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SIMULATION AND INVESTIGATION OF BOSE-EINSTEIN CONDENSATE USING VARIATIONAL MONTE CARLO METHOD
COMPUTATIONAL PHYSICS I FYS4411/FYS9411
PROJECT 1

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ABSTRACT

The present project is devoted to the simulation of a trapped boson gas and the investigation of its properties with implementation of Variational Monte Carlo (VMC) method coupled to the brute force Metropolis and Metropolis-Hastings algorithms (1).The case of independently moving bosons is considered alongside with the boson system with pair correlations taken into account. The system wave function is represented by the combination of single-particle Gaussian functions and the hard-sphere Jastrow factor (2). The bosons are considered to be trapped in spherical and elliptical harmonic oscillator. The study of the ground state, the one body density and the presence of the Jastrow factor, is performed for both analytical and numerical calculations of local energy. The results obtained are compared with the results on the base of Gross-Pitaevskii equitation and (3).

For the non-interacting bosons in the spherical harmonic potential the CPU performance time, for both analytical and numerical local energy, points to a significant delay for the numerical derivative calculation. For the same type of local energy calculation the Metropolis-Hastings algorithm is shown to be slower than the brute-force based Metropolis method, however the former is able to perform significantly higher step acceptance rate and, in principle, allows to speed the calculations up due to small reduction of number of Monte Carlo cycles. Including the Jastrow factor slightly increases the ground state energies and shifts the radial distribution of particles.

Subject headings: Bose-Einstein condensate — Variational Monte Carlo — Metropolis algorithm — blocking method — local energy — gradient descent method — one body density

1. INTRODUCTION

A matter consisting of bosons reveals particular behaviour as it is cooled down to some critical temperature and then becomes a Bose-Einstein condensate. Reaching this critical temperature all the bosons end up occupying the ground state, which can be described with a specific wave function, and it is of particular interest to calculate the ground state energy of the system. The theory for this was written down in a collaboration between Bose and Einstein in 1926, but one was not able to observe it until 1995, done by Anderson et. al., because of this condensed matter is one of the most studied fields in physics today.

A gas that is used to obtain the Bose-Einsten condensate consists of many particles that are trapped by a magnetic field, this is therefore a typical many body problem. For studying a real Bose-Einstein condensate it requires special and expensive equipment and this is not always possible to obtain. However, the problem can be studied by calculating it computationally. Monte Carlo simulations are known for being particularly applicable when it comes to many body problems, and in this case it was used together with two different types of metropolis algorithms to find the upper limit for the ground state energy of the system, which consisted of the alkali diluted gas ^{87}Rb. The traps used where a spherical and an elliptical trap. Further a modification of the algorithm was added, the importance sampling and the effects of its implementation were studied. To find the optimization of the parameter α for the energy minimization the gradient descent method was applied. In the end the interaction between the particles was also taken into account as well as the one body densities. The detailed discussion of the implementation in the program is presented in section 4. The results are represented in section 5, and under discussion in section 6 the results and errors found are examined in further detail.

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2. THEORETICAL BACKGROUND

2.1. *Bose-Einstein systems*

Systems of high temperatures and low densities behave according to Maxwell-Boltzmann statistics, that is, an ideal gas of bosons or fermions both behave as a classical gas described by the well known equation $PV =$

Nk_BT. When a system of density ρ is cooled down to a certain critical temperature T_c, quantum effects start to become important and the system of fermions will behave differently then that of bosons. The fermions are limited to single occupancy of the same state as they follow the Pauli exclusion principal. This is not the case for the bosons, because of their integer values of spin many bosons are able to occupy one state at a time. When undergoing a cooling an ideal Bose gas becomes a liquid, then the liquid becomes a solid, if it is cooled down even more, it becomes a Bose-Einstein Condensate (BEC), which follows the Bose-Einstein statistics (4)-(5).

For a system to behave as a BEC cooling it to around absolute zero is necessary. This is often done by hitting the system with lasers, that will cool the system down to a certain degree. To get the low temperatures needed a rather simple concept is used, illustrated often with a cup of coffee: By trapping warm coffee in a cup the warm particles will evaporate out, leaving the colder particles, which again leads to cold coffee in the cup. Using this simple concept one can make a trap for the particles in the system by using magnets. The warmer particles have the energy to evaporate out of the trap leaving only the cold particles in the ground state. Now the system stops behaving classically and starts showing quantum effects. The particles behave more like wave packets and as cooled down to absolute zero start to overlap into one continuous quantum state.

2.2. *The introduction to the potential and trial wave function*

In this study a system of N bosons was considered trapped in a harmonic oscillator potential, both spherical and elliptical. Since all the bosons are in ground state the aim was to estimate the energy in this particular state. The system chosen was the alkali gas ^{87}Rb which turns out to be particularly easy to trap in potentials, this because of the ground-state electronic structure: all electrons but one occupy closed shells, and the remaining one is in an s orbit (6). This makes the alkali gas easier to hit with lasers and cool down. For the actual trapping their scattering properties are also important. The cross sections of alkali are repulsive, thus highly elastic and have a constant scattering length (6). For low energies it is sufficient to look at the s-wave scattering length, which in this study was $a_{Rb} = 4.33 \times 10^{-3}$. The typical dimensions of a trap for ^{87}Rb is $a_{h0} = (\hbar/m\omega_\perp)^{\frac{1}{2}}$. The ratio between the scattering length and trap size gives $a_{Rb}/a_{h0} = 4.33 \times 10^{-3}$ but the values $\omega = \hbar = m$ where all scaled to one, therefore in this study $a_{h0} = 1$. The condition for diluteness to achieve BEC holds for ^{87}Rb

$$n \leq \frac{N}{V} \tag{1}$$

Where n is the number of atoms per cubic cm and here $n = 10^{12} - 10^{14}$. N is the number of particles and V is the volume. The critical temperature T_c for BEC is defined as the lowest temperature for which $\rho = \rho_{max}$, where both volume V and number of particles N play an important role (7). In this situation the physics is dominated by two-body collisions, which gives rise to the two-body Hamiltonian for the system. As well known the Hamiltonian is important for further calculations of the wave function and then the ground state energy of interest (3):

$$H = \sum_i^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 + V_{ext}\left(\mathbf{r}_i\right) \right) + \sum_{i<j}^N V_{int}\left(\mathbf{r}_i, \mathbf{r}_j\right) \tag{2}$$

. Where V_{ext} is the external trap potential mentioned above (3):

$$V_{ext}(\mathbf{r}_i) = \begin{cases} \frac{m\omega^2 r_i^2}{2} & \text{spherical case,} \\ \frac{m(\omega_\perp^2 (x_i^2 + y_i^2) + \omega_\parallel^2 (z_i^2)}{2} & \text{elliptical case.} \end{cases} \tag{3}$$

Here ω_{ho}^2 is the harmonic oscillator frequency. In the spherical case the dimensions have the same scales whereas in the elliptical case the z dimension has a different frequency ω_z. The values used for these in the calculation can be seen in Appendix B 10. The other potential included in the Hamiltonian (3):

$$V_{int}\left(\vec{r}_i, \vec{r}_j\right) = \begin{cases} 0 & \text{if } |\vec{r}_i - \vec{r}_j| \geq a \\ \infty & \text{if } |\vec{r}_i - \vec{r}_j| < a \end{cases} \tag{4}$$

, with $a = a_{Rb}$ in our calculations, this is the repulsive potential due to the interaction between the bosons. Short range corresponds to the strong interaction and the potential is infinite while if the distance between the bosons is too large, this will not have any effect on them.

To calculate the the ground state energy one needs a wave function, since it is unknown what it looks like a trial wave function (3) is created of the form

$$\Psi_T\left(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, \alpha, \beta\right) = \prod_i^N g\left(\alpha, \beta, \vec{r}_i\right) \prod_{i<j} f\left(a, r_{ij}\right), \tag{5}$$

, where the first part is the ground state wave function for an harmonic oscillator and the second part is the correlation wave function. This function together with the Hamiltonian play an important role in finding the true ground state energy. As seen in the equation above there is a parameter α, this is a variational parameter while β is treated as a constant in the present project. It can be shown (see Appendix B 10) alongside with the scaling of the Hamiltonian, that

$$\gamma = \beta = \frac{\omega_z}{\omega_{hn}}. \tag{6}$$

The first part of the wave function

$$g\left(\alpha, \beta, \mathbf{r}_i\right) = \exp\left[-\alpha\left(x_i^2 + y_i^2 + \beta z_i^2\right)\right], \tag{7}$$

is the one body ground state wave function for a harmonic oscillator. For the spherical trap β is set to one and for the elliptical case $\beta = 2.8284$. Since $\alpha = 0.5/a_{ho}^2$, and as previously stated $a_{ho} = 1$ in this study $\alpha = 0.5$ for the ground state energy. The correlation wave function is stated to be

$$f\left(a, |\mathbf{r}_i - \mathbf{r}_j|\right) = \begin{cases} 0 & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ \left(1 - \frac{a}{|\mathbf{r}_i - \mathbf{r}_j|}\right) & |\mathbf{r}_i - \mathbf{r}_j| > a \end{cases} \tag{8}$$

. So for the non-interacting case $a = 0$ and for the interacting case the whole wave function will be equal to zero.

2.3. *Local energy of the system and its analytical calculations*

The whole study evolves around finding the ground state energy, luckily it can be calculated analytically in this case, as is shown in appendix C 11. The variational principle claims that the $E_{exact} \leq \langle E \rangle$. Where $\langle E \rangle$ is the expectation value of the local energy as a function of the variational parameter α. The task at hand is then to find the minimum of the expectation value for the energy, and thus an estimation of the ground state energy. So for a function $f(x)$ the standard statistical definition of the expectation value is

$$\langle f \rangle = \int f(x)p(x)dx, \tag{9}$$

but the quantum mechanical value for the expectation value of the energy is

$$\langle E \rangle = \langle H \rangle = \frac{\int \Psi^*(\vec{r})H\Psi(\vec{r})d\vec{r}}{\int \Psi^*(\vec{r})\Psi(\vec{r})d\vec{r}}. \tag{10}$$

To make the expectation value for the energy look more like the standard statistical definition stated above, the local energy is defined as

$$E_L(\vec{r}) = \frac{1}{\Psi_T(\vec{r})}\hat{H}\Psi_T(\vec{r}). \tag{11}$$

This enables us to write the energy as

$$\langle E \rangle = \int \left|\Psi_T^2\right| E_L d\vec{r}. \tag{12}$$

Since the study involves large numbers, Bernoullis law can be applied and the integral thus becomes

$$\langle E \rangle = \int \Psi_T^2 E_L(r)dr \approx \frac{1}{M}\sum_{i=1}^{n} E(\overrightarrow{R}_i, \overrightarrow{\alpha}), \tag{13}$$

where the number M is the number of Monte Carlo cycles. To find the expression for the local energy for N number of particles, the second derivative for Ψ_T has to be found with respect to $\vec{r}_i$. This is calculated in Appendix C 11 along with the analytical expression for the local energy both for the elliptical and the spherical case, the latter shown below,

$$E_L(\mathbf{R}, \alpha) = \alpha N \cdot N_{\text{dim}} + \sum_{i=1}^{N} r_i^2 \left(\frac{1}{2} - 2\alpha^2\right). \tag{14}$$

Here $\beta = 1$ and $a = 0$.For the chosen case this relation can be written in the more familiar form of n-th level energy in the spherical harmonic oscillator in N_{dim} dimensions:

$$E(n) = \hbar\omega_{ho}\left(n + \frac{N_{dim}}{2}\right). \tag{15}$$

For the interacting case for N particles where $\beta = \gamma = \frac{\omega_z}{\omega_{hn}}$ and $a \neq 0$ it becomes more complicated, the calculations are again to be found in Appendix C 11 and the results shown below.

$$\begin{aligned}
E_L(\mathbf{R}, \alpha, \beta) = &\sum_{i=1}^{N}\Bigg(-\frac{\nabla_k^2\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \\
&+ 2\frac{\nabla_k\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\sum_{j\neq k} u'(r_{kj})\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} \\
&+ \sum_{j\neq k} u'(r_{kj})\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{ij}}\sum_{i\neq k} u'(r_{ki})\frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}} + \\
&+ \sum_{j\neq k}\left(u"(r_{kj}) + u'(r_{kj})\frac{2}{r_{kj}}\right) \\
&= \frac{\nabla_k^2\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + 2\frac{\nabla_k\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\sum_{j\neq k} u'(r_{kj})\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{kj}} + \\
&+ \sum_{j,j\neq k} u'(r_{kj})u'(r_{ki})\frac{\mathbf{r}_k - \mathbf{r}_j}{r_{ij}}\frac{\mathbf{r}_k - \mathbf{r}_i}{r_{ki}} + \\
&+ \sum_{j\neq k}\left(u"(r_{kj}) + u'(r_{kj})\frac{2}{r_{kj}}\right) \\
&+ V_{\text{exzt}}\ (\mathbf{r}_i)) + \sum_{i<j} V_{int}\left(\mathbf{r}_i, \mathbf{r}_j\right).
\end{aligned} \tag{16}$$

Despite of its visual complexity, this expression was proven to give good results in both the interacting and non-interacting case.

2.4. *Numerical calculations of the local energy*

The other approach implemented in this study was the calculation of the local energy E_L numerically. Here the energy was split up into two terms of the kinetic and potential energies

$$E_{L,i} = -\frac{\hbar^2}{2m}\frac{\nabla_i^2\Psi_T}{\Psi_T} + V_{ext}\left(\vec{r}_i\right) = E_{k,i} + E_{p,i}, \tag{17}$$

using (9):

$$\nabla^2 u \approx \frac{u(i+h) + h(i-h) - 2u(i)}{h^2} \tag{18}$$

for all the dimensions x, y, z when a grid $i = 0, 1...N_{x,y,z}$ is introduced. Even though this expression looks simpler than the analytical expression, it takes more time to compute. For more detailed discussion of this result in the scope of present project see 5.

2.5. *Gross-Pitaevskii equation*

The alkali gas of ^{87}Rb is a dilute boson gas, and the ground state energy could therefore be represented by the mean field Gross-Pitaevskii (GP) equation for dilute systems (10). The estimation for the energy is given by the integral over all the position

$$E[\Psi_T] = \int [-\frac{\hbar^2}{2m}|\nabla\Psi_T|^2 + \frac{m(\omega_\perp(x^2+y^2)+\omega_\parallel z^2)}{2}|\Psi_T|^2 + \\ + \frac{2\pi\hbar^2 a}{m}|\Psi_T|^4]d\mathbf{r}. \quad (19)$$

For the present study this equation was solved analytically for the simplest case and the derivation can be seen in Appendix E 13. The result for N non-interacting bosons in three dimensions is

$$E\left[\Psi_T\right] = \left(\alpha + \frac{1}{4\alpha}\right) N(\beta+2). \quad (20)$$

The latter equation holds for a system with few particles but when the number of particle increase the equation does not longer hold and it requires further modifications (see 6). The integral can be solved numerically with, for instance, the VMC. This was not implemented in this study but the results without interaction where compared to the GP solutions.

2.6. *Analysis of the Errors*

An inevitable part of each result to be obtained and subsequently published are the errors. The errors allows one to estimate the range of values and the actual result can be found within a certain increased probability. The errors are put into the categories of statistical and systematic errors. A statistical error is a difference between the achieved value in the experiment and the exact known (or usually unknown) value due to some statistical effects. As an example, the reason might be hidden in a lack of data points, the more data points are obtained, the closer to the true value one might get. The systematic errors are mostly due to a constant or systematically varying error or a shift which might occur in the machinery producing the data, or an inappropriate measurement method or the environment chosen. This type of error might be complicated to detect, however as long as it is detected it can be in principle minimized significantly. To analyze the statistical errors the central limit theorem was applied, and it can be practically formulated as: the larger amount of data points the closer the distribution of the results is to the normal distribution. So, if there is n measured data points, so that $\{x_1, \ldots, x_n\}$. The assumption is that these are independent and identically distributed (iid), this gives a likelihood function $p(x_1, x_2, \ldots, x_n) = p(x_i)$. In the discrete case this gives a mean value

$$\mu = \frac{1}{n}\sum_{i=1}^{n} p(x_i)x_i, \quad (21)$$

which correspond to a sample variance

$$\sigma^2 = \langle x^2 \rangle - \mu = \frac{1}{n}\sum_{i=1}^{n} p(x_i)(x_i-\mu)^2, \quad (22)$$

and standard deviation $= \frac{\sigma}{\sqrt{n}}$. For an iid case the correlation between the data points should be equal to zero. However, this is not the case and therefore the sample variance with a covariance term has to be added

$$\sigma_m = \frac{\sigma}{\sqrt{n}} + \text{covariance term} \quad (23)$$

,

Without the covariance term the error might noticeably underestimate the real error of the experiment. The covariance term is the challenging part in the analysis of the errors, however various methods can be applied, and therefore, one can approach better statistical estimation of the error. These are discussed in further depth in Methods 3.

2.7. *One body densities of the system*

One of the representative quantities characterizing the system is the distribution of particles over the observed volume attributed to ground state. This can be given by the one-body densities as follows:

$$\rho_i = \int |\Psi_T(\mathbf{R})|^2 d\mathbf{r}_1 d\mathbf{r}_2 \cdot \ldots \cdot d\mathbf{r}_{i-1} d\mathbf{r}_{i+1} \cdot \ldots \cdot d\mathbf{r}_N, \quad (24)$$

which can also reflect the relation between the particle localization and the hard sphere radius of the Jastrow factor included into the trial wave function. One body densities represent the simultaneous distribution of every particle in the system. In case of non-interacting bosons one body densities can be easily calculated analytically as follows:

$$\rho_i = \int \prod_j e^{-2\alpha(x_j^2+y_j^2+\beta z_j^2}} \prod_{j\neq i} d\mathbf{r}_i \\ = \left(\frac{\pi}{2\alpha}\right)^{3N/2} \frac{1}{\beta^{N/2}} e^{-2\alpha(x_i^2+y_i^2+\beta z_i^2}}. \quad (25)$$

For the case of interacting particles the integral can be calculated by means of variational Monte Carlo method.

In the present project the radial distribution of particles in the system was introduced as the part of general calculations in the program. For the range of radii of particles a grid is introduced thus the whole volume investigated is subdivided into the spherical segments enclosed by radii $\mathbf{r}_i$, and $\mathbf{r}_{i+1}$ within a thickness δr. The number of particles in each segment forms a histogram of particles within the thickness covered by each segment.

3. METHOD

3.1. *Variational Monte Carlo method*

The numerical Monte Carlo methods are the the widely used in the large variety of areas (physics, chemistry, biology,engineering etc).These methods imply the statistical simulation which allows to omit writing all differential equations that describe a system and its dynamics, since the process is simulated directly. If the given system can be described by a certain probability distribution functions the, the random sampling based on these functions allows pass through the number of steps and arrive in

or achieve the solution. However, the separate results of these samplings should be accumulated the way the final result will be obtained in the most efficient way, that is why Monte Carlo technique should be based on a combination of some sampling technique and a selection algorithm, or, in the present work, the Metropolis algorithm which governs the movement towards the most probable result. Unless this algorithm is implemented the step sizes and directions for movement of components of the system (particles in our case) are independent and random, thus the movement towards the equilibrium state is much less efficient.

The number of particles can be large, and one will not be able to obtain the exact solutions of a given many-body problem. The conventional integration methods (e.g. Gauss-Legendre method) are not efficient when the large number of dimensions is involved. In this case the quantum Monte Carlo methods are an excellent tool for studying of quantum mechanical systems or calculation various expectation values of interest i.e. calculation of multi-dimensional integrals. The method used in the present work is variational Monte Carlo approach for the estimation of the ground state energy of a system of N particles. Basing on the variation principle which for the given Hamiltonian and a trial wave function $\Psi_T(\mathbf{R},\alpha)$ claims (1):

$$E[H(\alpha)] = \frac{\int d\mathbf{R}\Psi_T^*(\mathbf{R},\alpha)\hat{H}(\mathbf{R})\Psi_T(\mathbf{R},\alpha)}{\int d\mathbf{R}\Psi_T^*(\mathbf{R},\alpha)\Psi_T(\mathbf{R},\alpha)} \geq E_0, \quad (26)$$

here E_0 is the true ground state energy of a system. This scheme implies the following principal steps:

1. Initialization of the trial wave of the system function $\Psi_T(\mathbf{R},\alpha)$ dependent on the variational parameter which is assumed to be as close to the true value as possible. Fixing of the number of Monte Carlo cycles and number of variational parameters and setting of initial position of particles for a given α.
2. Initialization of the energy and variance and start of the Monte Carlo cycles.
   (a) Proposal of the new step for one particle or all particles $\mathbf{R}' = \mathbf{R} + step \cdot r$, where r is a random variable $\in [0,1]$.
   (b) Calculation of the trial wave function and the probability distribution function for the new position.
   (c) Test of the new position in the Metropolis algorithm, the step is either rejected or accepted.
   (d) If the step is accepted, the initial position is assigned with the proposed step $\mathbf{R} = \mathbf{R}'$.
   (e) Update of the energy and variance.
3. End of Monte Carlo cycles, final calculation of the averages of interest.
4. Variation over the range of α selected and the repetition of steps described above to find the value corresponding to the minimum energy or application of the minimization algorithm.

In the present work these steps were performed for two different ways of sampling - the brute force sampling and the importance sampling, which are described in subsequent sections.

3.2. *Metropolis algorithm*

The Metropolis algorithm is the central driving algorithm in the Monte Carlo methods including the variational Monte Carlo exploited. It allows to sample a normalized probability distribution by a stochastic process (8). The base for the Metropolis algorithm is the Markovian process and the evolution of the probability distribution function in a random walk of the system from the state j to the state i is described by the transition matrix $W_{i\to j}$ and is not known initially. It can be decomposed into two multiplied probabilities:$A_{i\to j}$ - the probability of accepting a move from j towards i and $T_{i\to j}$ the probability of making the step from the state j to the state i:

$$W_{j\to i} = A_{j\to i} \cdot T_{j\to i}, \quad (27)$$

and for the the probability of the system to occur in the state i after the n steps denoted as $P_i^{(n)}$ can be obtained in two following ways: on the n-th step the system undergoes the accepted step from each of j states which the system can pass through or it attempts to undergo the transition from the state i to all the j states but the corresponding step is rejected. This can be mathematically written as:

$$P_i^{(n)} = \sum_j (P_j^{(n-1)} T_{j\to i} A_{j\to i} + P_i^{(n-1)} T_{i\to j}(1 - A_{i\to j})), \quad (28)$$

as the probability of making a transition is $\sum_j T_{j\to i} = 1$, thus:

$$P_i^{(n)} = P_i^{(n-1)} + \sum_j (P_j^{(n-1)} T_{j\to i} A_{j\to i} - P_i^{(n-1)} T_{i\to j} A_{i\to j}). \quad (29)$$

The system approaches the equilibrium position as the time goes to infinity, at the same time $P_i^{(n)}$ approaches the p_i – the value of desired probability distribution,that implies:

$$\lim_{t\to\infty} P_i^{(n)} = p_i = \lim_{t\to\infty} P_i^{(n-1)} + \sum_j (\lim_{t\to\infty} P_j^{(n-1)} T_{j\to i} A_{j\to i} -$$
$$- \lim_{t\to\infty} P_i^{(n-1)} T_{i\to j} A_{i\to j}) = p_i + \sum_j (p_j T_{j\to i} A_{j\to i} -$$
$$- p_i T_{i\to j} A_{i\to j}), \quad (30)$$

and thus we get the following:

$$\sum_j (p_j T_{j\to i} A_{j\to i} - p_i T_{i\to j} A_{i\to j}) = 0, \quad (31)$$

which can be rewritten in the following way:

$$\frac{A_{j\to i}}{A_{i\to j}} = \frac{p_i T_{i\to j}}{p_j T_{j\to i}}. \tag{32}$$

This relation defines the condition governing the movement towards the most probable state and in the present work is is treated in two different approaches which involve the two different ways of sampling – the brute force and the importance sampling.

3.2.1. *The brute force Metropolis algorithm*

The base of the brute force Metropolis algorithm is an assumption that the transition probability is symmetric i.e. $T_{i\to j} = T_{j\to i}$.The acceptance probabilities are still not known and it defines the ratio of different probabilities. However, the main idea of the algorithm considered is to move to the equilibrium state in the most efficient way, or, it terms of proposed steps, to have the maximum possible number of steps accepted. In the scope of present work the larger acceptance rate will correspond to the smaller value of energy of the state we are moving to, since the probability of the latter is higher.The ratio (32) will be larger than 1 in case we are moving towards the more probable state and it is smaller than 1 in the opposite case. this can be reflected by the following condition for the brute force approach (the normalization factors are eliminated $P(\mathbf{R}) = |\Psi_T(\mathbf{R})|^2 / \int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}$):

$$w = \frac{p_i}{p_j} = \frac{|\Psi_T(\mathbf{R}_i)|^2}{|\Psi_T(\mathbf{R}_j)|^2} > 1, \tag{33}$$

in this case the new step from the j state to the i state (for the further equations rthe corresponding positions are renamed as $\mathbf{R}$ and $\mathbf{R}'$) is accepted. However, it will be accepted in case:

$$w = \frac{p_i}{p_j} = \frac{|\Psi_T(\mathbf{R}')|^2}{|\Psi_T(\mathbf{R})|^2} \geq s, \tag{34}$$

where s is the random number and s$\in [0,1]$. Thus, the brute force approach will be the following in the case of the given problem:in each Monte Carlo cycle the new position is proposed:

$$\mathbf{R}' = \mathbf{R} + s \cdot \Delta R, \tag{35}$$

here s$\in [0,1]$ and ΔR is user defined step size for each particle in each direction, and then to calculate the wave functions for both new and old positions. Then the condition (34) is checked, if it is fulfilled, the step is accepted for a subsequent use, if no, the position remains the same. In both cases the energy and the variance are updated and then the calculation goes to the next Monte Carlo cycle. The drawback of this algorithm is the ΔR step size parameter which should be properly tuned to obtain the proper result for a given number of Monte Carlo cycles. The step proposal is not defined by the wave function of the system, and since it is manually adjusted, the brute force approach is not the most efficient way of point sampling.As a usual case the ΔR is chosen thus $\approx 50\%$ of Monte Carlo cycles (or step proposals) are accepted.

3.2.2. *The importance sampling*

The drawback of the previous algorithm can be eliminated, i.e. instead of choosing the the step size parameter and finding an appropriate value, the step can be defined by the trial wave function of the system. This algorithm is based on the Fokker-Planck equation and the Langevin equation. The latter equation is used in Monte Carlo calculations to define the new step proposed which will be dependent on the transition probability for a given point in space which will correspond to the initial state of the system. The new trial position is given as the solution of the Langevin equation (in one dimension) (1):

$$\frac{\partial x(t)}{\partial t} = DF(x(t)) + \eta, \tag{36}$$

where D has a meaning of factor in kinetic energy and equals to $1/2$, $F(x(t))$ is the drift force, η is the random variable. In general, the physical meaning of the following: a moving particle will constantly collide with other particles and these collisions will more likely occur on the front side preventing the particle from moving forward. This will result in a systematic force, proportional to velocity of a particle and having an opposite direction. In addition, the stochastic force is also present. Combining these factors, the evolution of the particle movement can be derived. The solution of the Langevin equation can be obtained by Euler's method and has the following form in one dimension:

$$x' = x + DF(x)\Delta t + \xi\sqrt{\Delta t}, \tag{37}$$

here ξ is gaussian random variable and the only parameter to be chosen is the time step Δt . The values of $\Delta t \in [0.001, 0.01]$ results in the relatively stable value of energy for the ground state.

On the other hand, the constant diffusion process a particle undergoes in all directions isotropically can be associated with the time-dependent probability density $P(\mathbf{R}, t)$. Taking into account that the initial condition of the system changes thus the system evolves to achieve the equilibrium state, it can be shown that the Fokker-Planck equation for $P(\mathbf{R}, t)$ takes place in many-dimensional case:

$$\frac{\partial P(\mathbf{R}, t)}{\partial t} = \sum_i D \frac{\partial}{\partial x_i} \left(\frac{\partial}{\partial x_i} - F_i \right) P(\mathbf{R}, t), \tag{38}$$

where x_i and F_i are the i-th components of the $\mathbf{R}$ position vector of the system and the drift force (or quantum force),which can be obtained from the Fokker-Planck equation in the form $\mathbf{F} = f() \frac{\partial P}{\partial \mathbf{x}}$ with the assumption of stationary densities :

$$\mathbf{F} = 2\frac{1}{\Psi_T} \nabla \Psi_T. \tag{39}$$

The importance sampling algorithm implies that the transition probabilities $T_{j\to i}$ (32) can no longer be omitted. And as the Langevin equation allows to obtain the new trial position, the Fokker-Planck equation provides with the transition probabilities in the form of the Green

function (written in one dimension):

$$G(x',x,t)=\frac{1}{(4\pi D\Delta t)^{3N/2}}\exp(-(x'-x-D\Delta tF(x))^2/4D\Delta t). \tag{40}$$

In this case the Metropolis algorithm is called the Metropolis-Hastings algorithm and assumes the condition for the selection of steps in form of:

$$w=\frac{G(\mathbf{R},\mathbf{R}',t)|\Psi_T(\mathbf{R'})|^2}{G(\mathbf{R}',\mathbf{R},t)|\Psi_T(\mathbf{R})|^2}\geq s, \tag{41}$$

with $s\in[0,1]$, and if this requirement is satisfied, the accepted move is accepted and used in subsequent calculations, otherwise the position remains the same.

3.3. *Energy minimization and gradient descent method*

The local energy computed in each Monte Carlo iteration is the function of several parameters - α and β related to the guess for the form of the trial wave function, the latter parameter reflects the deviations of the chosen harmonic potential from a spherical form. In case non-interacting bosons and spherical potential it is known that $\beta=1$ and α should correspond to value 0.5. However, the interaction between particles in the system is included, it is no longer obvious, what values should be chosen for calculations. In principle, one can variate these parameters over a chosen region of values, i.e. to calculate local energy $E_L(\alpha,\beta)$ for each variational parameter and find the minimum $E_L(\alpha,\beta)$ graphically. This plain method is,nevertheless, quite time consuming when it is not initially clear where the minimum can be found. For the sake of facilitation of parameter search, the various minimization methods can be applied.

In the present work one of the easiest for understanding approaches – the gradient descent (or steepest descent) method is used for minimization of the local energy with respect to parameter α. Its form applied to our particular problem is the following:

$$\hat{\alpha}=\alpha-\eta\cdot\frac{d\langle E(\alpha)\rangle}{d\alpha}, \tag{42}$$

where η is a step size (or learning rate in machine learning). The underlying idea is that $E_L(\alpha)$ decreases faster if one moves in variational parameter space towards the direction of negative gradient $\frac{d<E(\alpha)>}{d\alpha}$ and ideally the sequence of α converges to a global minimum of a given convex function. Despite relatively uncomplicated implementation this method is quite sensitive to a choice of initial guess for a parameter,learning rate and, moreover, it can be computationally expensive for large number of data involved. It also treats all directions in variational parameter space uniformly,faces struggles dealing with saddle points and defines only local minima in more complicated functions. This might become sensible problems when the machine learning is involved. However, in the present work the implementation excludes all the mentioned problems and there is no significant problem to choose the initial guess properly.

Implementation of the gradient descent in present work implies calculation of the following derivatives:

$$\bar{E_L}(\alpha)=\frac{d\langle E(\alpha)\rangle}{d\alpha}, \tag{43}$$

and as the local energy is presented as:

$$\langle E(\alpha)\rangle=\frac{\langle\Psi_T(\alpha)|\,\hat{H}\,|\Psi_T(\alpha)\rangle}{\langle\Psi_T(\alpha)|\Psi_T(\alpha)\rangle}, \tag{44}$$

differentiating one can obtain:

$$\bar{E_L}(\alpha)=2\left[\langle E_L(\alpha)\frac{\bar{\Psi}_T(\alpha)}{\Psi_T(\alpha)}\rangle-\langle E_L(\alpha)\rangle\langle\frac{\bar{\Psi}_T(\alpha)}{\Psi_T(\alpha)}\rangle\right], \tag{45}$$

here $\bar{\Psi}_T(\alpha)=\frac{d\Psi_T(\alpha)}{d\alpha}$.

The described procedure was realized in the program, and the gradient is calculated unless the minimum is reached, which is defined by the user chosen tolerance ϵ – if the energy derivative in a given step is less than ϵ the calculation is stopped. Additionally the stop of calculation if fluctuations of α over 10 last steps are less than ϵ is also included.

3.4. *Blocking method for variance estimation*

As it was already mentioned in the subsection 2.6 an appropriate method for obtaining the variance σ^2 in Monte Carlo experiments is required. For this aim the resampling methods are the inalienable tools which allow to efficiently obtain the variance by repeatedly drawing different samples from the given data set. Such popular methods as independent bootstrap and the jackknife (special case of independent bootstrap) can be used for independent, identically distributed random variables. However, for the large data sets they are not applicable because of increasing complexity, and the blocking method, which becomes even more accurate for increasing number of data, can be applied instead.

Let's consider the data set (stationary time series) $\vec{x}=\{x_1+x_2+...+x_n\}$, where $n=2^d$ and $d>1$ is some integer. The blocking transformations involve this initial vector to create the new vector $\vec{x}_1$ by taking the mean of subsequent pair of elements from $\vec{x}$. Taking the $\vec{x}_1$ vector as the base and repeating procedure for other base vectors we get in each iteration one can end up after k blocking transformations with d new vectors with elements:

$$\begin{aligned}(\vec{x}_0)_k&=(\vec{x})_k\\(\vec{x}_{i+1})_k&=\frac{(\vec{x}_i)_{2k-1}+(\vec{x}_i)_{2k}}{2}\end{aligned} \tag{46}$$

for $1\leq i\leq d-1$ and it can be shown that if the components of $\vec{x}$ are stationary time series, then the components of $\vec{x}_i$ with $1\leq i\leq d-1$ are the stationary time series as well.And if the initially chosen time series is asymptotically uncorrelated the kth series is also asymptotically uncorrelated. It can be shown that the variance of $\vec{x}_k$ is given as:

$$V(\bar{x}_k)=\frac{\sigma_k^2}{n_k}+\frac{2}{n_k}\sum_{h=1}^{n_k-1}\left(1-\frac{h}{n_k}\right)\gamma_k(h)=\frac{\sigma_k^2}{n_k}+e_k, \tag{47}$$

where e_k is called truncation error and $\gamma_{k+1}(h) = cov((x_{k+1})_i, x_{k+1})_j)$ and $h = |i-j|$,$\gamma_k(0) = \sigma_k^2$. It can be also proven that $V(\bar{x}_k) = V(\bar{x})$ for $0 \leq k \leq d-1$ and thus the variance of the sample mean we are looking for all $0 \leq k \leq d-1$ is:

$$V(\bar{x}) = \frac{\sigma_k^2}{n_k} + e_k. \tag{48}$$

As the number of blocking procedures increases (i.e. more measurements is inserted in each subsequent block) the e_k can be made small enough to make $V(\bar{x}) = \frac{\sigma_k^2}{n_k}$ a good estimate for the variance.

4. CODE

4.1. *Implementation*

This study revolves around being able to simulate real events by using VMC. The number of particles where set to variate from 1 to 500 and due to the amount of particles, an efficient code was needed. The code was first built in a methods.cpp where all the code for the VMC, without interaction implemented. To set the positions a class called Matrix was made in *matrix.h*. This class was tested against other solutions like the matrix class in armadillo, which was found to be slightly slower. By using the matrix class all the positions are set simultaneously and the energy then calculated, instead of picking a particle at random in the system for so calculating the energy. These options are two sides of the same coin, the only difference is the way particles move towards the most probable state. The *methods.cpp* includes the function with brute VMC with Metropolis algorithm where it is possible to calculate the local energy analytically or numerically. There is also a function with VMC including importance sampling where the Metropolis-Hastings algorithm is used, and then finally the VMC with gradient decent. On top of this, there is another file including largely the same code but with interactions. This file is simply called *methods$_i$nteraction.cpp*. Despite repeating code and not using object orientation, this showed itself to be the fastest way when implementing many particles to the system. On the other hand, it might be easy to get lost in the amount of code lines. In an attempt to make it more suitable there was implemented a switch function in *main.cpp*, where the user can choose which of the codes it wants to get data from. All the data that are presented in this study are generated from these functions, and to test the results the Gross-Pitaevskii equation is added in *main.cpp* to check if the results corresponds to the it.

```
switch (ind_2)
        {
        case 1:
          mc_sampling(stepSize, dim, numOfPart,
    numMCCycles, numVar, Etot, Etot2, ind_1,
    alpha, deltaAlpha, thermailization);
          writeToFile("E_average_LA.txt", Etot,
    Etot2, numVar, alpha, deltaAlpha);
          break;
        case 2:
          mc_sampling_IMS(stepSize, dim,
    numOfPart, numMCCycles, numVar, Etot, Etot2,
     ind_1, alpha, deltaAlpha, thermailization);
        // ......and so on
         //...
         default:
         cout << "Coose any option next time!";
         }
         cout << "Main running for " << " " <<
    double((clock()-time_start)/double(
    CLOCKS_PER_SEC)) << " seconds" << endl;

         alpha=alpha-numVar*deltaAlpha;
         if((ind_2==1)||(ind_2==2)){
         for(int i=0; i<numVar; i++){
             double e_GP=0;
             e_GP=numOfPart*(1/(4*alpha)+alpha)
    *(1+beta/2);
             if(fabs(e_GP-Etot[i])>5){
                 cout<<"Results do not correspond
    to the GP equation!Please, check the
    parameters!"<<endl;
             }
          }
         }
```

4.2. *Implementing Classes*

For learning and because of interests, a second program was which included the original code was written, but now it was attempted to make it more object oriented. The aim was mainly to learn how to make a suitable code and to use object orientation, which is how the $C++$ programming language is intended to be used. In the second code it was decided to keep the matrix class, and to hide the for loops where the matrices are filled with the positions of the particles, the machinery if one will, a Position class was made where these were put. Then the energy, numerical and analytical, together with the wave function was implemented into a System class. All these classes where used to shorten down the code significantly in *methods.cpp*, and if continued for all the original program, would have made it shorter and maybe easier to use by users.

Since this was mostly done for the learning experience the classes code was made for the brute VMC with the metropolis algorithm. What is interesting to illustrate is the difference in CPU time for the code with classes and the less polished code without. By running both codes with the variational parameters shown here:

```
int numVar=4;
double stepSize = 1;
double alpha=0.3, deltaAlpha=0.1;
```

, and by variating the number of particles from 1 to 20, for 1 dimension and one million Monte Carlo cycles the CPU for the two codes differ quite much. This is best illustrated in the figure below.

This illustrates plainly the difference, and might be interesting to know when making decisions on what to prioritize. Without classes the code might become hazardous to read, but it is quite good if efficiency is important. While with classes are definitely better regarding the future, for example if one builds it more general so it will work for both bosons and fermions, for example.

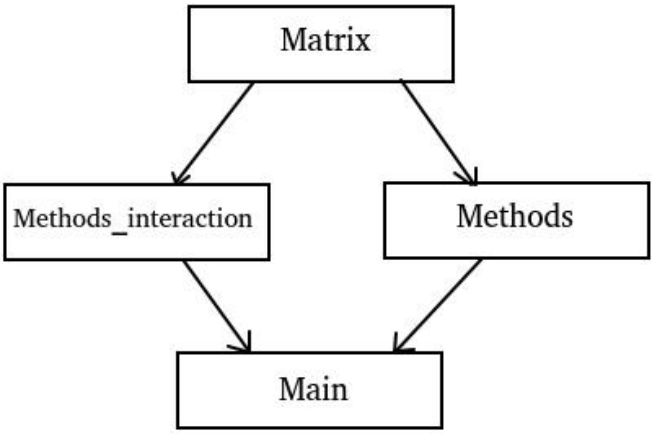

FIG. 1.— A scheme of the code and how it interacts is shown here.

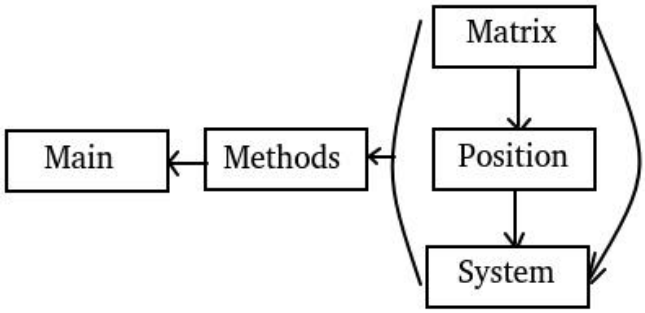

FIG. 2.— A scheme of the code with classes and how the different classes interact with each other is presented here.

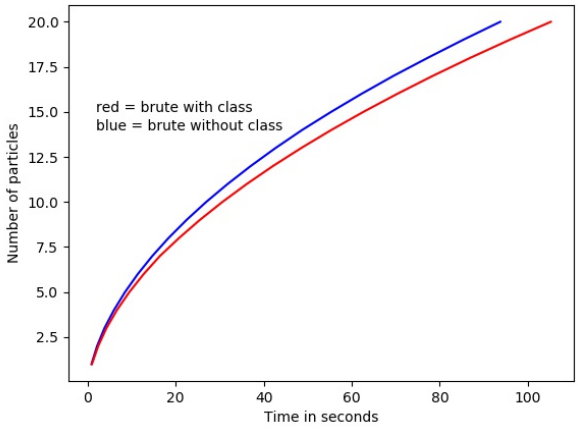

FIG. 3.— The energy is being calculated for the variational parameter $\alpha = 0.3$ to $\alpha = 0.7$, with one million Monte Carlo cycles for 1 up to 20 particles. It can look like the time complexity of the particles is a square root time complexity $O(n^{1/2})$.

5. RESULTS

In the present chapter the results of calculations performed by means of program developed are presented. Firstly, the results for the simplest system case (bosons do not interact with each other ($a = 1$) in a spherical harmonic oscillator potential ($\beta = 1$) are performed for two method modifications - the brute force and importance sampling, which imply different step proposal and selection procedures and were considered in more detail in previous chapters. Then, the better statistical analysis is performed for previously obtained results. The second and most relevant complicated and interesting part of the project is concerned with the case of deformed harmonic oscillator potential ($\beta = 2.82843$) and interacting bosons system ($a = 0.0043$), estimation of variational parameter α corresponding to the ground state energy for this system on the base of gradient descent method and estimation of one-body densities for interacting and non-interacting case.

5.1. *VMC with brute force sampling for non-interacting spherical case*

One of the most pictorial (but not exact at the same time) ways of variational parameter α corresponding to the minimum energy $E_L(\alpha)$ of the system (ground state energy) is to represent the dependence of $E_L(\alpha)$ on α graphically. Therefore, the local energy was calculated for 10 different values of α starting with $\alpha = 0.1$ with the step $\Delta\alpha = 0.1$. The variational Monte Carlo with brute force Metropolis algorithm with 10^6 cycles is used. The calculations of local energy and its variance for 1, 10,100,500 particles for 1,2,3-dimensional cases are presented and listed in TABLE 1 and TABLE 2. The first table includes the results of calculations with analytical calculation of the local energy involved, the second table contains similar results with corresponding numerical calculation. In addition the comparison with exact values for all cases are included in the tables as well. An important part of performed calculations is the comparison of CPU times for analytical and numerical approaches for local energy estimation. All the points are calculated for variational parameter $\alpha = 0.5$ which would give the minimum of local energy in all cases.

The parameters used for the two forst problems is the following:

```
// Parameters used for the program
// Initial alpha
double alpha = 0.1;
// Step for alpha
double deltaAlpha = 0.1;
// Initial beta
double beta = 1.0;
// Number of alpha-points for local energy
    calculation
int numVar = 0;
// Step size for the new step proposal
double stepSize = 1.0  //0.001 in case of
    importance sampling
// Number of dimensions
int dim = 3; //Number of dimensions 1,2,3
// Number of particles
int numOfPart = 10 //Number of particles 1, 10,
    100, 500
```

```
// Number of MC experiments
int numMCCycles = 1e6;
// Mass of a particle
double mass = 1.0;
// Frequency of HO potential
double omega = 1.0;
```

TABLE 1
THE ANALYTICAL RESULTS OBTAINED FOR LOCAL ENERGY E_L, VARIANCE $\sigma^2(E_L)$ AND CPU TIMES ON THE BASE VMC WITH BRUTE-FORCE BASED METROPOLIS ALGORITHM FOR 1, 10, 100 AND 500 PARTICLES IN THE SYSTEM WITH 1, 2, 3 DIMENSIONS. THE VARIATIONAL PARAMETER $\alpha = 0.5$, THE NUMBER OF MC CYCLES IS 10^6 AND THE STEP SIZE $r_{step} = 1.0$. THE RIGHT COLUMN CONTAINS EXACT VALUE FOR THE GIVEN SYSTEMS WHICH COINCIDES WITH THE VALUE OBTAINED WITH GROSS-PITAEVSKII EQUATION.

N_{part}	N_{dim}	E_L, $\hbar\omega_{h0}$	$\sigma^2(E_L)$, $(\hbar\omega_{h0})^2$	CPU, time,s	E_L^{exact}/GPE, $\hbar\omega_{h0}$
1	1	0.50000	0	0.050749	0.50000
1	2	1.0000	0	0.065422	1.0000
1	3	1.5000	0	0.072097	1.5000
10	1	5.0000	0	0.15762	5.0000
10	2	10.000	0	0.22656	10.000
10	3	15.000	0	0.31355	15.000
100	1	50.000	0	1.3552	50.000
100	2	100.00	0	1.8791	100.00
100	3	150.00	0	2.7665	150.00
500	1	250.00	0	5.1662	250.00
500	2	500.00	0	9.3791	500.00
500	3	750.00	0	13.611	750.00

TABLE 2
THE NUMERICAL RESULTS OBTAINED FOR LOCAL ENERGY E_L, VARIANCE $\sigma^2(E_L)$ AND CPU TIMES ON THE BASE VMC WITH BRUTE-FORCE BASED METROPOLIS ALGORITHM FOR 1, 10, 100 AND 500 PARTICLES IN THE SYSTEM WITH 1, 2, 3 DIMENSIONS. THE VARIATIONAL PARAMETER $\alpha = 0.5$, THE NUMBER OF MC CYCLES IS 10^6 AND THE STEP SIZE $r_{step} = 1.0$. THE RIGHT COLUMN CONTAINS EXACT VALUE FOR THE GIVEN SYSTEMS WHICH COINCIDES WITH THE VALUE OBTAINED WITH GROSS-PITAEVSKII EQUATION.

N_{part}	N_{dim}	E_L, $\hbar\omega_{h0}$	$\sigma^2(E_L)$, $(\hbar\omega_{h0})^2$	CPU, time,s	E_L^{exact}/GPE, $\hbar\omega_{h0}$
1	1	0.50000	1.7431e-14	0.32015	0.50000
1	2	1.0000	2.4008e-14	0.34433	1.0000
1	3	1.5000	1.0258e-13	0.41041	1.5000
10	1	5.0000	2.5864e-12	1.9816	5.0000
10	2	10.000	2.6290e-11	2.7879	10.000
10	3	15.000	2.7171e-11	4.1920	15.000
100	1	50.000	1.9599e-10	41.395	50.000
100	2	100.00	1.1340e-08	107.97	100.00
100	3	150.00	2.4216e-07	225.37	150.00
500	1	250.00	3.8425e-07	658.38	250.00
500	2	500.00	7.6540e-06	2393.4	500.00
500	3	750.00	1.1366e-06	6996.5	750.00

This fact is reflected at FIG.4 and 5. The Local energy dependence on α is presented for MC 10^6 cycles and 10 particles in three dimensions for non-interacting case. Here $\alpha = 0.5$ represents a clear minimum (within $\Delta\alpha = 0.1$ step interval). In addition the corresponding values obtained with Gross-Pitaevskii equation (2.5).The variance dependence on α reflects the minimum value $(V(E_L(\alpha)) \approx 0)$ for $\alpha = 0.5$ as well. This is in coincidence with zero variance in case of exact energy value.

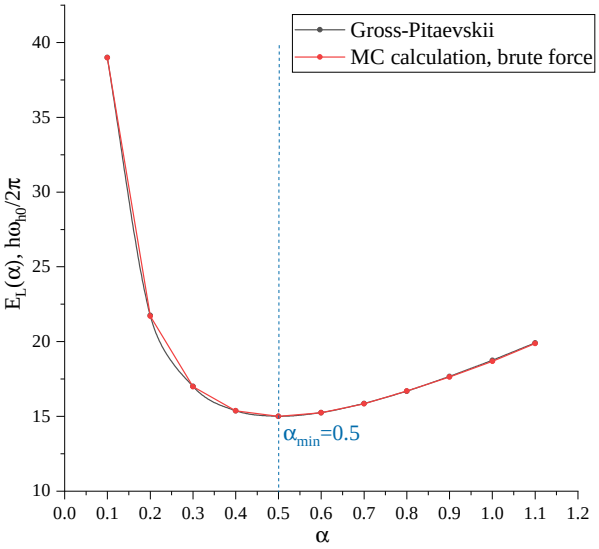

FIG. 4.— Local energy $E_L(\alpha)$ as a function of α calculated for 10 particles in 3 dimensions with VMC with brute force Metropolis algorithm for non-interacting case. The analytical calculations for Gross-Pitaevskii equation are included.

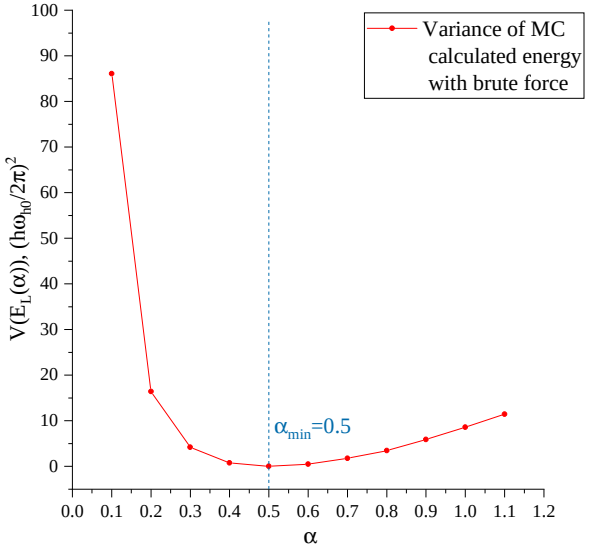

FIG. 5.— Variance of local energy $E_L(\alpha)$ as a function of α calculated for 10 particles in 3 dimensions with VMC with brute force Metropolis algorithm.

The efficiency of brute-force Metropolis algorithm is strongly dependent on the choice of step size which was chosen in our calculations to be equal to 1.0 in units of $a_{h0} = \sqrt{\frac{\hbar}{m\omega_{h0}}} = 1.0$ with $\hbar = m = \omega_{h0} = 1.0$ chosen for the sake of simplicity. This choice of step size demonstrates quite high acceptance rate i.e. a quite large number of purposed steps is accepted. The sensitivity of chosen method to the size of spatial step is shown at FIG.6.

The acceptance rate drops nearly linearly with increase of the step size. However, even though the smaller step

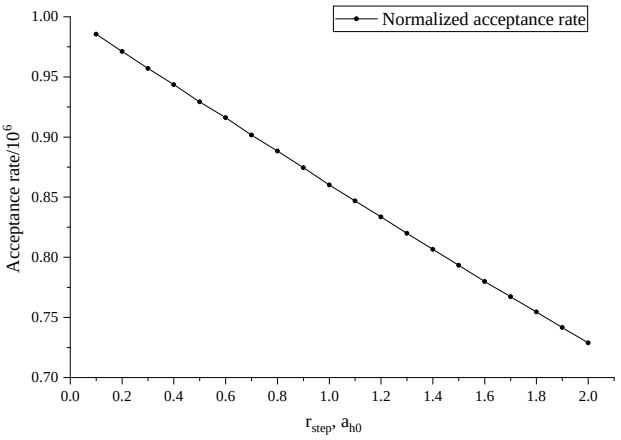

FIG. 6.— The relative acceptance rate (normalized by 10^6) as a function of step size calculated for 1 particle in 1 dimension.

size corresponds to the higher acceptance rate, the results obtained for too small step sizes reveal an inappropriate jumping as the local energy is considered as a function of α, at the same time the size step comparable with the characteristic characteristic length of the trap is proved to provide stable meaningful results.

5.2. *VMC with importance sampling for non-interacting spherical case*

The next step of further improvement of the program involves change of brute force Metropolis algorithm with importance sampling based one. The results obtained for cases of 1, 10, 100 and 500 particles in 1, 2 and 3 dimensions are for both analytically and numerically calculated local energies. In both cases the drift force was calculated analytically since an additional numerical calculation implemented was significantly slowing the program down, which was quite critical for large number of particles and dimensions. The values of local energies and the corresponding variances calculated in the program are presented in TABLE 3 and TABLE 4 where they are also compared with exact values.

Due to additional calculations related to the appearance and evaluation of the drift force and the Green function, the part of the program involving the importance sampling algorithm is slightly slower, however the acceptance rate is significantly high and close to 10^6 for the chosen time step $t_{step} = 0.001$. even though the importance sampling does not require an additional tuning of step size parameter, it is still dependant of the time step size. The sensitivity of acceptance rate was studied for different time steps in a wide range of $[10^{-4}, 10]$ (see FIG.6). An acceptance rate remains high (above $0.9{\cdot}10^6$ for 10^6 MC cycles) for $t_{step} \in [10^{-4}, 0.1]$ and then drops fast as the time step size increases. The step size for the calculations provided was chosen for the middle part of purposed interval.

TABLE 3
THE ANALYTICAL RESULTS OBTAINED FOR LOCAL ENERGY E_L, VARIANCE $\sigma^2(E_L)$ AND CPU TIMES ON THE BASE VMC WITH IMPORTANCE SAMPLING BASED METROPOLIS ALGORITHM FOR 1, 10, 100 AND 500 PARTICLES IN THE SYSTEM WITH 1, 2, 3 DIMENSIONS. THE VARIATIONAL PARAMETER $\alpha = 0.5$, THE NUMBER OF MC CYCLES IS 10^6 AND THE TIME STEP SIZE $r_{step} = 0.001$. THE RIGHT COLUMN CONTAINS EXACT VALUE FOR THE GIVEN SYSTEMS WHICH COINCIDES WITH THE VALUE OBTAINED WITH GROSS-PITAEVSKII EQUATION.

N_{part}	N_{dim}	E_L, $\hbar\omega_{h0}$	$\sigma^2(E_L)$, $(\hbar\omega_{h0})^2$	CPU, time,s	E_L^{exact}/GPE, $\hbar\omega_{h0}$
1	1	0.50000	0	0.078061	0.50000
1	2	1.0000	0	0.11374	1.0000
1	3	1.5000	0	0.13772	1.5000
10	1	5.0000	0	0.38130	5.0000
10	2	10.000	0	0.64532	10.000
10	3	15.000	0	0.90542	15.000
100	1	50.000	0	3.1951	50.000
100	2	100.00	0	5.9035	100.00
100	3	150.00	0	8.6738	150.00
500	1	250.00	0	15.610	250.00
500	2	500.00	0	29.313	500.00
500	3	750.00	0	42.488	750.00

TABLE 4
THE NUMERICAL RESULTS OBTAINED FOR LOCAL ENERGY E_L, VARIANCE $\sigma^2(E_L)$ AND CPU TIMES ON THE BASE VMC WITH IMPORTANCE SAMPLING BASED METROPOLIS ALGORITHM FOR 1, 10, 100 AND 500 PARTICLES IN THE SYSTEM WITH 1, 2, 3 DIMENSIONS. THE VARIATIONAL PARAMETER $\alpha = 0.5$, THE NUMBER OF MC CYCLES IS 10^6 AND THE TIME STEP SIZE $r_{step} = 0.001$. THE RIGHT COLUMN CONTAINS EXACT VALUE FOR THE GIVEN SYSTEMS WHICH COINCIDES WITH THE VALUE OBTAINED WITH GROSS-PITAEVSKII EQUATION.

N_{part}	N_{dim}	E_L, $\hbar\omega_{h0}$	$\sigma^2(E_L)$, $(\hbar\omega_{h0})^2$	CPU, time, s	E_L^{exact}/GPE, $\hbar\omega_{h0}$
1	1	0.5000	1.7902e-14	0.34074	0.50000
1	2	1.0000	2.0317e-14	0.39135	1.0000
1	3	1.5000	1.9540e-13	0.48607	1.5000
10	1	5.0000	1.6094e-12	2.2277	5.0000
10	2	10.000	2.7569e-12	3.1587	10.000
10	3	15.000	5.4570e-12	4.7094	15.000
100	1	50.000	9.5497e-12	42.684	50.000
100	2	100.00	2.2010e-10	112.44	100.00
100	3	150.00	4.2601e-09	232.25	150.00
500	1	250.00	3.0122e-09	682.11	250.00
500	2	500.00	1.8103e-08	2836.2	500.00
500	3	750.00	1.3853e-08	7439.8	750.00

5.3. *The better statistical analysis*

In order to evaluate the variance for each calculated result properly the blocking method was used. This method was interpreted by Marius Jonsson (12) in the python written program used for this project and attached. The calculations are performed for 1, 10, 100 and 500 particles in three dimensions with local energy calculated numerically. Both the blocking method and conventional variance evaluation described above (3.4) were used. As the results of Monte Carlo calculations are written to the file used by blocking.py program each 100 iterations, it turned out that the previously selected grid step for numerical calculation $h = 0.001$ gives the result so close to analytical one that the variance calculated

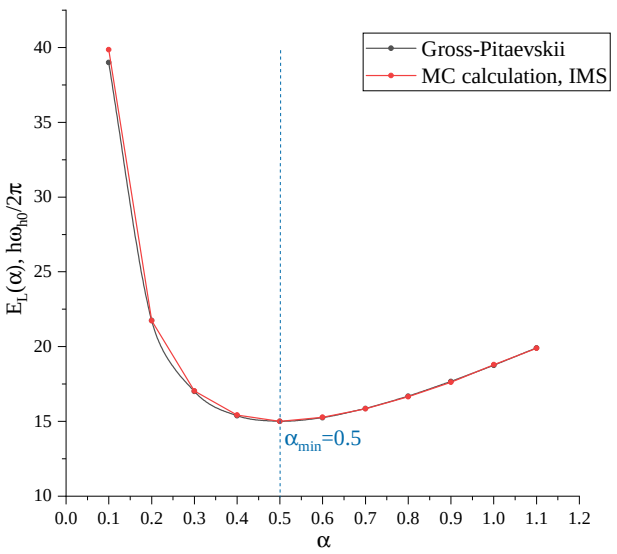

FIG. 7.— Local energy $E_L(\alpha)$ as a function of α calculated for 10 particles in 3 dimensions with VMC with brute force Metropolis algorithm for non-interacting case. The analytical calculations for Gross-Pitaevskii equation are included.

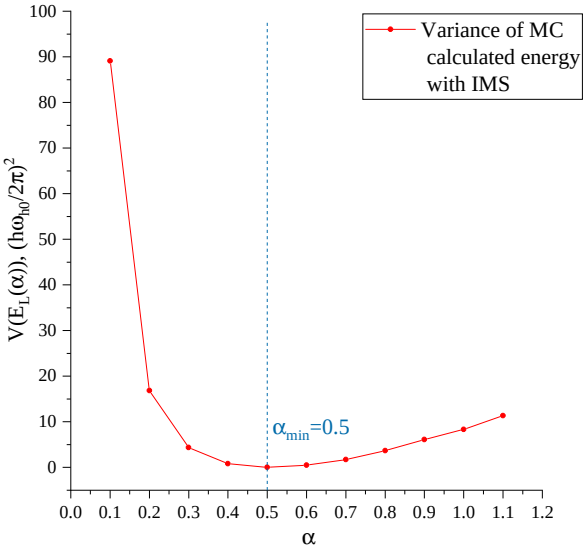

FIG. 8.— Variance of local energy $E_L(\alpha)$ as a function of α calculated for 10 particles in 3 dimensions with VMC with brute force Metropolis algorithm.

by blocking method is 0, which is not a sensible result. Thus, two other grids were used $h = 0.01$ and $h = 0.1$ to obtain the results which are presented in TABLE 5.

5.4. *VMC calculation for interacting elliptical case*

The next step in further complication and making the program more realistic is introducing the interaction between bosons in the system. The hard sphere radius is fixed as $a/a_{h0} = 0.0043$ (3),(13) with $a = 1.0$ according to initial choice of $\omega = m = \hbar = 1.0$. The variational parameter is still fixed, but its value is $\beta = 2.82843$ which

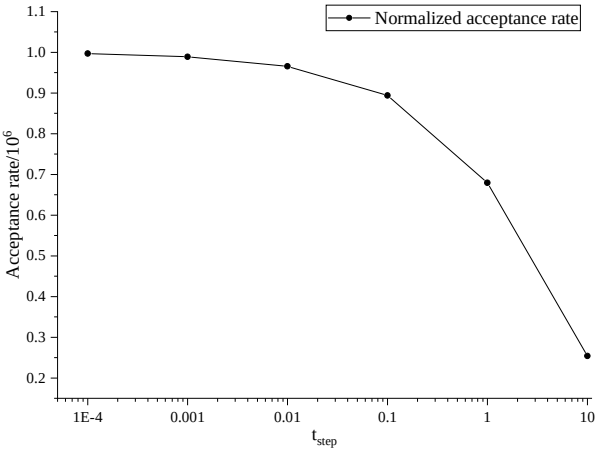

FIG. 9.— The relative acceptance rate (normalized by 10^6) as a function of time step size calculated for 1 particle in 1 dimension.

TABLE 5
THE NUMERICAL RESULTS OBTAINED FOR LOCAL ENERGY E_L, VARIANCE $\sigma^2(E_L) = \langle E_L^2\rangle - \langle E_L\rangle$ AND THE VARIANCE CALCULATED WITH THE BLOCKING METHOD. THE CALCULATIONS ARE BASED ON THE VMC WITH IMPORTANCE SAMPLING BASED METROPOLIS ALGORITHM FOR 1, 10, 100 AND 500 PARTICLES IN THE SYSTEM WITH 3 DIMENSIONS. THE VARIATIONAL PARAMETER $\alpha = 0.5$, THE NUMBER OF MC CYCLES IS 10^6 AND THE TIME STEP SIZE $r_{step} = 0.001$. THE RIGHT COLUMN CONTAINS EXACT VALUE FOR THE GIVEN SYSTEMS.

N_{part}	$\langle E_L\rangle$, $\hbar\omega_{h0}$	$\sigma^2(E_L)$, $(\hbar\omega_{h0})^2$	$\sigma^2_{blocking}(E_L)$ $(\hbar\omega_{h0})^2$
	h=0.001		
1	1.5000	2.0872e-13	0.0000
10	15.000	5.9686e-12	0.0000
100	150.00	1.7826e-10	0.0000
500	750.00	1.3853e-08	0.0000
	h=0.01		
1	1.5000	3.1661e-10	1.9512e-08
10	15.000	3.0304e-09	7.7512e-07
100	150.00	9.1148e-07	5.8364e-06
500	750.00	5.2677e-06	8.8750e-05
	h=0.1		
1	1.4990	3.1182e-06	1.8652e-05
10	14.991	3.1039e-05	2.5862e-04
100	149.69	5.3179e-04	9.4456e-04
500	749.57	1.7584e-03	9.0905-03

reflects the elliptical shape of the potential trap. The parameter α is still the only actually variable parameter altered to find the ground state energy. The calculations are performed on the base of brute force Metropolis algorithm. When the initial positions for each α are set the possibility for two particles accidentally occurring within the same a^3 volume is taken into account. The systems of 10, 50 and 100 interacting bosons in 3 dimensional elliptical trap are presented in TABLE 6,TABLE 7, and TABLE 8.

5.5. *Finding the minimum energy of the system*

The variational parameter $\alpha = 0.5$ corresponding to the ground state (i.e. minimum) energy was verified

TABLE 6
THE ANALYTICAL RESULTS OBTAINED FOR LOCAL ENERGY E_L, VARIANCE $\sigma^2(E_L)$ FOR INTERACTING (I) AND NON-INTERACTING (NI) CASES. THE CALCULATIONS ARE BASED ON THE VMC BASED ON THE BRUTE FORCE METROPOLIS ALGORITHM FOR 10 PARTICLES IN THE SYSTEM WITH 3 DIMENSIONS. THE VARIATIONAL PARAMETER $\alpha = 0.5$, THE NUMBER OF MC CYCLES IS 10^6 AND THE STEP SIZE $r_{step} = 1.0$.

Interacting vs non-interacting 10 Particles					
α	E_L^i $\hbar\omega_{h0}$	$\sigma^2(E_L)^i$ $(\hbar\omega_{h0})^2$	E_L^{ni} $\hbar\omega_{h0}$	$\sigma^2(E_L)^{ni}$ $(\hbar\omega_{h0})^2$	GPE $\hbar\omega_{h0}$
0.3	27.489	14.106	27.284	13.951	27.361
0.4	24.919	2.6072	24.749	2.4981	24.746
0.5	24.288	0.0030919	24.142	1.0215e-08	24.142
0.6	24.714	1.7108	24.534	1.6869	24.545
0.7	25.649	5.9751	25.526	5.9073	25.522

TABLE 7
THE ANALYTICAL RESULTS OBTAINED FOR LOCAL ENERGY E_L, VARIANCE $\sigma^2(E_L)$ FOR INTERACTING (I) AND NON-INTERACTING (NI) CASES. THE CALCULATIONS ARE BASED ON THE VMC BASED ON THE BRUTE FORCE METROPOLIS ALGORITHM FOR 50 PARTICLES IN THE SYSTEM WITH 3 DIMENSIONS. THE VARIATIONAL PARAMETER $\alpha = 0.5$, THE NUMBER OF MC CYCLES IS 10^6 AND THE STEP SIZE $r_{step} = 1.0$.

Interacting vs non-interacting 50 Particles					
α	E_L^i $\hbar\omega_{h0}$	$\sigma^2(E_L)^i$ $(\hbar\omega_{h0})^2$	E_L^{ni} $\hbar\omega_{h0}$	$\sigma^2(E_L)^{ni}$ $(\hbar\omega_{h0})^2$	GPE $\hbar\omega_{h0}$
0.3	140.40	90.680	135.81	85.619	136.81
0.4	125.84	14.998	123.34	13.044	123.73
0.5	123.06	0.046789	120.71	9.8462e-09	120.71
0.6	125.72	10.897	122.81	9.1911	122.72
0.7	130.89	30.749	127.90	27.504	127.61

TABLE 8
THE ANALYTICAL RESULTS OBTAINED FOR LOCAL ENERGY E_L, VARIANCE $\sigma^2(E_L)$ FOR INTERACTING (I) AND NON-INTERACTING (NI) CASES. THE CALCULATIONS ARE BASED ON THE VMC BASED ON THE BRUTE FORCE METROPOLIS ALGORITHM FOR 100 PARTICLES IN THE SYSTEM WITH 3 DIMENSIONS. THE VARIATIONAL PARAMETER $\alpha = 0.5$, THE NUMBER OF MC CYCLES IS 10^6 AND THE STEP SIZE $r_{step} = 1.0$.

Interacting vs non interacting 100 Particles					
α	E_L^i $\hbar\omega_{h0}$	$\sigma^2(E_L)^i$ $(\hbar\omega_{h0})^2$	E_L^{ni} $\hbar\omega_{h0}$	$\sigma^2(E_L)^{ni}$ $(\hbar\omega_{h0})^2$	GPE $\hbar\omega_{h0}$
0.3	275.51	177.88	268.97	168.92	273.61
0.4	258.13	37.988	246.17	30.302	247.46
0.5	246.58	0.23568	241.42	3.9384e-08	241.42
0.6	251.18	26.865	245.66	22.460	245.44
0.7	266.55	84.875	255.24	75.960	255.22

in the previous sections graphically. However, this way of minimum parameter search is inefficient and can be substituted by the gradient descent method. The latter based on the brute force VMC was implemented in order to find the value of the parameter α corresponding to the ground state energy in case of 1, 10, 50 and 100 particles in 3 dimensional elliptical harmonic oscillator trap. The results are presented in the TABLE 9.

5.6. *Radial distribution of particles*

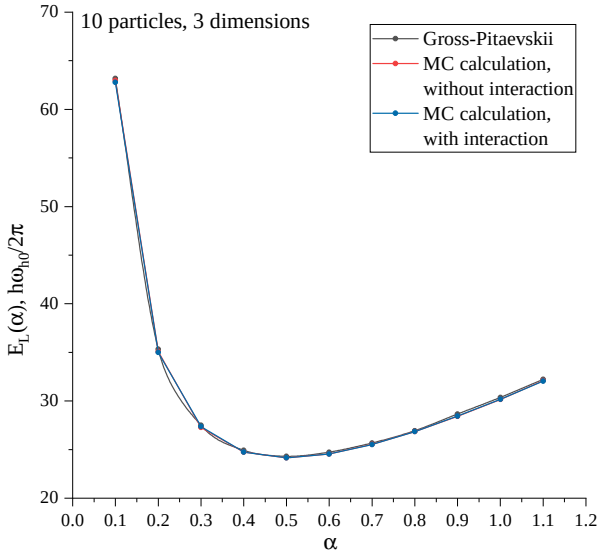

FIG. 10.— Local energy $E_L(\alpha)$ as a function of α calculated for 10 particles in 3 dimensions for case of interacting and non-interacting particles with VMC with brute force Metropolis algorithm. The analytical calculations for Gross-Pitaevskii equation are included.

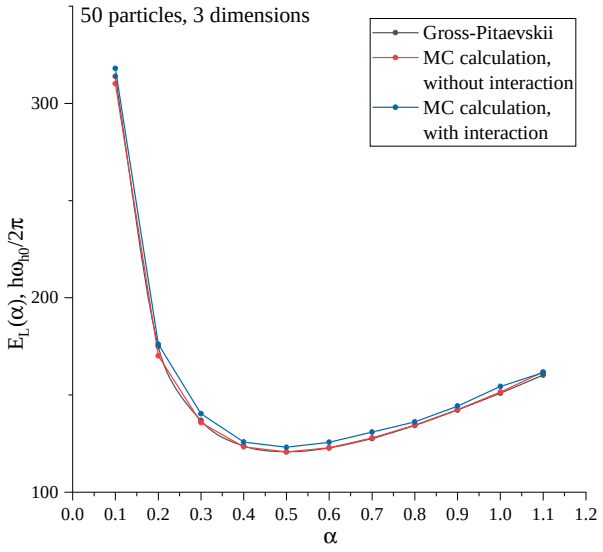

FIG. 11.— Local energy $E_L(\alpha)$ as a function of α calculated for 10 particles in 3 dimensions for case of interacting and non-interacting particles with VMC with brute force Metropolis algorithm. The analytical calculations for Gross-Pitaevskii equation are included.

The optimal parameter α found for the systems of 1, 10, 50, and 100 particles is close to 0.5, thus for the systems of 10 and 50 particles chosen for example calculation of particle distribution,it is assumed to be close to 0.5 as well.

```
// Number of bins inserted for counting
int numOfBins =120;
// Maximal range for density calculation
double radMax =3;
```

The radial distributions for the chosen number of particles in 3 dimensions are presented on figures 13 and 14.

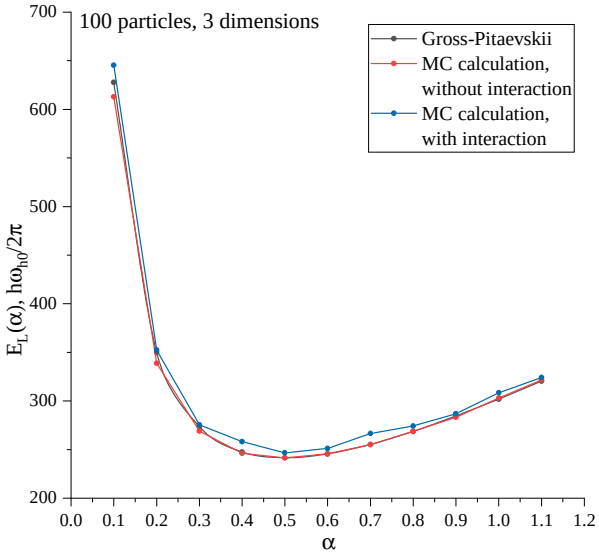

FIG. 12.— Local energy $E_L(\alpha)$ as a function of α calculated for 10 particles in 3 dimensions for case of interacting and non-interacting particles with VMC with brute force Metropolis algorithm. The analytical calculations for Gross-Pitaevskii equation are included.

TABLE 9
THE ANALYTICAL RESULTS OBTAINED FOR GROUND STATE ENERGY E_L AND GRADIENT FOR α_{min}.THE NUMBER OF MC CYCLES IS 10^6 AND THE STEP SIZE $r_{step} = 1.0$.

N_{part}	α_{min}	E_L^{min} $\hbar\omega_{h0}$	$-\partial E_L(\alpha)/\partial\alpha$ $\hbar\omega_{h0}$
1	0.50000	2.414(20)	9.30076e-08
10	0.50614	24.274(56)	9.9750e-07
50	0.51958	123.67(22)	2.2001e-05
100	0.52981	246.90(48)	9.7408e-03

In addition the actual distribution of particles in space in the ground state for spherical and elliptical harmonic oscillator is also presented on figures 15 and 16.

6. DISCUSSION OF THE RESULTS

The simulation of N particle systems of bosons in the present project undergoes a series of subsequent modifications, yielding in approaching of previously assumed behaviour to a more realistic case. The starting point for this process is the assumption of the absence of interaction for N bosons enclosed in the simplest spherical HO potential trap. The trial wave function chosen (7) presents the renormalized single-particle Gaussian function which is an harmonic oscillator ground-state function including two variational parameters α and β. The latter corresponds to $\beta = 1.0$ for spherical symmetry of the whole system. The α-dependence of the trial wave function makes it indeed corresponding to the ground state of the system for $\alpha = \frac{1}{2a_{h0}^2} = \frac{1}{2}$ as the choice of $\hbar = m = \omega_{h0} = 1$ is taken. However it might be interesting to study the sensitivity of the systems energy calculated to variations of α. As is shown in figures 4 and 5 the parameter $\alpha = 0.5$ indeed yields the minimum of

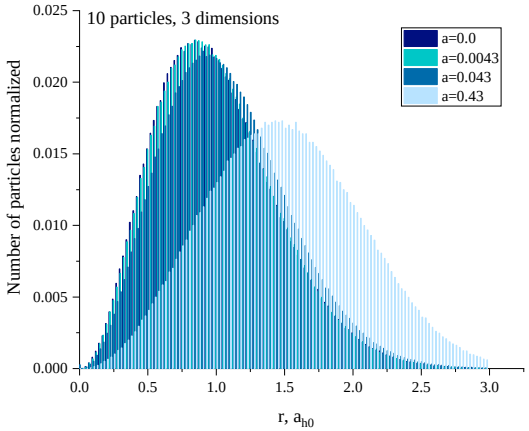

FIG. 13.— Radial distribution of 10 bosons in 3 dimensions in ground state calculated for the elliptic potential trap. The calculations are performed by means of variational Monte Carlo with 10^6 cycles for different radii of hard-sphere interaction $a/a_{h0} = 0.0043, 0.043, 0, 43$ and non-interacting case.

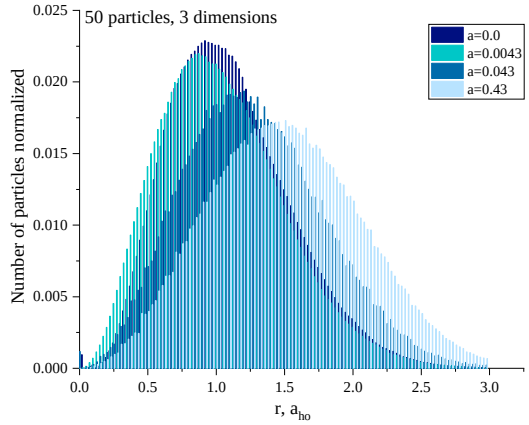

FIG. 14.— Radial distribution of 50 bosons in 3 dimensions in ground state calculated for the elliptic potential trap. The calculations are performed by means of variational Monte Carlo with 10^6 cycles for different radii of hard-sphere interaction $a/a_{h0} = 0.0043, 0.043, 0, 43$ and non-interacting case.

the systems energy, corresponding to the ground state, and the variance for this calculated as $\sigma^2 = \langle E^2\rangle - \langle E\rangle^2$ equals to exact zero for analytical local energy calculation. This is a benchmark of exact value achieved. As α decreases to zero or increases to infinity both local energy and variance increase to infinity. As the numerical evaluation of local energy is involved the estimated variance deviates from 0 due to inevitable uncertainty arising from numerical derivative calculation, however $\alpha = 0.5$ still corresponds to its clear minimum value.

The first simulation attempt was carried out by the means of VMC with the brute force approach implemented for both numerical and analytical approaches to the local energy evaluation. Since the considered system is quite simple, we can easily obtain the analytical form of the local energy and subsequently use it in the program. The local energy obtained for different combinations of

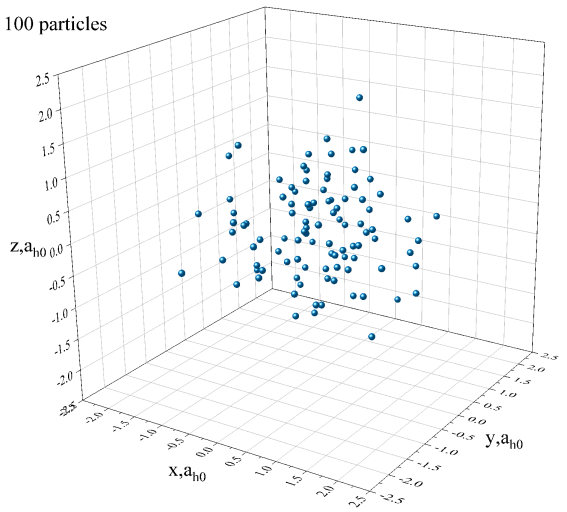

FIG. 15.— Spatial locations of 100 bosons in 3 dimensions in ground state calculated for the spherical potential trap. The calculations are performed by means of variational Monte Carlo with 10^6 cycles for hard-sphere interaction radius $a/a_{h0} = 0.0043$.

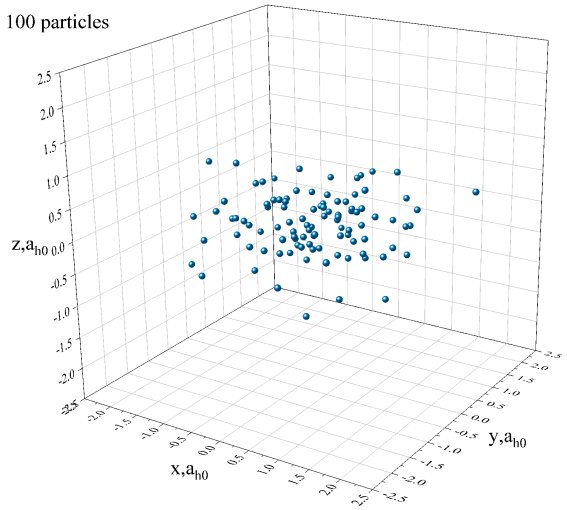

FIG. 16.— Spatial locations of 100 bosons in 3 dimensions in ground state calculated for the elliptical potential trap. The calculations are performed by means of variational Monte Carlo with 10^6 cycles for hard-sphere interaction radius $a/a_{h0} = 0.0043$.

particles and dimensions for $\alpha = 0.5$ coincides with exact values for each case (22) as is shown in TABLE 1. The numerically evaluated local energy reproduces the exact values as well, however the optimization error is present (see TABLE 2) and strongly depends on the grid bin size chosen for calculation. In present project $h = 0.001$ is selected since the larger size $h = 0.01$ results in slight deviation from exact value and $h = 0.1$ in "jumping" behaviour of $E_L(\alpha)$ function. The CPU calculation time for both analytical and numerical evaluation increases fast with increasing number of dimensions and particles involved, however this increase is much more noticeable for the latter case. Comparing the CPU times for these to cases one can notice that the maximal difference reaches $\frac{CPU_{num}}{CPU_{analyt}} \approx 10^3$, which might be critical for large number of particles in 3 dimensions. For the sake of time saving the analytical local energy expression was used for all calculations where the opposite is not required. Nevertheless, when the interaction between particles is included, the analytical expression becomes much more bulky and time consuming to solve, and in some cases systems with more complicated internal behaviour can not be found. The numerical evaluation might then be helpful for cases up to 100 particles.

As it is shown on FIG 6, acceptance rate for the brute force algorithm chosen drops linearly with the proposed step size increasing but it is still high for $\Delta r = 1.0$ which corresponds to the characteristic trap size in chosen units and could chosen for all calculations involving the brute force algorithm.

The similar calculations performed for importance sampling with Metropolis-Hastings algorithm involved demonstrating similar results and compare to the brute force: both analytical and numerical local energy evaluations yield the exact values and the only difference between them is still in non-zero variance for numerical calculation. The maximum CPU time difference is still $\frac{CPU_{num}}{CPU_{analyt}} \approx 10^3$. An additional comparison with the results obtained with the mean field Gross-Pitaevskii equation was introduced. In the considered case of spherical symmetry and absence of interaction it completely coincides with exact value. Comparing the corresponding CPU times for the brute force and importance sampling algorithms it can be easily seen that the latter is slightly slower. The reason for this is hidden in the additional calculations assumed by the Metropolis-Hastings algorithm. This involves the calculation of the drift force governing the direction of most probable move of a particle (or set of particles) towards the ground state. Since it involves the first derivative of the wave function it can also be calculated numerically and analytically, however the numerical evaluation will make the whole process even more time consuming, therefore the analytical way was chosen. An additional calculation covers the evaluation of the Green function taking into account non-equal transition probabilities for the Metropolis-Hastings algorithm. Despite that these factors make each program run slightly slower, the Meropolis-Hastings algorithm allows to define the direction of most probable subsequent steps which would let the system evolve to the ground state. Since this process defined by the drift force introduced is much more efficient than the random direction choice for the brute force approach, quite high acceptance rates can be easily achieved. In other words, the MC cycles are more efficiently exploited, thus one can achieve the better statistics for the same number of MC cycles as compared to the brute force method. In principle the speed loss can be compensated by certain decrease of MC cycles number. Nevertheless, if the time difference is not significant the number of MC cycles should be as high as possible to provide the better statistic for the final result estimation.

The acceptance rate for the Metropolis-Hastings algorithm remains considerably high for a large interval of time steps, but the physically reasonable results can be obtained for $\Delta t \in [0.001; 0.1]$. Further increasing the time step results in considerable decrease of acceptance

rate presumably because of time step dependence hidden in the Green function, which implies that if the the larger time it takes for particle to move from the initial position to the proposed one, the less of such steps are accepted since they do not necessarily lead towards the ground state.

The variance estimated in the previously considered cases does not include the the covariance term and, therefore, might significantly underestimate the uncertainty for some cases. For the simplest case of non-interacting bosons in spherical symmetric HO trap the variances obtained with the blocking method are listed in TABLE 5. The calculations were performed with the numerical evaluation of the local energy for $\alpha = 0.5$ since the analytical evaluation leads to the exact value in even cases of small number of MC cycles. As it turned out, the first one demonstrates the similar behaviour for the numerical grid step $h = 0.001$, thus the input used for blocking presented a row of exact values which resulted in zero variance for the blocking method. For the larger grid step the value obtained as an output used for blocking oscillates under the level of exact value for low number of MC cycles and tends to reach it for larger number of MC cycles. The results for $h = 0.01, 0.1$ demonstrate that the blocking based variance exceeds the simple version of variance calculated as $\sigma^2 = \langle E^2 \rangle - \langle E \rangle^2$ with the factor of 10 in average, so the simple variance indeed underestimates the value of an uncertainty to be reported. However, the latter still serves as a good and simple estimate for the error of the results that can be easily performed in the program alongside with the mean value of local energy.

The variational Monte Carlo with standard Metropolis algorithm was also exploited to investigate more realistic case of interacting bosons in the three dimensional elliptic potential trap (3). The trial wave function, and the local energy as a consequence, is now the function of two variational parameters α and β. However the latter parameter reflecting the deformation scale for the potential was kept constant $\beta = 2.82843$ throughout all calculations. The radius of hard sphere interaction is chosen to be one for ^{87}Rb atoms in an elliptical trap $a/a_{ho} = 0.0043$ from (3),(13). The direct comparison of interacting and non-interacting case demonstrates that for all cases considered ($N = 10, 50, 100$) the average energy for the case with interaction included is slightly larger than the average energy on non-interacting bosons in three dimensional deformed potential. The more particles are conciser the larger this deviation which can be plainly seen on figures 11,12 and 13, since the probability of interaction increases with the number of objects to interact. This difference remains almost the same as we run through the chosen values of α. The similar behaviour is observed for the calculated variance. The minimum value of energy corresponding to the ground state remains in the vicinity of $\alpha \approx 0.5$ what is also confirmed by noticeable decrease of the energy variance approaching to almost zero value. The results for interacting and non-interacting case were also compared to those obtained on the base of Gross-Pitaevskii equation. In the present project we have considered the simplest solution for it which excludes the interaction between the particles. This is the reason for similar deviations of it from the case of interacting particles. The Gross-Pitaevskii results are in the perfect agreement with the non-interacting case for $N = 10, 50, 100$ in the vicinity of the ground state and the larger the number of particles the larger the deviation between energies for $\alpha > 0.5$ and $\alpha < 0.5$. This might be related to the area of GP equation applications which assumes a system to be considerably dilute (or gas parameter for a system with local density $n(\mathbf{r})$ satisfies $x(\mathbf{r} = n(\mathbf{r})a^3 < 10^{-3}$. In some specific cases of the Feshbach resonance presence (14), this value is exceeded. The arising problem of inability to apply the GP equation is overcome by introducing the modified GP equation which takes an additional term of low-density expansion of the energy density (only the first one is used to derive the simple GP equation (see 2.5)) As it was shown in (13) the results of MGP and VMC calculations in a good agreement for both ground and excited states.

The results obtained were also benchmarked with the corresponding results from (3) which in its own turn were compared with the GP calculations for interacting bosons from (15).Since the first paper focuses mainly on larger numbers of particles, one can only visually compare results from the figure 2 in (3) with the results obtained in this project. The approximated values are in a good agreement. As comparing an increase of energy per particle,in (3) it demonstrates significantly steep rise with increasing number of particles. A certain rise is also observed for the results from TABLE 6,7,8, however it is not as steep as in (3). Indeed, the GP result from (15) for 100 $E/N = 2.66$ demonstrates that the value obtained in this project $E/N = 2.46$ underestimates energy per particle in the ground state. The rate of interactions simulated seems to be slightly lower than it is predicted by GP equation in (15).

Since keeping α as the only variable parameter only and graphical search to the minimum energy and corresponding optimal value for α is quite inaccurate and inefficient, the gradient descent method was implemented. As it is shown in TABLE 9 the optimal α value shifts slightly towards $\alpha = 0.53$ from $\alpha = 0.5$ as the number of particles increases. For $N = 1$ and $N = 10$ the optimal α is located in the immediate vicinity of 0.5 which is confirmed by TABLE 6. For $N = 1$ the energy obtained coincide and for $N = 10$ the energy obtained on the base of GD method is even smaller, however, for the larger numbers of particles $N = 50$ and $N = 100$ does not yield in the minimum energy. It might be related to the incorrectly chosen combination of starting point for the minimization of α, η and stop-point (tolerance) of the calculation. In the present project it was confirmed that the gradient descent method is extremely sensitive to the first two parameters since exactly they are defying the framework or the "path" and steps for the α minimization, as the gradient itself sets the direction.

The distribution of particles in the ground state might also serve an important result reflecting the effect of interaction. As it is shown on figures 15 and 16 an increasing radius of hard sphere the number of particles possessing larger values of $\mathbf{r}$ increases. It is consistent

with (3), which implies that the larger values of na^3 result in shifting of condensate towards the edges of the trap. As density remains the same for both cases, for the larger radii of interaction radius a the particles are indeed shifted towards the larger values of $\mathbf{r}$ i.e. further from the central part of the trap.

7. PERSPECTIVES FOR FUTURE IMPROVEMENTS

While the aim for the project was to evaluate the Bose-Einstein condensate it was also to learn how to write and construct a working program. Starting from the simplest structure without object orientating the code, one soon came to the realization that this might have been easier to work with had it been done. The object orientated part of the program was made, but only for the brute Metropolis algorithm and not for the rest of the code. In future endeavors one could make great improvements by making more classes like a Hamiltonian class, and a wave function class. This would help to generalise the code for other types of particles, like for instance fermions. The class Position and Matrix can also be evaluated and maybe replaced with the already existing vector class from $C++$.

8. CONCLUSIONS

Under the present study the VMC method was applied for the calculation of the ground state energy for the quantum mechanical system of bosons, both interacting and non-interacting cases. The brute force Metropolis algorithm and the Metropolis-Hastings algorithm where applied to both cases and both proved to be efficient and coinciding with exact values and results obtained by mean field GP equation. The Metropolis-Hastings algorithm showed itself to be slightly slower than the brute Metropolis algorithm. However, the acceptance rate for the former with the right choice of time step can be significantly higher. The energy was calculated both numerically and analytically, where the latter was a much faster option when the expression was derived. The statistical errors where found by the use of the blocking method and provided an improved the upper limit for the error estimate. Including the Jastrow factor into the wave function affects the energy and makes it larger, this can be interpreted as an interaction. The gradient decent method was applied to find the optimal variable parameter α corresponding to the ground state energy. This parameter was slightly shifted from 0.5 as the number of particles where increased. However, it does not correspond to an exact minimum this due to the difficulties related to setting the initial conditions for the gradient decent. The radial distribution of the particles is shifted when the radius of the interaction increases.

9. APPENDIX A: LINK TO ALL PROGRAMS

Link to the project in Github

10. APPENDIX B: SCALING OF THE HAMILTONIAN

The present appendix is devoted to rescaling of initial general form of the Hamiltonian for the system of N particles trapped in the three dimensional elliptical trap:

$$\begin{aligned}\hat{H} &= \sum_{i=1}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+V_{ext}(\mathbf{r}_i)\right)+\sum_{i<j}^{N}V_{int}(\mathbf{r}_i,\mathbf{r}_j)= \\ &= \sum_{i=1}^{N}\left(-\frac{\hbar^2\nabla_i^2}{2m}+\frac{m\omega_{ho}^2(x_i^2+y_i^2)}{2}+\frac{m\omega_z z_i^2}{2}\right)+ \\ &+ \sum_{i<j}^{N}V_{int}(\mathbf{r}_i,\mathbf{r}_j).\end{aligned} \tag{49}$$

The first step aims at making energies dimensionless dividing the Hamiltonian by $\hbar\omega_{ho}$:

$$\begin{aligned}\frac{\hat{H}}{\hbar\omega_{ho}} &= \sum_{i=1}^{N}\left(-\frac{\hbar\nabla_i^2}{2m\omega_{ho}}+\frac{m\omega_{ho}(x_i^2+y_i^2)}{2\hbar}+\frac{m\frac{\omega_z^2}{\omega_{ho}}z_i^2}{2\hbar}\right)+ \\ &+ \sum_{i<j}^{N}V_{int}(\mathbf{r}_i,\mathbf{r}_j).\end{aligned} \tag{50}$$

The second step to be performed is making the length dimensionless by dividing by characteristic size of the trap given as:

$$a=\sqrt{\frac{\hbar}{m\omega_{ho}}}, \tag{51}$$

therefore the dimensionless Hamiltonian is presented as following:

$$\begin{aligned}\hat{H}^{dl} &= \sum_{i=1}^{N}\left(-\frac{\nabla_i^2}{2}+\frac{(x_i^2+y_i^2)}{2}+\frac{\omega_z^2 z_i^2}{2\omega_{ho}^2}\right)+ \\ &+ \sum_{i<j}^{N}V_{int}(\mathbf{r}_i,\mathbf{r}_j)= \\ &= \sum_{i=1}^{N}\frac{1}{2}\left(-\nabla_i^2+x_i^2+y_i^2+\frac{\omega_z^2}{\omega_{ho}^2}z_i^2\right)+ \\ &+ \sum_{i<j}^{N}V_{int}(\mathbf{r}_i,\mathbf{r}_j),\end{aligned} \tag{52}$$

therefore the parameter γ cited in the theoretical chapter is defined as:

$$\gamma=\beta=\frac{\omega_z}{\omega_{ho}}. \tag{53}$$

11. APPENDIX C: ANALYTICAL DERIVATION OF LOCAL ENERGY

This appendix is devoted to the detailed analytical derivation of local energy presented in the theoretical background section (see 2) and applied for the computationally performed calculations in the program. The derivation is subdivided into two cases corresponding to the systems of interacting and non-interacting particles correspondingly. The first sub-case to be considered is the simplest 1 dimensional comprising of 1 particle in the spherical harmonic potential trap. This case will be subsequently extended to 3 dimensional case of 1 particle system. The next step is to write generalized form of expression for local energy in 3 dimensional case of arbitrary number of particles N applied in the program used. Similar equation is written for the case of elliptical potential trap as well. Then, moving to more complicated case, we have inserted the interaction between the particles present in the system on the basis of equations listed in the theoretical chapter. For the interacting system the general case of 3 dimensions and N particles is considered, and this expression was used in the program assuming user to switch on and of the parameters of the system depending on whether the interacting or non-interacting, spherical or elliptical case is considered.

11.1. *Non-interacting case, 1 dimension, 1 particle*

Given the general form of the Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{ext}(\mathbf{r}_i)\right) + \sum_{i<j}^{2} V_{int}(\mathbf{r}_i,\mathbf{r}_j), \quad (54)$$

excluding the interaction potential ($a = 0$) and given the external potential trap as:

$$V_{ext}(\mathbf{r}_i) = \begin{cases} \frac{m\omega^2 r_i^2}{2} & \text{spherical case,} \\ \frac{m(\omega_\perp^2(x_i^2+y_i^2)+\omega_\parallel^2(z_i^2)}{2} & \text{elliptical case.} \end{cases} \quad (55)$$

The trial wave function of a system presented as the product of one body wave functions:

$$\Psi_T(\mathbf{R}) = \prod_i^N e^{-\alpha(x_i^2+y_i^2+\beta z^2)}, \quad (56)$$

and in the simplest case of one particle trapped in the one dimensional spherical potential ($\beta = 1$) it transforms into:

$$\Psi_T(x) = e^{-\alpha x^2}. \quad (57)$$

The expression for the local energy $E_L = \frac{1}{\Psi}\hat{H}\Psi$ requires the calculation of second derivative of $\Psi(x)$ with respect to x:

$$\frac{d\Psi_T}{dx} = -2\alpha x e^{-\alpha x^2}, \quad (58)$$

$$\frac{d^2\Psi_T}{dx^2} = (4\alpha^2x^2 - 2\alpha)e^{-\alpha x^2}, \quad (59)$$

and therefore in dimensionless case considered ($\hbar = m = \omega = 1$) the Hamiltonian can be rewritten as:

$$\begin{aligned}\hat{H} &= -\frac{\nabla^2}{2} + \frac{x^2}{2} = \\ &= -\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2},\end{aligned} \quad (60)$$

and the local energy corresponding to this Hamiltonian as:

$$\begin{aligned}E_L(x,\alpha) &= \frac{1}{\Psi_T(x)}\hat{H}\Psi(x) = \\ &= \frac{1}{\Psi_T(x)}\left(-\frac{1}{2}\frac{d^2\Psi_T(x)}{dx^2} + \frac{x^2}{2}\Psi_T(x)\right) = \\ &= \frac{1}{e^{-\alpha x^2}}\left(\alpha - 2x^2\alpha^2 + \frac{x^2}{2}\right)e^{-\alpha x^2} = \\ &= \alpha + x^2\left(\frac{1}{2} - 2\alpha^2\right).\end{aligned} \quad (61)$$

Thus, the local energy for one particle described by one spatial dimension dimensionless Hamiltonian in case of the spherical harmonic oscillator trap is the following:

$$E_L(x,\alpha) = \alpha + x^2\left(\frac{1}{2} - 2\alpha^2\right). \quad (62)$$

11.2. *Non-interacting case, 3 dimensions, 1 particle*

The previously discussed case of one dimension can be easily be extended to three dimensions. The Laplace operator $\Delta = \nabla^2$ present the Hamiltonian can be easily rewritten as:

$$\Delta = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}, \quad (63)$$

and acting on the wave function of the system:

$$\Psi(\mathbf{r}) = e^{-\alpha(x^2+y^2+z^2)}, \quad (64)$$

one may easily obtain in the similar way the following expression for the Hamiltonian:

$$\begin{aligned}\hat{H} &= -\frac{\nabla^2}{2} + \frac{r^2}{2} = \\ &= \left(3\alpha + (x^2+y^2+z^2)\left(\frac{1}{2} - 2\alpha^2\right)\right) = \\ &= \left(3\alpha + r^2\left(\frac{1}{2} - 2\alpha^2\right)\right),\end{aligned} \quad (65)$$

and the following expression for the local energy in three dimensional case of one particle in the spherical harmonic oscillator:

$$\begin{aligned}E_L(\mathbf{r},\alpha) &= \frac{1}{\Psi_T(\mathbf{r})}\hat{H}\Psi_T(\mathbf{r}) = \\ &= \frac{1}{e^{-\alpha(r^2)}}\left(3\alpha + r^2\left(\frac{1}{2} - 2\alpha^2\right)\right)e^{-\alpha(r^2)} = \\ &= 3\alpha + r^2\left(\frac{1}{2} - 2\alpha^2\right).\end{aligned} \quad (66)$$

11.3. *Non-interacting case, general form, 3 dimensions, N particles*

The next step to be considered is the subsequent extension of the previous situation to an arbitrary number of particles N which can be easily performed if the following for of the Laplace operator and Hamiltonian as the sum over the Laplace operators acting on the single particles in three dimensions and single particle Hamiltonians is taken into account:

$$\Delta = \sum_{i=1}^{N} \Delta_i = \sum_{i=1}^{N} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right), \tag{67}$$

and the corresponding Hamiltonian as:

$$\begin{aligned} \hat{H} &= \sum_{i=1}^{N} \left(-\frac{\nabla^2}{2} + \frac{r^2}{2} \right) = \\ &= \sum_{i=1}^{N} \left(3\alpha + (x^2 + y^2 + z^2) \left(\frac{1}{2} - 2\alpha^2 \right) \right) = \\ &= \sum_{i=1}^{N} \left(3\alpha + r^2 \left(\frac{1}{2} - 2\alpha^2 \right) \right), \end{aligned} \tag{68}$$

The wave function of the three dimensional system of N particles presents the product of the corresponding single-particle wave-functions, it was already discussed in the theoretical section. The local energy in this case can be written as following:

$$\begin{aligned} E_L(\mathbf{R}, \alpha) &= \frac{1}{\prod_i \phi(\mathbf{r}_i)} \sum_{i=1}^{N} \hat{H} \prod_i \phi(\mathbf{r}_i) = \sum_{i=1}^{N} E_L^i(\alpha) = \\ &= \sum_{i=1}^{N} \left(3\alpha + r_i^2 \left(\frac{1}{2} - 2\alpha^2 \right) \right) = \\ &= 3\alpha N + \sum_{i=1}^{N} r_i^2 \left(\frac{1}{2} - 2\alpha^2 \right). \end{aligned} \tag{69}$$

Thus, the general expression for the local energy for number of dimensions N_dim and number of particles N for the spherical symmetric harmonic oscillator trap with the only parameter α is proved to correspond to:

$$E_L(\mathbf{R}, \alpha) = \alpha N \cdot N_{dim} + \sum_{i=1}^{N} r_i^2 \left(\frac{1}{2} - 2\alpha^2 \right). \tag{70}$$

In addition the relation for the elliptical harmonic oscillator (see 3) trap can be obtained in the similar set of steps implying the following form of the wave function (see 7) including and additional parameter β in front of z coordinate introduced to take the elliptical form of the potential into account. The local energy in such case is given as following:

$$\begin{aligned} E_L(\mathbf{R}, \alpha) = 2\alpha N + \alpha\beta N + \sum_{i=1}^{N} (x_i^2 + y_i^2) \left(\frac{1}{2} - 2\alpha^2 \right) + \\ + \sum_{i=1}^{N} z_i^2 \beta^2 \left(\frac{1}{2} - 2\alpha^2 \right), \end{aligned} \tag{71}$$

however, this form of the local energy was not required in the calculations performed.

11.4. *Interacting case, general form, 3 dimensions, N particles*

The more realistic behaviour of bosons in the spherical or elliptical potential trap (the latter is considered in the present work) assumes the interaction between particles taken into account. As the introduction is introduced the general form for the Hamiltonian and the trial wave function becomes more complicated and cumbersome and we are no longer able to find an exact analytical solution. However, some of the steps of simplification towards obtaining the solution can be performed analytically and, therefore, partially speed the program up as compared to bare numerical calculation. The general case of three dimensions and N particles trapped in the elliptical harmonic potential assumes the following form of the Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{\hbar^2 \nabla_i^2}{2m} + V_{ext}(\mathbf{r}_i) \right) + \sum_{i<j}^{N} V_{int}(\mathbf{r}_i, \mathbf{r}_j), \tag{72}$$

and the wave function (see theoretical section):

$$\begin{aligned} \Psi_T(\mathbf{R}) &= \prod_i^N e^{-\alpha(x_i^2 + y_i^2 + \beta z^2)} \prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \\ &= \prod_i^N g(\alpha, \beta, \mathbf{r}_i) \prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \\ &= \prod_i^N \phi(\mathbf{r}_i) exp\left(\sum_{i<j} u(r_{ij}) \right), \end{aligned} \tag{73}$$

where $\phi(\mathbf{r}_i) = g(\alpha, \beta, \mathbf{r}_i) = e^{-\alpha(x_i^2 + y_i^2 + \beta z^2)}$ and $exp(u(r_{ij})) = f(r_{ij})$ is the Jastrow factor describing the interaction part of the wave function, and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. One of the most complicated step of calculation of the local energy in this case is the calculation of the kinetic part of the Hamiltonian. This step involves the simplification of $\nabla_k \Psi_T(\mathbf{R})$ first derivative value for an arbitrary

k-particle:

$$\begin{aligned}\nabla_k\Psi_T(\mathbf{R}) &= \nabla_k\left[\prod_i^N\phi(\mathbf{r}_i)exp\left(\sum_{i<j}u(r_{ij})\right)\right] = \\ &= \nabla_k\phi(\mathbf{r}_k)\left[\prod_{i\neq k}^N\phi(\mathbf{r}_i)\right]\prod_i^N exp\left(\sum_{i<j}u(r_{ij})\right)+ \\ &= \left[\prod_i^N\phi(\mathbf{r}_i)\right]\nabla_k\left[\prod_i^N exp\left(\sum_{i<j}u(r_{ij})\right)\right] \\ &= \nabla_k\phi(\mathbf{r}_k)\left[\prod_{i\neq k}^N\phi(\mathbf{r}_i)\right]\prod_i^N exp\left(\sum_{i<j}u(r_{ij})\right)+ \\ &= \prod_i^N\phi(\mathbf{r}_i)exp\left(\sum_{i<j}u(r_{ij})\right)\sum_{j\neq k}\nabla_k u(r_{kj}).\end{aligned} \tag{74}$$

The next step involves the derivation of the second derivative based on the previously performed derivation of the first derivative:

$$\begin{aligned}\nabla_k^2\Psi_T(\mathbf{R}) &= \nabla_k^2\phi(\mathbf{r}_k)\left[\prod_{i\neq k}^N\phi(\mathbf{r}_i)\right]\prod_i^N exp\left(\sum_{i<j}u(r_{ij})\right)+ \\ &+\nabla_k\phi(\mathbf{r}_k)\left[\prod_{i\neq k}^N\phi(\mathbf{r}_i)\right]\prod_i^N exp\left(\sum_{i<j}u(r_{ij})\right)\sum_{j\neq k}\nabla_k u(r_{kj})+ \\ &+\nabla_k\phi(\mathbf{r}_k)\left[\prod_{i\neq k}^N\phi(\mathbf{r}_i)\right]\prod_i^N exp\left(\sum_{i<j}u(r_{ij})\right)\sum_{j\neq k}\nabla_k u(r_{kj})+ \\ &+\prod_i^N\phi(\mathbf{r}_i)exp\left(\sum_{i<j}u(r_{ij})\right)\sum_{j\neq k}\nabla_k u(r_{kj})\sum_{i\neq k}\nabla_k u(r_{ki})+ \\ &+\prod_i^N\phi(\mathbf{r}_i)exp\left(\sum_{i<j}u(r_{ij})\right)\sum_{j\neq k}\nabla_k^2 u(r_{kj}).\end{aligned} \tag{75}$$

In order to proceed with further simplification one should consider the following relations:

$$\begin{aligned}\nabla_k u(r_{kj}) &= u'(r_{kj})\nabla_k r_{kj} = u'(r_{kj})\nabla_k\sqrt{(\mathbf{r}_k-\mathbf{r}_j)^2} = \\ &= u'(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{\sqrt{(\mathbf{r}_k-\mathbf{r}_j)^2}} = u'(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{r_{kj}},\end{aligned} \tag{76}$$

$$\begin{aligned}\nabla_k u(r_{kj}) &= \nabla_k\left(u'(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{|\mathbf{r}_k-\mathbf{r}_j|}\right)+ \\ &+u"(r_{kj})-u'(r_{kj})\frac{(\mathbf{r}_k-\mathbf{r}_j)(\mathbf{r}_k-\mathbf{r}_j)}{r_{ij}^3}+ \\ &+u'(r_{kj})\frac{div_k(\mathbf{r}_k-\mathbf{r}_j)}{r_{kj}} = u"(r_{kj})+\frac{2}{r_{kj}}.\end{aligned} \tag{77}$$

Applying these equations and the form of the second derivative of the trial wave function, one may obtain:

$$\begin{aligned}\frac{\nabla_k^2\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} &= \frac{\nabla_k^2\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}+2\frac{\nabla_k\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\sum_{j\neq k}u'(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{r_{kj}}+ \\ &+\sum_{j\neq k}u'(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{r_{ij}}\sum_{i\neq k}u'(r_{ki})\frac{\mathbf{r}_k-\mathbf{r}_i}{r_{ki}}+ \\ &+\sum_{j\neq k}\left(u"(r_{kj})+u'(r_{kj})\frac{2}{r_{kj}}\right) \\ &= \frac{\nabla_k^2\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}+2\frac{\nabla_k\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\sum_{j\neq k}u'(r_{kj})\frac{\mathbf{r}_k-\mathbf{r}_j}{r_{kj}}+ \\ &+\sum_{j,j\neq k}u'(r_{kj})u'(r_{ki})\frac{\mathbf{r}_k-\mathbf{r}_j}{r_{ij}}\frac{\mathbf{r}_k-\mathbf{r}_i}{r_{ki}}+ \\ &+\sum_{j\neq k}\left(u"(r_{kj})+u'(r_{kj})\frac{2}{r_{kj}}\right).\end{aligned} \tag{78}$$

This relation can be subsequently used in the general relation for the local energy:

$$\begin{aligned}E_L(\mathbf{R},\alpha,\beta) &= \frac{1}{\Psi_T(\mathbf{R})}\sum_{i=1}^N\left(-\frac{\nabla_i^2}{2}+V_{ext}(\mathbf{r}_i)\right)\Psi_T(\mathbf{R}) \\ &+\frac{1}{\Psi_T(\mathbf{R})}\sum_{i<j}V_{int}(\mathbf{r}_i,\mathbf{r}_j)\Psi_T(\mathbf{R}) = \\ &= \sum_{i=1}^N\left(-\frac{\nabla_i^2\Psi_T(\mathbf{R})}{2\Psi_T(\mathbf{R})}+V_{ext}(\mathbf{r}_i)\right)+\sum_{i<j}V_{int}(\mathbf{r}_i,\mathbf{r}_j),\end{aligned} \tag{79}$$

this relation was performed computationally in the present work.

12. APPENDIX D: ANALYTICAL DERIVATION OF DRIFT FORCE

The present appendix is devoted to the derivation of the drift force realized in the importance sampling approach:

$$\mathbf{F} = \frac{2\nabla\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})}, \tag{80}$$

starting from the simplest case of one dimensional system of one particle in the case of spherical trap.

12.1. *Spherical case, 1 dimension, 1 particle*

In order to derive the quantum drift force for this case one should consider the first derivative of the corresponding wave function:

$$\nabla\Psi_T(x) = \frac{\partial}{\partial x}e^{-\alpha x^2}\mathbf{e}_x = -2\alpha x\mathbf{e}_x e^{-\alpha x^2}, \tag{81}$$

therefore the expression for the drift force is given as following:

$$\mathbf{F} = \frac{2\nabla\Psi_T(x)}{\Psi_T(x)} = -4\alpha x\mathbf{e}_x, \tag{82}$$

12.2. *Spherical case, 3 dimensions, 1 particle*

The case considered above can be easily extended to the case of three dimensions in the following way:

$$\begin{aligned}\nabla\Psi_T(\mathbf{r}) &= \left(\frac{\partial}{\partial x}\mathbf{e}_x + \frac{\partial}{\partial y}\mathbf{e}_y + \frac{\partial}{\partial z}\mathbf{e}_z\right) e^{-\alpha(x^2+y^2+z^2)} \\ &= -2\alpha\mathbf{r}e^{-\alpha r^2},\end{aligned} \tag{83}$$

and then the drift force is given as:

$$\mathbf{F} = \frac{2\nabla\Psi_T(\mathbf{r})}{\Psi_T(\mathbf{r})} = -4\alpha\mathbf{r}, \tag{84}$$

12.3. *General case, 3 dimensions, N particles*

Finally, one can obtain the general form of the drift force for an arbitrary number of particles N in three dimensions for the case of spherical symmetry:

$$\begin{aligned}\nabla\Psi_T(\mathbf{R}) &= \sum_{i=1}^{N}\left(\frac{\partial}{\partial x_i}\mathbf{e}_x + \frac{\partial}{\partial y_i}\mathbf{e}_y + \frac{\partial}{\partial z_i}\mathbf{e}_z\right)\prod_i e^{-\alpha(r_i^2)} \\ &= -2\alpha\sum_{i=1}^{N}\mathbf{r}e^{-\alpha r^2},\end{aligned} \tag{85}$$

and the quantum drift force is obtained as:

$$\mathbf{F} = \frac{2\nabla\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} = -4\alpha\sum_{i=1}^{N}\mathbf{r}_i. \tag{86}$$

Taking the elliptical form of the potential affecting the form of the trail function chosen (including β parameter into account) one can derive the following form of the first derivative of the trial wave function:

$$\begin{aligned}\nabla\Psi_T(\mathbf{R}) &= \sum_{i=1}^{N}\left(\frac{\partial}{\partial x_i}\mathbf{e}_x + \frac{\partial}{\partial y_i}\mathbf{e}_y + \frac{\partial}{\partial z_i}\mathbf{e}_z\right)\prod_i e^{-\alpha(x^2+y^2+\beta z^2)} \\ &= -2\alpha\sum_{i=1}^{N}(x\mathbf{e}_x + y\mathbf{e}_y + \beta z\mathbf{e}_z)e^{-\alpha(x^2+y^2+\beta z^2)}.\end{aligned} \tag{87}$$

The quantum force in this case:

$$\mathbf{F} = \frac{2\nabla\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})} = -4\alpha\sum_{i=1}^{N}(x\mathbf{e}_x + y\mathbf{e}_y + \beta z\mathbf{e}_z). \tag{88}$$

13. APPENDIX E: THE DERIVATION OF THE GROSS-PITAEVSKII EQUATION

In the framework of mean field Gross-Pitaevskii equation the ground state energy for a dilute system of condensed bosons can be represented by the following functional (13),(10):

$$\begin{aligned}E[\Psi_T] = \int[-\frac{\hbar^2}{2m}|\nabla\Psi_T|^2 + \frac{m(\omega_\perp(x^2+y^2)+\omega_\parallel z^2)}{2}|\Psi_T|^2 + \\ + \frac{2\pi\hbar^2 a}{m}|\Psi_T|^4]d\mathbf{r},\end{aligned} \tag{89}$$

for the simplest case of non-interacting system ($a = 0$) of bosons described by the normalized trial wave function for N particles:

$$\Psi_T = \left(\frac{2\alpha}{\pi}\right)^{3N/4}\beta^{N/4}\prod_i e^{-\alpha(x_i^2+y_i^2+\beta z_i^2)}, \tag{90}$$

and its gradient:

$$\begin{aligned}\nabla\Psi_T = \left(\frac{2\alpha}{\pi}\right)^{3N/4}\beta^{N/4}\prod_i e^{-\alpha(x_i^2+y_i^2+\beta z_i^2)}\cdot \\ \cdot\sum_i(-2\alpha(x_i\mathbf{e}_x + y_i\mathbf{e}_y + \beta z_i\mathbf{e}_z)),\end{aligned} \tag{91}$$

and therefore the Gross-Pitaevskii equation can be written as following:

$$\begin{aligned}E[\Psi_T] = \sum_i\int\left(2\alpha^2+\frac{1}{2}\right)(x_i^2+y_i^2+\beta z_i^2)|\Psi_T|^2 d\mathbf{r} = \\ = \left(2\alpha^2+\frac{1}{2}\right)\left(\frac{2\alpha}{\pi}\right)^{3N/2}\beta^{N/2}N_{part}(2+\beta)\cdot \\ \cdot\left(\frac{\pi}{2\alpha}\right)^{3N/2}\beta^{-N/2}\frac{1}{4\alpha} = \left(\alpha+\frac{1}{4\alpha}\right)N(\beta+2).\end{aligned} \tag{92}$$

This form of equation is used for benchmarking the results calculated for the spherical and elliptical HO trap for N particles in 3 dimensional case.

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