure as in the 10 particle case. The results are presented in Tab. 6, where we show also the ground state energies computed with these optimal variational parameters. The table shows that the optimal α tends to increase with the number of particles. This is a strange tendency. According to equation 1, one would expect the optimal α to be the same for all the N's since the macroscopic wavefunction $\Psi(\mathbf{r}, \alpha)$ is independent on N. The calculations for the spherical trap ($\beta = 1$) produce the same optimal α's. This fits with the theory.

The gradient descent method is also be applied to the system of non-interacting bosons. The algorithm finds $\alpha_{optimal} = 0.5 \pm (1 \times 10^{-6})$ in good agreement with the results in Fig. (1) and the calculations in section 3.2.1.

Table 6: Optimal variational parameters α for systems of interacting bosons found by using the gradient descent method together with the local energy computed using 10^6 MC cycles. The data indicates that the optimal alpha increases with the number of particles.

N	Optimal α	Ground state local energy
10	0.50018 ± 0.00001	24.1917 ± 0.0002
50	0.50093 ± 0.00001	120.929 ± 0.005
100	0.5021 ± 0.0006	241.77 ± 0.02

4.4 One-body density

The one-body density is computed by sampling the radial distance for each particle for each MC step after calibration into bins and normalization.

4.4.1 Interacting and non-interacting bosons

The one-body density matrix computed for the interacting and non-interacting bosons in a spherical harmonic oscillator potential ($\beta = 1$) is presented in Fig. (7). The figure shows that in both cases the probability of finding a boson is largest at the typical length scale of the harmonic oscillator potential: a_{ho}.

The result is surprising. One would expect that the interaction of the bosons would cause them to move further apart, however that does not seem to be the case. As it has been found, the energy is much higher for the interacting bosons than for the non-interacting. This effect does not appear to affect the mean particle distribution.

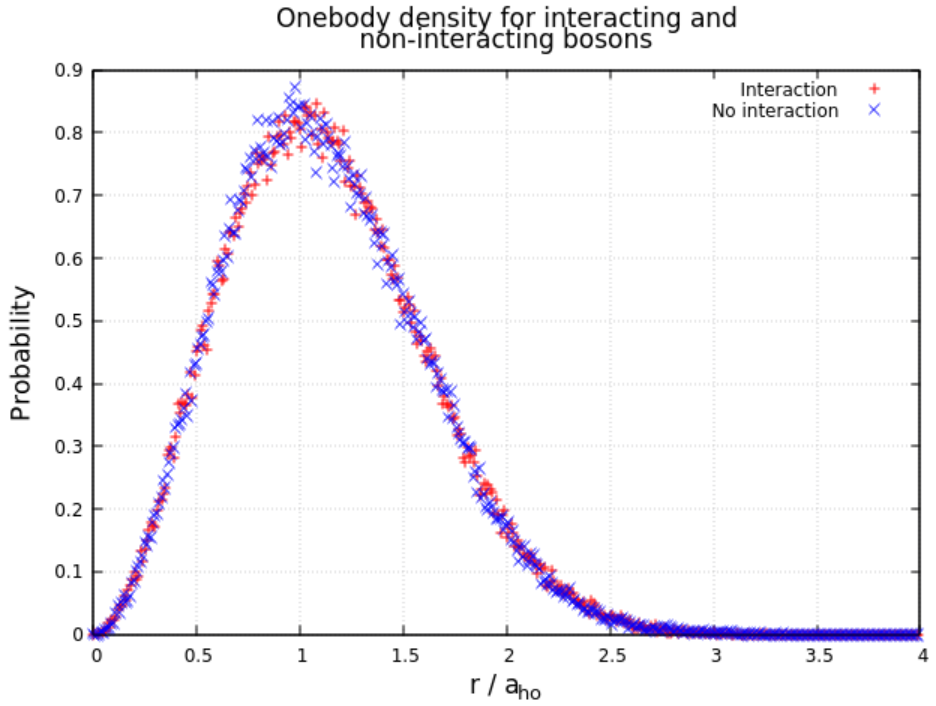

Figure 7: One-body density for interacting and non-interacting bosons computed using 5×10^5 MC cycles. The figure shows no clear difference between the two cases.

4.4.2 Interacting bosons in spherical and elliptical traps

Fig. (8) shows the one-body density for interacting bosons in spherical and elliptical traps. The figure shows that the spherical trap peaks at the typical length scale whereas the elliptical trap peaks at a lower r. This makes sense, because the elliptical trap is a squeezed version of the spherical trap. So the bosons find it harder to move outward z-direction of the potential. The result is that the bosons on average are closer to the origin.

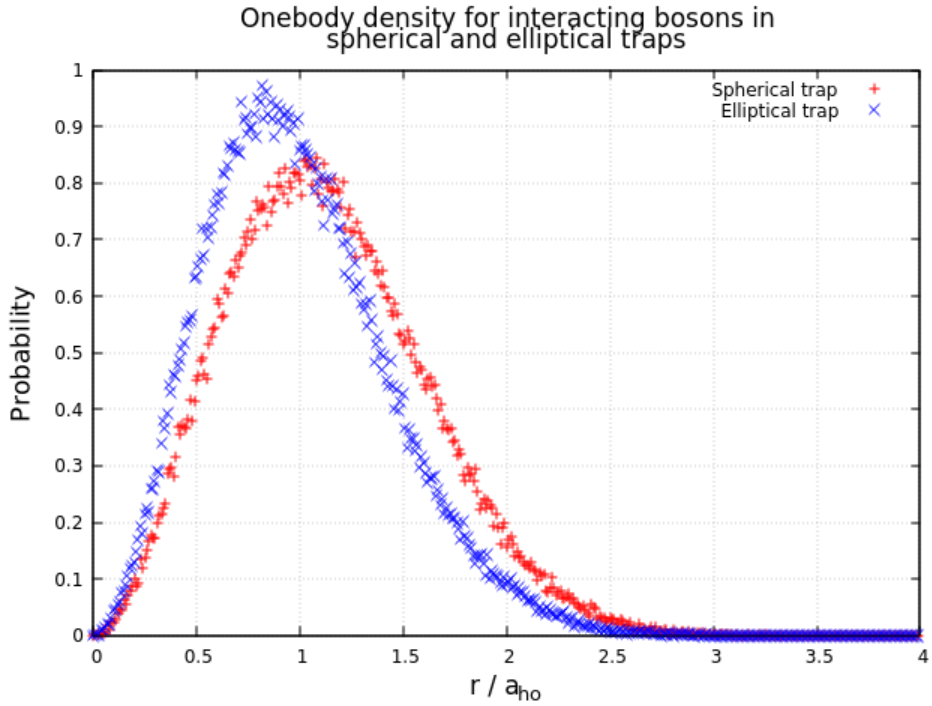

Figure 8: One-body density for interacting bosons in spherical and elliptical traps. In the elliptical case $\beta = 2.82843$. The figure shows the ellipse pushes the bosons closer together.

5 Conclusions

The goal of this report was to compute the ground state energy of a system of interacting bosons in an elliptical harmonic oscillator. Even though our results are not compatible with the benchmarks, since the discrepancies are small, we can state that we were able to write a program which compute the ground state energy of this system. The implementation of the Importance Sampling was also successful since it reproduced the results obtained with Brute Force Metropolis with a higher acceptance ratio. Moreover the discussion of the time step leaded us to consider as optimal $\Delta t \in [0.01, 0.1]$.

Furthermore with gradient descent we found the optimal parameters to be

$$\alpha = 0.50018 \pm 0.00001 \quad \text{for } N = 10$$
$$\alpha = 0.50093 \pm 0.00001 \quad \text{for } N = 50$$
$$\alpha = 0.5021 \pm 0.0006 \quad \text{for } N = 100$$

We noted the weird tendency of the optimal variational parameter to increase as we increase the number of particles which shouldn't happen since we should obtain the same ground state energy per particle. However

the ground state energies corrected with these optimal parameters were computed

$$E_L = 24.1917 \pm 0.0002 \quad \text{for } N = 10$$
$$E_L = 120.929 \pm 0.005 \quad \text{for } N = 50$$
$$E_L = 241.77 \pm 0.02 \quad \text{for } N = 100.$$

Eventually we compared the one-body densities with the interacting and non-interacting bosons in a spherical trap and for the interacting bosons in spherical and elliptical traps. In the first case, we found that the two densities overlap: this is weird, we would have expected that the interaction between bosons would move them further with respect to the case of non-interacting bosons. In the second case, we found that the peak of the density in the elliptical trap is at a lower r than the peak with the spherical trap: this is reasonable since the elliptical trap is somewhat squeezed version of a spherical one.

The next step might be to introduce a variational parameter to the correlation wavefunction. It is perhaps a bit naive to think that the Jastrow factor acts only as $(1 - a/r_{ij})$. It might be interesting to consider multiplying it by a variational parameter. We have now studied bosons in a harmonic oscillator potential, it would be interesting and also straightforward (given the object-orientation of the program) to study fermions in the same potential and compare the results. Another step would be to parallelize the program which also should be easy and direct.

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