FYS4411 - Project 1

Variational Monte Carlo Simulation of Bosonic System

Gabriel S. Cabrera – Eirill S. Hauge

(Dated: March 24, 2020)

The goal of this project was to find the ground state energy of a trapped, hard sphere Bose gas, using the Variational Monte Carlo method. Both the Metropolis and the Metropolis-Hastings algorithms were implemented.

Both the implementation of Metropolis and Metropolis-Hastings algorithm successfully computed the ground state energy of a system of non-interacting bosons given the correct value of $\alpha = 0.5$. For every system with dimensionality $d_r = 1$, 2, or 3 with N = 1, 10, 100, or 500 bosons, it was found that the numerical energy expectation value always matched the analytical expectation value ($\langle E \rangle / N d_r = 0.5$) exactly, with an extremely small variance. Additionally, the implementation of importance sampling managed to improve the performance of the algorithm by a significant amount; in short, the random walk acceptance rate was raised from an approximate average of 60% to over 99% in the 3-D case.

Upper-bound estimates for the ground state energy for the interacting bosons with radius $a/a_{ho} = 0.0043$ in the elliptical trap with parameters $\beta = \gamma = 2.82843$ and optimized values for α using Newton's method were produced using the Metropolis algorithm. The upper-bound estimates were found to be $24.3985/(\hbar\omega_{ho})$ when the system consisted of 10 particles and $\alpha = 0.4975$. The upper-bound energy for the same system containing 50 particles and using $\alpha = 0.4891$ was $127.264/(\hbar\omega_{ho})$. Lastly, for a system of 100 particles and $\alpha = 0.4829$, the upper bound-energy was found to be $266.196/(\hbar\omega_{ho})$. The relative deviance of the computed lower-bound energy compared to the ideal non-interacting bosons in the same kind of trap and potential using $\alpha = 0.5$ was found to be increasing as the number of particles in the system was increased (relative deviance of 0.01, 0.05 and 0.1 for 10, 50 and 100 particles respectively), confirming the results of DuBois and Glyde [1].

I. INTRODUCTION

Gases consisting of bosonic particles may form a Bose-Einstein condensate, in which the majority of the bosons occupy the ground state, making the total energy converge towards the zero-point energy of the gas. For the gas to form a Bose-Einstein condensate it must have very low density and be cooled down to extremely low temperatures. It has been shown that certain isotopes of alkali metals, such as ^{7}Li, ^{23}Na and ^{87}Rb, have formed Bose-Einstein condensates when confined in magnetic traps. In this project, we will investigate the ground state energies of such systems.

We will study systems of N bosons confined in a harmonic trap, using the variational Monte Carlo method. The *ground state energy* will be investigated using quantum mechanical descriptions of the system, and the minimization of the energy with respect to *variational parameters* included in the description of the state of the bosons.

The Monte Carlo simulations can be considered *computer experiments*, where we treat the results in a way reminiscent of experimental measurements. The accuracy of the obtained ground state energy must be validated by calculating the statistical error.

In the next section we will begin by describing the system of bosons by introducing the Hamiltonian with a corresponding trial wave function. The methods for performing the computer experiments will then be introduced, as will some tools used in evaluating the results' accuracies. We will then move on to a section briefly describing details of the implementation. The results will then be presented, followed by a discussion regarding their significance and accuracy. Lastly, we will present a conclusion for this project.

II. METHOD

This section describing the methods used is largely based on Morten H. Jensen's lecture notes. [2]

We will study a system of N bosons, which gives us an eigenvalue problem to solve, known as *Schrödinger's equation*

$$\hat{H}\Psi(\mathbf{R}) = E\Psi(\mathbf{R}). \tag{1}$$

The *Hamiltonian*, $\hat{H}$, is a complete description of the system. The *eigenstate* (also known as the *wave function*) $\Psi(\mathbf{R})$ is a function of the coordinates for every boson in the system $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$ and E is the energy of the system in the corresponding state.

Schrödinger's equation will typically have many solutions for a given Hamiltonian. These correspond to different energy levels. The equilibrium state (or *ground state*) is the desired solution to the Schrödinger equation in which the energy of the system is at its lowest. Given a trial wave function, we will use the *variational Monte Carlo method* to minimize the energy. This method will eventually be discussed, but first we must introduce the Hamiltonian and trial wave function.

A. The Bosonic Many-Body Hamiltonian

The non-interacting Hamiltonian $\hat{H}_0$, for a system consisting of N bosonic particles, consists of the sum over the potential and kinetic energy contributions from each particle. The system we will study consists of indistinguishable particles of equal mass, and its non-interacting Hamiltonian is given by

$$\hat{H}_0 = \sum_{i=1}^{N} \left(\frac{-\hbar^2}{2m} \nabla_i^2 + V_{ext}(\mathbf{r}_i) \right), \tag{2}$$

where $\hbar$ is proportional to the Planck constant $\hbar = \frac{h}{2\pi}$, and where m is the mass of a single boson. The left term shows the kinetic operator of the i^{th} particle.

The external potential energy operator of the i^{th} particle, $V_{ext}(\mathbf{r}_i)$, will be given by the spherical (S) or elliptical (E) harmonic trap. The harmonic trap in three dimensions is given by

$$V_{ext}(\mathbf{r}) = \begin{cases} \frac{1}{2} m \omega_{ho}^2 r^2 & (S) \\ \frac{1}{2} m \left[\omega_{ho}^2 (x^2 + y^2) + \omega_z^2 z^2 \right] & (E), \end{cases} \tag{3}$$

where ω_{ho} defines the trap potential strength, and ω_z gives the elongation in the z-direction in the case of the elliptical potential.

Now, to mitigate the occurrence of floating-point operation errors, we will convert the Hamiltonian to natural units by providing the energy units of $\hbar\omega_{ho}$ such that $E\prime = E/\hbar\omega_{ho}$. The coordinates will be rewritten as $\mathbf{r}\prime = \mathbf{r}/a_{ho}$, where $a_{ho} \equiv \sqrt{\hbar/m\omega_{ho}}$ is the characteristic length of the trap. This in turn means that $\nabla_i\prime = a_{ho}\nabla_i$.

Dividing both sides of the Schrödinger equation by a factor $\hbar\omega_{ho}$ and rewriting the Hamiltonian with the new units we get

$$\hat{H}_0 = \frac{1}{2} \sum_{i=1}^{N} \left(-\nabla_i^2 + x_i^2 + y_i^2 + \gamma^2 z_i^2 \right), \tag{4}$$

where $\gamma = \omega_z/\omega_{ho}$. Note that we have omitted the prime symbol ($\prime$) on the gradient and the coordinates – from now on, the reader should assume natural units and thus that $\mathbf{r} \equiv \mathbf{r}\prime$.

We choose the trial wave function of this Hamiltonian to be the *one-body* wave function

$$\Psi_{OB}(\mathbf{R}) = \prod_{i=1}^{N} \phi(\alpha, \beta, \mathbf{r}_i), \tag{5}$$

where α and β are positive *variational parameters*; this concept will be presented and explained later on. The function $\phi(\alpha, \beta, \mathbf{r})$ is the exact one-particle wave function given by

$$\phi(\alpha, \beta, \mathbf{r}) = \exp\left[-\alpha(x^2 + y^2 + \beta z^2) \right], \tag{6}$$

where $\beta = 1$ in the case of spherical trap and $\beta \neq 1$ corresponds to an elliptic trap. In the case of the non-interacting bosons we have $\alpha = 1/2$. Both variables α and β are dimensionless.

Adding repulsive forces between the bosons we get the full Hamiltonian

$$\hat{H} = \hat{H}_0 + \sum_{i<j}^{N} V_{int}(r_{ij}), \tag{7}$$

where $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j|$ is the distance between the i^{th} and j^{th} bosonic particles, and $V_{int}(r_{ij})$ is the potential energy contribution caused by their interaction. Note that the shorthand notation

$$\sum_{i<j}^{N} = \sum_{i=1}^{N} \sum_{j=i+1}^{N}$$

is used throughout the text. The pairwise repulsive force between pairs of bosons is given by

$$V_{int}(r_{ij}) = \begin{cases} \infty & r_{ij} \leq a \\ 0 & r_{ij} > a, \end{cases} \tag{8}$$

where a, given in units of a_{ho}^{-1}, is the hard-core diameter of the bosons. The repulsive force is hence zero unless the two particles attempt to occupy the same space, in which case the force is infinitely large.

The complete trial wave function is given by

$$\Psi_T(\mathbf{R}) = \Psi_{OB}(\mathbf{R}) \prod_{i<j}^{N} f(a, r_{ij}) \tag{9}$$

where $f(a, r_{ij})$ is the correlation wave function between the i^{th} and the j^{th} particle, given by

$$f(a, r_{ij}) = \begin{cases} 0 & r_{ij} \leq a \\ 1 - \frac{a}{r_{ij}} & r_{ij} > a. \end{cases} \tag{10}$$

We separate the trial wave function into $\Psi_{OB}(\mathbf{R})$ and $\Psi_C(\mathbf{R})$, such that $\Psi_T(\mathbf{R}) = \Psi_{OB}(\mathbf{R})\Psi_C(\mathbf{R})$. We already know $\Psi_{OB}(\mathbf{R})$ as the *one-body* factor of the wave function, while the remaining part $\Psi_C(\mathbf{R})$ is the *correlation* factor (also known as the *Jastrow factor*) of the wave function. We can rewrite the correlation factor as

$$\Psi_C(\mathbf{R}) = \prod_{i<j}^{N} f(a, r_{ij}) = \exp\left(\sum_{i<j}^{N} u(a, r_{ij}) \right), \tag{11}$$

where $u(a, r_{ij}) \equiv \ln f(a, r_{ij})$.

Now that the Hamiltonian and trial wave function have been introduced, we move on to the variational Monte Carlo method, and how we can make the trial wave function converge towards the ground state.

B. Variational Monte Carlo

The energy of the system in a given state is the *expectation value* of the Hamiltonian itself

$$E = \langle \hat{H} \rangle = \int \Psi^*(\mathbf{R}) \hat{H} \Psi(\mathbf{R}) d\mathbf{r}_1 d\mathbf{r}_2 ... d\mathbf{r}_N, \tag{12}$$

which through the *variational principle* provides an upper bound of the ground state energy of the system. The variational principle states that this expectation value for the energy of the system must be greater than or equal to the ground state energy E_{gs}, formulated by

$$E_{gs} \leq \langle \hat{H} \rangle. \tag{13}$$

Should $\langle \hat{H} \rangle = E_{gs}$, then the state $\Psi(\mathbf{R})$ would be the ground state of the system: this property is a feature of the *Variational Monte Carlo* (VMC) calculations. Given the Hamiltonian of the system, the energy of the system is minimized with respect to the *variational parameters* of some trial wave function.

In this project, we will limit ourselves to the study of the variational parameter α. The Variational Monte Carlo method aims to let a reasonable trial wave function converge towards the ground state of the system.

To show how the energy of the system is computed, we must introduce *Monte Carlo integration*. Monte Carlo integration of any function $g(x)$ with a corresponding *probability distribution* $P(x)$ can be computed as the average of a set $\{x^1, x^2, ..., x^M\}$ in accordance with the probability distribution. The Monte Carlo integration is given by

$$\int P(x)g(x)dx \approx \frac{1}{M}\sum_{m=1}^{M} g(x^m), \tag{14}$$

where M is the number of *Monte Carlo cycles*. The accuracy of the approximation depends on the number of Monte Carlo cycles, and will converge to the exact solution as $M \to \infty$.

The integral of the energy in Eq. 12 is an integral over $d_r \times N$ dimensions, where d_r is the *dimensionality factor* (the number of dimensions of the coordinates). This is extremely computationally expensive, and it is therefore convenient to use Monte Carlo integration. With this in mind, we introduce the definition of the local energy

$$E_L(\mathbf{R}, \alpha, \beta) = \frac{1}{\Psi(\mathbf{R}, \alpha, \beta)}\hat{H}\Psi(\mathbf{R}, \alpha, \beta), \tag{15}$$

for which the expressions have been derived in the appendix for the one-body wave function, as well as the wave function containing the correlation factor. We will also need the probability distribution

$$P(\mathbf{R}, \alpha, \beta) = |\Psi(\mathbf{R}, \alpha, \beta)|^2. \tag{16}$$

Using these new properties, we can rewrite the expression for the expectation value of the energy of the system

$$\begin{aligned} E(\alpha, \beta) &= \int \Psi^*(\mathbf{R}, \alpha, \beta)\frac{\Psi(\mathbf{R}, \alpha, \beta)}{\Psi(\mathbf{R}, \alpha, \beta)}\hat{H}\Psi(\mathbf{R}, \alpha, \beta)d\mathbf{R} \\ &= \int P(\mathbf{R}, \alpha, \beta)E_L(\mathbf{R}, \alpha, \beta)d\mathbf{R}. \end{aligned} \tag{17}$$

This multidimensional integral can then be approximated using Monte Carlo integration

$$E(\alpha, \beta) \approx \frac{1}{M}\sum_{m=1}^{M} E_L(\mathbf{R}^m, \alpha, \beta) \equiv \mathbb{E}[\hat{H}], \tag{18}$$

where each $\mathbf{R}^m$ is a complete set of N coordinates corresponding to the N particles in the system. The sets of coordinates $\mathbf{R}^m$, can be found using the Metropolis algorithm.

C. The Metropolis Algorithm

The Metropolis algorithm can be initialized by generating random coordinates for all the particles in the system. Using the probability distribution from Eq. 16, the Metropolis algorithm performs a so-called *random walk* to step-wise alter the set positions $\mathbf{R}$. A given number of Monte Carlo cycles is initially made in order to bring the system into a state that more closely fits our physical expectations. Once an equilibrium is reached, the sampling for the Monte Carlo integration begins.

A single Monte Carlo cycle loops through all N particles in the system and proposes a new position with a given step length $\Delta\mathbf{r}$ from the previous position. The initial set $\mathbf{R}^{old}$ in the m^{th} cycle will be those found in the previous cycle $\mathbf{R}^{m-1}$, and the last accepted configuration $\mathbf{R}^{new}$ after all particles have been considered will be the new set $\mathbf{R}^m$. Looping through all the particles, the new proposed position of the i^{th} particle is given by

$$\mathbf{r}_i^{new} = \mathbf{r}_i^{old} + \mathbf{s}\Delta\mathbf{r}, \tag{19}$$

where $\mathbf{s}$ is a set of size d_r of uniformly distributed random numbers. Each time a new position is proposed, the new position is either accepted or rejected depending on the acceptance probability, which as mentioned depends on the probability distribution. The acceptance probability of the new state is given by

$$A_{old \to new} = \min\left(1, \frac{P(\mathbf{R}^{new})}{P(\mathbf{R}^{old})}\right), \tag{20}$$

where $\mathbf{R}^{new}$ and $\mathbf{R}^{old}$ only differ by the coordinates of a single particle. The new coordinate $\mathbf{r}_i^{new}$ is accepted if the acceptance probability is larger than the random acceptance threshold $h \in [0, 1]$. We can see that if $P(\mathbf{R}^{new}) > P(\mathbf{R}^{old})$ then $\mathbf{r}_i^{new}$ must always be accepted. At the end of the cycle the sample $\mathbf{R}^m$ will contain both new proposed coordinates $\mathbf{r}^{new}$ as well as coordinates $\mathbf{r}^{m-1}$ from the previous sample.

This procedure is often referred to as *brute force* sampling, which is likely to be inefficient; we will therefore introduce *importance sampling* – an improved way of choosing new samples in order to save computational power.

D. The Metropolis-Hastings Algorithm

We will now reduce the number of Monte Carlo cycles needed for the Monte Carlo integration by implementing a natural bias in the random walk procedure: specifically, we need a bias determined by the wave function. To accomplish this, we introduce the *Fokker-Planck* equation, which describes the time-dependency of the probability distribution and is defined as

$$\frac{\partial P(\mathbf{R},t)}{\partial t} = D\sum_{i=1}^{N}\nabla_i\left(\nabla_i - \mathbf{F}_i\right)P(\mathbf{R},t), \tag{21}$$

where $D = \frac{1}{2}$ is the diffusion constant, and $\mathbf{F}_i$ is the drift force of the i^{th} particle. We can find the stationary probability density by setting the time derivative to zero, yielding

$$D\sum_{i=1}^{N}\nabla_i\left(\nabla_i - \mathbf{F}_i\right)P(\mathbf{R},t) = 0. \tag{22}$$

For the sum to amount to zero, it is a strict requirement that *all* the individual terms must equal zero – we can therefore focus on solving the general equation for any arbitrary particle. Slightly rewriting the equation for a single particle, we get

$$\nabla_i^2 P(\mathbf{R},t) = P(\mathbf{R},t)\nabla_i\mathbf{F}_i + \mathbf{F}_i\nabla_i P(\mathbf{R},t). \tag{23}$$

Knowing that the drift vector should be of the form $\mathbf{F}_i = g(\mathbf{R})\nabla_i P(\mathbf{R},t)$, we again rewrite and get

$$\begin{aligned}\nabla_i^2 P(\mathbf{R},t) = P(\mathbf{R},t)\frac{\partial g(\mathbf{R})}{\partial P(\mathbf{R},t)}\cdot\left(\nabla_i P(\mathbf{R},t)\right)^2 \\ + P(\mathbf{R},t)g(\mathbf{R})\nabla_i^2 P(\mathbf{R},t) + g(\mathbf{R})\left(\nabla_i P(\mathbf{R},t)\right)^2.\end{aligned} \tag{24}$$

For this equation to hold, we need to find a $g(\mathbf{R})$ such that the right-hand side of the equation becomes equivalent to $2\left[(\nabla_i\Psi(\mathbf{R}))^2 + \Psi(\mathbf{R})\nabla_i^2\Psi(\mathbf{R})\right]$. The equation is fulfilled if $g(\mathbf{R}) = \frac{1}{P(\mathbf{R},t)}$, which gives us the final expression for the drift force for the i^{th} particle

$$\mathbf{F}_i = \frac{2}{\Psi(\mathbf{R})}\nabla_i\Psi(\mathbf{R}), \tag{25}$$

for which the expressions have been derived in the appendix for both the one-body wave function as well as the wave function containing the correlation factor.

To create our biased random walk, we use the *Langevin equation*, given by

$$\frac{\partial\mathbf{r}_i(t)}{\partial t} = D\mathbf{F}(\mathbf{r}_i(t)) + \eta, \tag{26}$$

where η is a random variable. We create a new expression for $\mathbf{r}_i^{new}$ by using the time-derivative in the Langevin equation in a simple Euler Scheme. *Euler's Method* yields a prediction of the form $y(x+\Delta x) = y(x)+\Delta x y'(x)$. The new and biased guess is then

$$\mathbf{r}_i^{new} = \mathbf{r}_i^{old} + \Delta t D\mathbf{F}_i^{old} + \sqrt{\Delta t}\xi, \tag{27}$$

where Δt is the time step, typically set to some value $\Delta t \in [0.001, 0.01]$ and ξ is a Gaussian random variable.

The acceptance probability when using importance sampling will be that of the *Metropolis - Hastings* algorithm, given by

$$A_{old\to new} = \min\left(1, \frac{G(\mathbf{r}_i^{old},\mathbf{r}_i^{new},\Delta t)P(\mathbf{R}^{new})}{G(\mathbf{r}_i^{new},\mathbf{r}_i^{old},\Delta t)P(\mathbf{R}^{old})}\right), \tag{28}$$

where $G(\mathbf{r}_i^{new},\mathbf{r}_i^{old},\Delta t)$ is *Green's function*. Green's function describes the *transition probability* and is given by

$$\begin{aligned}&G(\mathbf{r}_i^{new},\mathbf{r}_i^{old},\Delta t) = \\ &\quad\frac{1}{(4\pi D\Delta t)^{3N/2}}\exp\left(-\frac{(\mathbf{r}_i^{new}-\mathbf{r}_i^{old}-D\Delta t F_i^{old})^2}{4D\Delta t}\right).\end{aligned} \tag{29}$$

Next we will discuss how to optimize our variational parameters.

E. Optimization of Variational Parameters

We will use Newton's method in order to optimize the variational parameter α; Newton's method is an iterative scheme for approximating the root of an arbitrary continuous real-valued function $g(x)$, given its first derivative $g\prime(x)$ and an initial *guess* x_0. The n^{th} iteration updates the value of x according to

$$x_{n+1} = x_n - \frac{g(x_n)}{g\prime(x_n)}, \tag{30}$$

which will make $g(x_n)$ converge towards a root, as long as no local minima or maxima get in the way. Now, finding the root of the expectation value of the energy is futile, as we know it is positive, but Newton's method can also be used for optimization by searching for the root $g\prime(x) = 0$. The algorithm for finding the stationary point of $g(x)$ is

$$x_{n+1} = x_n - \frac{g\prime(x_n)}{g\prime\prime(x_n)}. \tag{31}$$

A decent guess x_0 is crucial to ensure that the Newton's method converges towards the *correct* root. In our case, this should not be an issue, but in general a good initial value is necessary for the algorithm to converge fast enough.

We will need both the first and second derivatives of the expectation value of the energy with respect to α.

The first derivative can be written as

$$\bar{E}_\alpha \equiv \frac{\partial\langle E_L(\mathbf{R},\alpha)\rangle}{\partial\alpha} = 2\langle\frac{E_L(\mathbf{R},\alpha)}{\Psi(\mathbf{R},\alpha)}\frac{\partial\Psi(\mathbf{R},\alpha)}{\partial\alpha}\rangle - 2\langle E_L(\mathbf{R},\alpha)\rangle\langle\frac{1}{\Psi(\mathbf{R},\alpha)}\frac{\partial\Psi(\mathbf{R},\alpha)}{\partial\alpha}\rangle, \tag{32}$$

where the derivative of the trial wave function with respect to α is given by

$$\frac{\bar{\Psi}_\alpha}{\Psi} \equiv \frac{1}{\Psi(\mathbf{R},\alpha)}\frac{\partial\Psi(\mathbf{R},\alpha)}{\partial\alpha} = -\sum_{k=1}^{N}(x_k^2 + y_k^2 + \beta z_k^2), \tag{33}$$

in both the correlated and the uncorrelated cases. The proof of this can be found in the appendix. Note that this derivative is independent of α.

The second derivative will be divided into smaller chunks, starting with the first term

$$\frac{\partial}{\partial\alpha}\langle E_L(\mathbf{R},\alpha)\frac{\bar{\Psi}_\alpha}{\Psi}\rangle = 2\langle E_L(\mathbf{R},\alpha)\left(\frac{\bar{\Psi}_\alpha}{\Psi}\right)^2\rangle - 2\langle E_L(\mathbf{R},\alpha)\frac{\bar{\Psi}_\alpha}{\Psi}\rangle\langle\frac{\bar{\Psi}_\alpha}{\Psi}\rangle, \tag{34}$$

moving on to the latter term using the product rule, we get

$$\frac{\partial}{\partial\alpha}\langle E_L(\mathbf{R},\alpha)\rangle\langle\frac{\bar{\Psi}_\alpha}{\Psi}\rangle = \langle\frac{\bar{\Psi}_\alpha}{\Psi}\rangle\bar{E}_\alpha + 2\langle E_L(\mathbf{R},\alpha)\rangle\left[\langle\left(\frac{\bar{\Psi}_\alpha}{\Psi}\right)^2\rangle - \langle\frac{\bar{\Psi}_\alpha}{\Psi}\rangle^2\right]. \tag{35}$$

The final expression for the second derivative is therefore

$$\bar{E}_{\alpha\alpha} \equiv \frac{\partial^2\langle E_L(\mathbf{R},\alpha)\rangle}{\partial\alpha^2} = 4\langle E_L(\mathbf{R},\alpha)\left(\frac{\bar{\Psi}_\alpha}{\Psi}\right)^2\rangle - 4\langle E_L(\mathbf{R},\alpha)\frac{\bar{\Psi}_\alpha}{\Psi}\rangle\langle\frac{\bar{\Psi}_\alpha}{\Psi}\rangle - 2\langle\frac{\bar{\Psi}_\alpha}{\Psi}\rangle\bar{E}_\alpha - 4\langle E_L(\mathbf{R},\alpha)\rangle\left[\langle\left(\frac{\bar{\Psi}_\alpha}{\Psi}\right)^2\rangle - \langle\frac{\bar{\Psi}_\alpha}{\Psi}\rangle^2\right]. \tag{36}$$

The iterative scheme for optimizing α to obtain the ground state energy is then given by

$$\alpha_{n+1} = \alpha_n - \frac{\bar{E}_\alpha}{\bar{E}_{\alpha\alpha}}, \tag{37}$$

where $\alpha_0 = 0.5$.

Next we will look at how to assess the statistical errors in this project.

F. Statistical Methods and Errors

The local energies found through the Monte Carlo simulations of the bosonic system should be treated similarly to experimental measurements. This section will therefore introduce measurements for the accuracy of the expectation value of the ground state energy.

The variance of the local energies is given by

$$\sigma^2 \equiv \mathrm{var}(E_L) = \frac{1}{M}\sum_{m=1}^{M}(E_L(\mathbf{R}^m) - \mathbb{E}[\hat{H}])^2. \tag{38}$$

An estimate of the error of the expectation value of the energy can be computed as $\sqrt{\frac{\sigma^2}{M}}$. This is a rough estimate, and will be lower than the real standard deviation, as the local energies are not uncorrelated. We will need to implement more powerful methods for a more accurate measure of the expectation value's error.

1. *Bootstrapping*

To extract more meaningful means and variances from smaller datasets, it can be helpful to implement resampling techniques. These techniques work in a variety of way: in simplified terms, they artificially increase the size of a dataset through the random sampling of existing datapoints, which improves the reliability of the dataset's mean and variance.

More specifically, we will begin with the *bootstrapping* technique; assuming we have a dataset containing L elements, and we choose a number of iterations N_{BOOT}, then:

Algorithm 1: Bootstrap Algorithm

```
Result: Bootstrapped Mean and Variance
mean_sum = 0.0;
var_sum = 0.0;
i = 0;
while i < N_boot do
    j = 0;
    iter = 0.0;
    squared_iter = 0.0;
    while j < L do
        idx = randint(0, L-1);
        iter += data[idx];
        squared_iter += data[idx]^2;
        j++;
    end
    mean_sum += iter/L;
    var_sum += (iter/L)^2 - squared_iter/L;
    i++;
end
bootstrap_mean = mean_sum / N_boot ;
bootstrap_var = var_sum / N_boot ;
```

As seen in Algorithm 1, this method involves the random selection of L elements *with replacement* – this

means that while some elements may be selected multiple times, others may never be selected. The simplicity of this method is something to be wary of however, as this method can be misleading in some datasets: some cases in which bootstrapping can lead to issues are small datasets, datasets with extreme points, and datasets whose elements are correlated.

In the case of a small dataset, the sample might not be large enough to represent its true probability distribution, which means that bootstrapping might lead to a mean and variance that is inaccurate.

Regarding outliers – if these values are unimportant in accurately portraying the dataset (i.e. they are statistical noise) then bootstrapping will cause the mean to underrepresent these values; if they are significant, then this will in turn cause the mean to inaccurately disregard these outliers.

Finally, bootstrapping as a technique is unable to correctly replicate the correlations in a dataset, as it selects its datapoints at random. This is a problem that can be resolved through the implementation of *blocking*.

2. Blocking

To mitigate the loss of correlation in a dataset, a dataset can be divided into *blocks*, rather than randomly selected groups of individual samples – this allows variables to retain their relation to nearby values.

We can see in Algorithm 2 that blocking is similar to bootstrapping, except that it removes both

- The selection of random datapoints
- The need to repeat the process an indeterminate number of times

The first point is quite important, as the lack of stochasticity will allow correlations to remain during the resampling. As for the second point, performance is key, and having an upper limit in terms of the number of iterations is an important factor when selecting a resampling technique.

Algorithm 2: Blocking Algorithm

```
Result: Blocking Mean and Variance
mean_sum = 0.0;
var_sum = 0.0;
i = min_block_size;
while i < max_block_size do
    j = 0;
    while j < N_boot do
        k = 0;
        iter = 0.0;
        squared_iter = 0.0;
        while k+i < L do
            l = 0;
            block = 0.0;
            squared_block= 0.0;
            while l < i do
                block += data[k];
                squared_block += data[k]^2;
                k++;
                l++;
            end
            iter += block/i;
            squared_iter += squared_block/i;
        end
        mean_sum += iter/L;
        var_sum += (iter/L)^2 - squared_iter/L;
        j++;
    end
    i++;
end
bootstrap_mean = mean_sum / N_boot ;
bootstrap_var = var_sum / N_boot ;
```

We will now move on to a short description of the implementation.

III. IMPLEMENTATION

The code for the variational Monte Carlo simulations was implemented in `C++`. The implementation was mostly object-oriented, and generalized for anything from one to three spacial dimensions.

The energy sampling was parallelized using `MPI`, where each processor created its own subset of values for the local energy. The implementation of Newton's method for optimizing α was parallelized by allowing all processors to run separate sets of Newton iterations, and then choosing their respective final α values as their means.

The statistical analysis on the other hand was implemented in `Python`, where the plots were generated using the `matplotlib` library.

A. Mathematical Optimization

Some of the expressions can be simplified by canceling terms and factors, which reduces the computational cost of the simulations. An important consideration is the excessive expense of mathematical operations such as the exponential function and square roots, which should be avoided or reduced as much as possible. Here we will introduce some of the mathematical simplifications used in the implementation.

The ratios of the probability density function can be considerably simplified by using properties of the exponential function. As $\mathbf{R}^{old}$ and $\mathbf{R}^{new}$ only differ by the coordinates a single particle, let's say the k^{th} particle, the ratio of the one-body factor can be rewritten as

$$\frac{\Psi_{OB}(\mathbf{R}^{new})}{\Psi_{OB}(\mathbf{R}^{old})} = \exp\big\{\ln\phi(\mathbf{r}_k^{new}) - \ln\phi(\mathbf{r}_k^{old})\big\}. \tag{39}$$

Similarly, the ratio of the correlation factor can be reduced to

$$\frac{\Psi_C(\mathbf{R}^{new})}{\Psi_C(\mathbf{R}^{old})} = \prod_{i\neq k}\frac{f(r_{ik}^{new})}{f(r_{ik}^{old})}. \tag{40}$$

From these results, the ratio of the probability density can be vastly simplified.

The Green's function ratio can also be slightly reduced to

$$\frac{G(\mathbf{R}^{old},\mathbf{R}^{new},\Delta t)}{G(\mathbf{R}^{new},\mathbf{R}^{old},\Delta t)} = \exp\left(\Big[\big(\mathbf{r}_k^{new} - \mathbf{r}_k^{old} - D\Delta t F_k^{old}\big)^2 - \big(\mathbf{r}_k^{old} - \mathbf{r}_k^{new} - D\Delta t F_k^{new}\big)^2\Big]\frac{1}{4D\Delta t}\right). \tag{41}$$

We will now present the results of the virtual labwork.

IV. RESULTS

A study of the non-interacting bosons was made using the Metropolis algorithm. Several different values for α were used. The result of this study in *one* dimension can be found in table I, while the results when simulated in *two* dimensions can be found in table II. Lastly, the results of the *three*-dimensional simulations can be found in table III.

TABLE I: The expectation values $\langle E\rangle$, in units of $1/\hbar\omega_{ho}$, were obtained by $M = 10^6$ Monte Carlo cycles using the Metropolis algorithm. The estimate of the error of the expectation value is given by $\sqrt{\frac{\sigma^2}{M}}$. The column *Reject Ratio* shows the ratio of rejected moves in the random walk. The number of particles N, and the variational parameter α were varied, while the other parameters were kept constant at $\beta = \gamma = 1$. The system was that of the non-interacting Hamiltonian $\hat{H}_0$ and wave function $\Psi_{OB}(\mathbf{R})$ in one dimension, $d_r = 1$.

N	α	$\langle E\rangle$	Error	Reject Ratio
1	0.45	0.50292	7×10^{-5}	0.21
1	0.50	0.50000	4×10^{-20}	0.22
1	0.55	0.50222	7×10^{-5}	0.23
10	0.45	5.02747	2×10^{-4}	0.21
10	0.50	5.00000	3×10^{-19}	0.22
10	0.55	5.02346	2×10^{-4}	0.23
100	0.45	50.2757	7×10^{-4}	0.21
100	0.50	50.0000	4×10^{-18}	0.22
100	0.55	50.2293	7×10^{-4}	0.23
500	0.45	252.318	0.04	0.21
500	0.50	250.000	2×10^{-17}	0.22
500	0.55	251.130	0.002	0.23

TABLE II: The expectation values $\langle E\rangle$, in units of $1/\hbar\omega_{ho}$, were obtained by $M = 10^6$ Monte Carlo cycles using the Metropolis algorithm. The estimate of the error of the expectation value is given by $\sqrt{\frac{\sigma^2}{M}}$. The column *Reject Ratio* shows the ratio of rejected moves in the random walk. The number of particles N, and the variational parameter α were varied, while the other parameters were kept constant at $\beta = \gamma = 1$. The system was that of the non-interacting Hamiltonian $\hat{H}_0$ and wave function $\Psi_{OB}(\mathbf{R})$ in two dimensions, $d_r = 2$.

N	α	$\langle E\rangle$	Error	Reject Ratio
1	0.45	1.00607	1×10^{-4}	0.32
1	0.50	1.00000	7×10^{-20}	0.33
1	0.55	1.00495	1×10^{-4}	0.35
10	0.45	10.0564	3×10^{-4}	0.32
10	0.50	10.0000	5×10^{-19}	0.33
10	0.55	10.0446	3×10^{-4}	0.35
100	0.45	100.556	1×10^{-3}	0.32
100	0.50	100.000	7×10^{-18}	0.33
100	0.55	100.456	1×10^{-3}	0.35
500	0.45	552.815	1.15	0.32
500	0.50	500.000	3×10^{-17}	0.33
500	0.55	502.260	2×10^{-3}	0.35

TABLE III: The expectation values $\langle E \rangle$, in units of $1/\hbar\omega_{ho}$, were obtained by $M = 10^6$ Monte Carlo cycles using the Metropolis algorithm. The estimate of the error of the expectation value is given by $\sqrt{\frac{\sigma^2}{M}}$. The column *Reject Ratio* shows the ratio of rejected moves in the random walk. The number of particles N, and the variational parameter α were varied, while the other parameters were kept constant at $\beta = \gamma = 1$. The system was that of the non-interacting Hamiltonian $\hat{H}_0$ and wave function $\Psi_{OB}(\mathbf{R})$ in three dimensions, $d_r = 3$.

N	α	$\langle E \rangle$	Error	Reject Ratio
1	0.45	1.50921	1×10^{-4}	0.40
1	0.50	1.50000	1×10^{-19}	0.42
1	0.55	1.50677	1×10^{-4}	0.43
10	0.45	15.0800	4×10^{-4}	0.40
10	0.50	15.0000	1×10^{-18}	0.42
10	0.55	15.0683	4×10^{-4}	0.43
100	0.45	150.834	1×10^{-3}	0.40
100	0.50	150.000	4×10^{-20}	0.42
100	0.55	150.681	1×10^{-3}	0.43
500	0.45	1001.440	5	0.40
500	0.50	750.000	6×10^{-17}	0.42
500	0.55	753.403	3×10^{-3}	0.43

The same study was made using importance sampling, adding different values for the step length, Δt. The result of this study in *one* dimension can be found in table IV, the results when simulated in *two* dimensions can be found in table V and lastly the results of the *three*-dimensional simulations can be found in table VI.

TABLE IV: The expectation values $\langle E \rangle$, in units of $1/\hbar\omega_{ho}$, were obtained by $M = 10^6$ Monte Carlo cycles using the Metropolis-Hastings algorithm. The estimate of the error of the expectation value is given by $\sqrt{\frac{\sigma^2}{M}}$. The column *Reject Ratio* shows the ratio of rejected moves in the random walk. The number of particles N, the step length Δt and the variational parameter α were varied, while the other parameters were kept constant at $\beta = \gamma = 1$. The system was that of the non-interacting Hamiltonian $\hat{H}_0$ and wave function $\Psi_{OB}(\mathbf{R})$ in one dimension, $d_r = 1$.

N	α	$\langle E \rangle$	Error	Reject Ratio	Δt
1	0.50	0.50000	4×10^{-20}	3×10^{-6}	0.001
1	0.50	0.50000	4×10^{-20}	9×10^{-5}	0.005
1	0.50	0.50000	4×10^{-20}	2×10^{-4}	0.010
1	0.55	0.50271	7×10^{-5}	7×10^{-6}	0.001
1	0.55	0.50288	7×10^{-5}	9×10^{-5}	0.005
1	0.55	0.50148	7×10^{-5}	3×10^{-4}	0.010
10	0.50	5.00000	3×10^{-19}	8×10^{-6}	0.001
10	0.50	5.00000	3×10^{-19}	8×10^{-5}	0.005
10	0.50	5.00000	3×10^{-19}	2×10^{-4}	0.010
10	0.55	5.01912	2×10^{-4}	1×10^{-5}	0.001
10	0.55	5.02460	2×10^{-4}	9×10^{-5}	0.005
10	0.55	5.02533	2×10^{-4}	3×10^{-4}	0.010
100	0.50	50.0000	4×10^{-18}	7×10^{-6}	0.001
100	0.50	50.0000	4×10^{-18}	8×10^{-5}	0.005
100	0.50	50.0000	4×10^{-18}	2×10^{-4}	0.010
100	0.55	50.2518	7×10^{-4}	8×10^{-6}	0.001
100	0.55	50.2216	7×10^{-4}	9×10^{-5}	0.005
100	0.55	50.2320	7×10^{-4}	3×10^{-4}	0.010
500	0.50	250.000	3×10^{-17}	7×10^{-6}	0.001
500	0.50	250.000	2×10^{-17}	8×10^{-5}	0.005
500	0.50	250.000	2×10^{-17}	2×10^{-4}	0.010
500	0.55	251.052	1×10^{-3}	8×10^{-6}	0.001
500	0.55	251.120	2×10^{-3}	9×10^{-5}	0.005
500	0.55	251.130	2×10^{-3}	3×10^{-4}	0.010

TABLE V: The expectation values $\langle E \rangle$, in units of $1/\hbar\omega_{ho}$, were obtained by $M = 10^6$ Monte Carlo cycles using the Metropolis-Hastings algorithm. The estimate of the error of the expectation value is given by $\sqrt{\frac{\sigma^2}{M}}$. The column *Reject Ratio* shows the ratio of rejected moves in the random walk. The number of particles N, the step length Δt and the variational parameter α were varied, while the other parameters were kept constant at $\beta = \gamma = 1$. The system was that of the non-interacting Hamiltonian $\hat{H}_0$ and wave function $\Psi_{OB}(\mathbf{R})$ in two dimensions, $d_r = 2$.

N	α	$\langle E \rangle$	Error	Reject Ratio	Δt
1	0.50	1.00000	7×10^{-20}	9×10^{-6}	0.001
1	0.50	1.00000	7×10^{-20}	1×10^{-4}	0.005
1	0.50	1.00000	7×10^{-20}	4×10^{-4}	0.010
1	0.55	1.00607	9×10^{-5}	9×10^{-6}	0.001
1	0.55	1.00603	9×10^{-5}	1×10^{-4}	0.005
1	0.55	1.00559	9×10^{-5}	4×10^{-4}	0.010
10	0.50	10.0000	5×10^{-19}	1×10^{-5}	0.001
10	0.50	10.0000	5×10^{-19}	1×10^{-4}	0.005
10	0.50	10.0000	5×10^{-19}	4×10^{-4}	0.010
10	0.55	10.0573	3×10^{-4}	1×10^{-5}	0.001
10	0.55	10.0452	3×10^{-4}	1×10^{-4}	0.005
10	0.55	10.0457	3×10^{-4}	4×10^{-4}	0.010
100	0.50	100.000	7×10^{-18}	1×10^{-5}	0.001
100	0.50	100.000	7×10^{-18}	1×10^{-4}	0.005
100	0.50	100.000	7×10^{-18}	4×10^{-4}	0.010
100	0.55	100.443	9×10^{-4}	1×10^{-5}	0.001
100	0.55	100.467	1×10^{-3}	1×10^{-4}	0.005
100	0.55	100.469	1×10^{-3}	4×10^{-4}	0.010
500	0.50	500.000	4×10^{-17}	1×10^{-5}	0.001
500	0.50	500.000	3×10^{-17}	1×10^{-4}	0.005
500	0.50	500.000	3×10^{-17}	4×10^{-4}	0.010
500	0.55	502.237	2×10^{-3}	1×10^{-5}	0.001
500	0.55	502.256	2×10^{-3}	1×10^{-4}	0.005
500	0.55	502.322	2×10^{-3}	4×10^{-4}	0.010

TABLE VI: The expectation values $\langle E \rangle$, in units of $1/\hbar\omega_{ho}$, were obtained by $M = 10^6$ Monte Carlo cycles using the Metropolis-Hastings algorithm. The estimate of the error of the expectation value is given by $\sqrt{\frac{\sigma^2}{M}}$. The column *Reject Ratio* shows the ratio of rejected moves in the random walk. The number of particles N, the step length Δt and the variational parameter α were varied, while the other parameters were kept constant at $\beta = \gamma = 1$. The system was that of the non-interacting Hamiltonian $\hat{H}_0$ and wave function $\Psi_{OB}(\mathbf{R})$ in three dimensions, $d_r = 3$.

N	α	$\langle E \rangle$	Error	Reject Ratio	Δt
1	0.50	1.50000	1×10^{-19}	9×10^{-6}	0.001
1	0.50	1.50000	1×10^{-19}	2×10^{-4}	0.005
1	0.50	1.50000	1×10^{-19}	5×10^{-4}	0.010
1	0.55	1.50780	1×10^{-4}	2×10^{-5}	0.001
1	0.55	1.50755	1×10^{-4}	2×10^{-4}	0.005
1	0.55	1.50703	1×10^{-4}	5×10^{-4}	0.010
10	0.50	15.0000	1×10^{-18}	1×10^{-5}	0.001
10	0.50	15.0000	1×10^{-18}	2×10^{-4}	0.005
10	0.50	15.0000	1×10^{-18}	5×10^{-4}	0.010
10	0.55	15.0525	4×10^{-4}	1×10^{-5}	0.001
10	0.55	15.0679	4×10^{-4}	2×10^{-4}	0.005
10	0.55	15.0691	4×10^{-4}	5×10^{-4}	0.010
100	0.50	150.000	0	1×10^{-5}	0.001
100	0.50	150.000	0	2×10^{-4}	0.005
100	0.50	150.000	0	5×10^{-4}	0.010
100	0.55	150.746	1×10^{-3}	2×10^{-5}	0.001
100	0.55	150.673	1×10^{-3}	2×10^{-4}	0.005
100	0.55	150.687	1×10^{-3}	5×10^{-4}	0.010
500	0.50	750.000	1×10^{-16}	1×10^{-5}	0.001
500	0.50	750.000	6×10^{-17}	2×10^{-4}	0.005
500	0.50	750.000	6×10^{-17}	4×10^{-4}	0.010
500	0.55	753.523	3×10^{-3}	2×10^{-5}	0.001
500	0.55	753.507	3×10^{-3}	2×10^{-4}	0.005
500	0.55	753.385	3×10^{-3}	5×10^{-4}	0.010

A statistical analysis was performed for the *three*-dimensional case of non-interacting bosons using importance sampling. The results can be found in table VII.

TABLE VII: The expectation values $\langle E \rangle$, in units of $1/\hbar\omega_{ho}$ with corresponding uncertainty calculated using *blocking* and *bootstrapping*. The set of local energy values were obtained by $M = 10^6$ Monte Carlo cycles using the Metropolis-Hastings algorithm. The number of particles N, the step length Δt and the variational parameter α were varied, while the other parameters were kept constant at $\beta = \gamma = 1$. The system was that of the non-interacting Hamiltonian $\hat{H}_0$ and wave function $\Psi_{OB}(\mathbf{R})$ in three dimensions, $d_r = 3$.

N	α	Δt	$\langle E \rangle_{\text{block}}$	$\langle E \rangle_{\text{boot}}$
1	0.50	0.001	1.5 ± 0	1.5 ± 0
1	0.50	0.005	1.5 ± 0	1.5 ± 0
1	0.50	0.010	1.5 ± 0	1.5 ± 0
1	0.55	0.001	1.511 ± 0.002	1.5113 ± 0.0001
1	0.55	0.005	1.509 ± 0.001	1.5088 ± 0.0001
1	0.55	0.010	1.507 ± 0.001	1.5067 ± 0.0001
10	0.50	0.001	15 ± 0	15 ± 0
10	0.50	0.005	15 ± 0	15 ± 0
10	0.50	0.010	15 ± 0	15 ± 0
10	0.55	0.001	15.071 ± 0.006	15.0710 ± 0.0004
10	0.55	0.005	15.059 ± 0.004	15.0592 ± 0.0004
10	0.55	0.010	15.063 ± 0.003	15.0628 ± 0.0005
100	0.50	0.001	150 ± 0	150 ± 0
100	0.50	0.005	150 ± 0	150 ± 0
100	0.50	0.010	150 ± 0	150 ± 0
100	0.55	0.001	150.68 ± 0.02	150.681 ± 0.001
100	0.55	0.005	150.69 ± 0.01	150.692 ± 0.001
100	0.55	0.010	150.67 ± 0.01	150.672 ± 0.001
500	0.50	0.001	750 ± 0	750 ± 0
500	0.50	0.005	750 ± 0	750 ± 0
500	0.50	0.010	750 ± 0	750 ± 0
500	0.55	0.001	753.46 ± 0.04	753.455 ± 0.003
500	0.55	0.005	753.34 ± 0.03	753.341 ± 0.003
500	0.55	0.010	753.42 ± 0.02	753.420 ± 0.003

Repulsive forces were added and the brute force Monte Carlo simulations in *three* dimensions were repeated. The results of the simulations can be found in table VIII.

TABLE VIII: The expectation values $\langle E \rangle$, in units of $1/\hbar\omega_{ho}$, were obtained by $M = 10^6$ Monte Carlo cycles using the Metropolis algorithm. The estimate of the error of the expectation value is given by $\sqrt{\frac{\sigma^2}{M}}$. The column *Reject Ratio* shows the ratio of rejected moves in the random walk. The number of particles N and the variational parameter α were varied, while the other parameters were kept constant at $\beta = \gamma = 2.82843$ and the hard-core radius of the particles were set to $a = 0.0043$. The system was that of the full Hamiltonian $\hat{H}$ and wave function $\Psi_T(\mathbf{R})$ in three dimensions, $d_r = 3$.

N	α	$\langle E \rangle$	Error	Reject Ratio
10	0.45	24.5219	7×10^{-4}	0.47
10	0.50	24.3988	5×10^{-5}	0.49
10	0.55	24.5218	7×10^{-4}	0.51
50	0.45	127.701	2×10^{-3}	0.46
50	0.50	127.294	5×10^{-4}	0.48
50	0.55	128.153	2×10^{-3}	0.50
100	0.45	266.862	2×10^{-3}	0.45
100	0.50	266.361	1×10^{-3}	0.47
100	0.55	268.470	3×10^{-3}	0.49

For comparison, the analytical values for the energy was calculated for the ideal, or non-interacting, case. The formula for this energy is $E = \frac{N(2+\beta)}{2}$ in *three* dimensions when $\alpha = 0.5$. These values can be found in table IX.

TABLE IX: The analytical expressions for the energy, in units of $1/\hbar\omega_{ho}$, of non-interacting bosons in a elliptical trap. The parameters used were $\alpha = 0.5$ $\beta = \gamma = 2.82843$. The system was that of the non-interacting Hamiltonian $\hat{H}_0$ and wave function $\Psi_{OB}(\mathbf{R})$ in three dimensions, $d_r = 3$.

N	E
10	24.1422
50	120.717
100	241.422

The variational parameter was optimized using Newton's method. The calculated α-values and their corresponding energy expectation values can be found in table X.

TABLE X: The values for α optimized using Newton's method. The expectation values $\langle E \rangle$, in units of $1/\hbar\omega_{ho}$, were obtained by $M = 10^6$ Monte Carlo cycles using the Metropolis algorithm. The estimate of the error of the expectation value is given by $\sqrt{\frac{\sigma^2}{M}}$. The column *Reject Ratio* shows the ratio of rejected moves in the random walk. The parameters used were $\beta = \gamma = 2.82843$ and $a = 0.0043$. The system was that of the full Hamiltonian $\hat{H}$ and wave function $\Psi_T(\mathbf{R})$ in three dimensions, $d_r = 3$.

N	α	$\langle E \rangle$	Error	Reject Ratio
10	0.4975	24.3985	2×10^{-4}	0.49
50	0.4891	127.264	1×10^{-3}	0.48
100	0.4829	266.196	3×10^{-3}	0.47

The particle density of both the correlated and the uncorrelated bosons was visualized, separating the three dimensions. Figure 1 shows the one-body density in the x-axis, figure 2 shows the y-axis and figure 3 shows the one-body density on the z-axis.

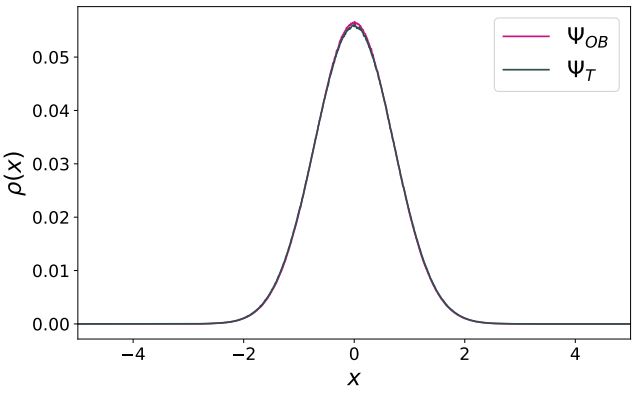

FIG. 1: The density ρ as a function of x. The densities were calculated using 10^7 Monte Carlo cycles with the Metropolis algorithm, using 100 particles. In the case of uncorrelated bosons, Ψ_{OB}, the parameters $\alpha = 0.5$ and $\beta = \gamma = 1$ were used. In the case of correlated bosons, Ψ_T, the parameters $\alpha = 0.4829$, $\beta = \gamma = 2.82843$ and $a = 0.0043$ were used.

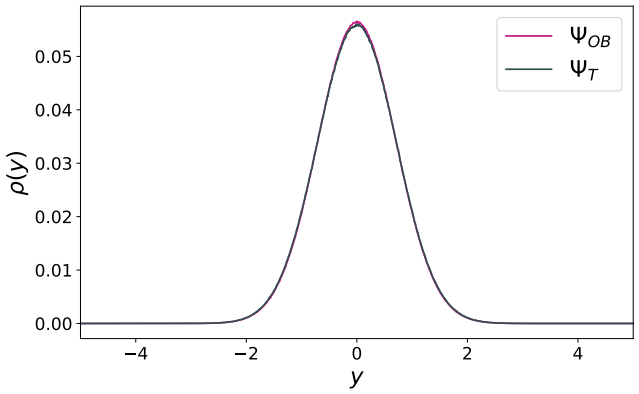

FIG. 2: The density ρ as a function of y. The densities were calculated using 10^7 Monte Carlo cycles with the Metropolis algorithm, using 100 particles. In the case of uncorrelated bosons, Ψ_{OB}, the parameters $\alpha = 0.5$ and $\beta = \gamma = 1$ were used. In the case of correlated bosons, Ψ_T, the parameters $\alpha = 0.4829$, $\beta = \gamma = 2.82843$ and $a = 0.0043$ were used.

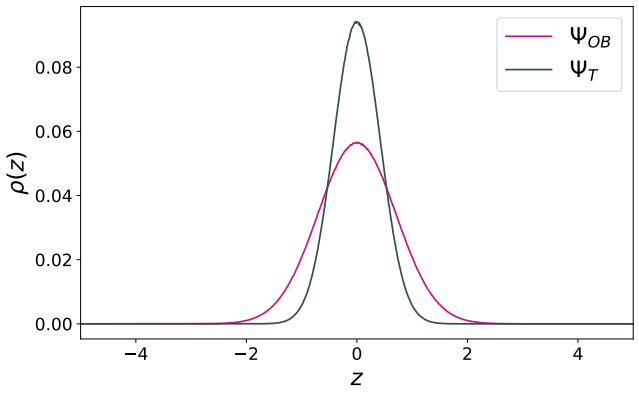

FIG. 3: The density ρ as a function of z. The densities were calculated using 10^7 Monte Carlo cycles with the Metropolis algorithm, using 100 particles. In the case of uncorrelated bosons, Ψ_{OB}, the parameters $\alpha = 0.5$ and $\beta = \gamma = 1$ were used. In the case of correlated bosons, Ψ_T, the parameters $\alpha = 0.4829$, $\beta = \gamma = 2.82843$ and $a = 0.0043$ were used.

V. DISCUSSION

Overall, the results we found for the energy of the non-interacting bosonic system were completely successful. As seen in Tables I, II, and III, the cases where $\alpha = 0.5$ always yields $\langle E \rangle / N d_r = 0.5$, which is the analytical solution for the expectation value of a boson's energy in a spherical harmonic potential. The energy expectation values are slightly higher when $\alpha \neq 0.5$, which is as expected.

It is also worth noting that the *error* for the $\alpha = 0.5$ rows are negligibly small, which implies that the results are exact. The errors found are likely due to numerical

error, which becomes more significant as the number of particles increases.

On the other hand, we see that the error for $\alpha \neq 0.5$ is far more significant, which is due to the stochastic nature of the Metropolis algorithm being implemented for the case of an incorrect hyperparameter. We see that in the case of large N this even leads to numerical instability, as the error reaches a maximum value that is very large in Tables I, II, and III for $N = 500$, and for $\alpha = 0.45$. Some caution in interpreting these errors is advised, as they do not account for correlation. The error will be artificially low, and should only be used for comparing the results when using different values for α and different Monte Carlo methods.

Finally, we see in all three of these aforementioned tables that the rejection rate for the particles' random walk increases quite a bit as a function of the number of dimensions d_r and α, and is quite large in some cases (e.g over 40% of all moves were rejected in Table III).

While the previous tables were all calculated using the brute-force Metropolis algorithm, the values in Tables IV, V, and VI were found more efficiently by implementing *importance sampling*. We see that the movement rejection ratio for these three tables are significantly smaller than for those in I, II, and III, which is already a good sign that our algorithm is functioning correctly. It is also worth noting that we are still getting the exact analytical solution for $\alpha = 0.5$ in Tables IV, V, and VI, which further suggests that the program is performing correctly.

Additionally, we can see that there exists a trend in these three tables relating the time-step Δt to the rejection rate; specifically, as the time-step increases so does the rejection rate – this is likely due to overshooting in the correct movement direction.

Unfortunately, while the trends outlined above are significant, the exact values of the errors in all the aforementioned tables are misleading due to the fact that no resampling techniques were implemented before the post-processing phase of this computer experiment. This has been mitigated to a degree in Table VII, where *bootstrapping* and *blocking* were applied to the energy values as recorded on a per-cycle basis.

As has been the case in all the previous tables, we are still looking at a system with no inter-particle interactions, and as such our energies are exact at $\alpha = 0.5$ – what has changed however is that the errors (denoted by the values after $\pm$) are consistently larger once resampling techniques were implemented, which once more point to flaws in the errors calculated previously.

Having confirmed the success of the non-interacting model, Table VIII shows the initial results of the run with an inter-particle interaction. Given that we are observing the 3-D case ($d_r = 3$) we can compare the values in Table VIII to the analytical values in the non-interacting system (Table IX).

When comparing results between the interacting model with the analytical results, we can see that the particle interaction tends to make the system more energetic per-particle compared to the non-interacting system – this makes sense, as all the particles always repel each other – a trend in accordance with the results of DuBois and Glyde [1]. It seems that $\alpha = 0.5$ is still the best choice of the three α-values, as this consistently yielded the lowest expectation values for the energy. The movement rejection ratio also appears to decrease as N increases, which implies that having more particles in the interacting case leads to less strict movement conditions.

Given that the results in Table VIII appear reasonable, the application of Newton's method (with respect to the parameter α) in order to find an energy minimum yields the values in Table X. Other than a more finely-tuned set of hyperparameters, this table also demonstrates an interesting trend: as the number of particles increases, so decreases the ideal value of α. The energy expectation values in table X are, to a different extent, lower than the previously found expectation values found in Table VIII. This gives an improved upper-bound for the energies. The relative difference between the ideal cases found in Table IX and the computed upper-bound energies are 0.01 when $N = 10$, 0.05 when $N = 50$ and 0.1 when $N = 100$. This shows a trend of linear increase in relative deviance from the ideal case as a function of number of particles.

Our last items of interest are Figures 1, 2, and 3, which show the one-body and interacting densities ρ as a function of the coordinates x, y, and z, respectively. In both the one-body and interacting cases, their respective ideal parameters α were used in order to show the systems' ground states as compared to one-another.

We can see that the plots for x and y (Figures 1 and 2) are essentially identical to one-another, implying that our density is (very nearly) circular on the xy-plane for all cases. The plots do not show much difference in ρ due to the Jastrow factor, but a small difference can be observed at the center of the trap. The interacting system shows lower density at the middle of the trap compared to the ideal system. Although not prominently, this shows the same trend as observed by DuBois and Glyde [1].

As for Figure 3, we see that the plot for ρ of Ψ_{OB} is the same as the two previous plots, but that ρ of Ψ_T is taller than its counterparts along the x and y axes. This phenomenon seems to be due to the elongation factor in the elliptical interacting potential, which affects the density's dependence on z.

VI. CONCLUSION

Overall, it appears that this computer experiment was successful – benchmarking with respect to the non-interacting bosonic system showed us that we could perfectly reproduce the analytical energy expectation values (given by $\langle E \rangle / N d_r = 0.5$) numerically for $\alpha = 0.5$. Specifically, we were able to reproduce this result exactly in systems of one, two, and three dimensions for 1, 10, 100, and 500 particle systems.

In addition to our benchmarking successes, we also managed to optimize our program by guiding our particles' random walk through the usage of a *quantum force*. This implementation of importance sampling motivated our particles to move in more reasonable directions, thus increasing our movement acceptance rate from an approximate average of 60% (in three dimensions) to values greater than 99% (also in three dimensions). This allowed us to obtain excellent results, with far fewer computational cycles.

The upper-bound energy for the interacting bosons with radius $a/a_{ho} = 0.0043$ in the elliptical trap with parameters $\beta = \gamma = 2.82843$ and optimized value for α using Newton's method was found to be $24.3985/(\hbar\omega_{ho})$ when the system consisted of 10 particles and $\alpha = 0.4975$. The upper-bound energy for the same system containing 50 particles and using $\alpha = 0.4891$ was $127.264/(\hbar\omega_{ho})$. Lastly, for a system of 100 particles and $\alpha = 0.4829$, the upper bound-energy was found to be $266.196/(\hbar\omega_{ho})$.

The relative deviance of the computed lower-bound energy compared to the ideal non-interacting bosons in the same kind of trap and $\alpha = 0.5$ was found to increase with the number of particles, confirming the results of DuBois and Glyde [1].

The particle density in the middle of the trap was slightly lower for the system of interacting bosons compared to the non-interacting bosons in the x and y-direction. Although weak, this demonstrates the same trend as found by DuBois and Glyde [1]. The difference was significant in the z-direction, but this is assumed to be due to the elliptical trap used (only) on the interacting particles.

[1] J. L. DuBois and H. R. Glyde. Bose-einstein condensation in trapped bosons: A variational monte carlo analysis. *Phys. Rev. A*, 63(023602), 2001.

[2] Morten Hjorth-Jensen. Computational Physics — Lecture Notes Fall 2015. `https://github.com/CompPhysics/ComputationalPhysics2/blob/gh-pages/doc/Literature/lectures2015.pdf`, 2015.

VII. APPENDIX

The appendix includes three parts. The first part shows the derivation of the gradient and Laplacian of the one-body wave function, the correlation factor and the full trial function. The second and third parts use the results from the first part to derive expressions for the local energy and drift force. While the second part uses the case of non-interacting bosons in a spherical potential, the third part shows the more general results for interacting bosons.

A. The Gradients of the Wave Function

We will look at the gradients and Laplacian of the one-body wave function, the correlation factor and the full trial function. For the correlation factor in the trial wave function, note that the trivial cases where $r_{ij} < a$ for any two particles have been omitted. In such a case, the correlation factor would effectively collapse the wave function and the probability density would be zero. Not only is the transition from a *good* state to one where two particles occupy the same space physically impossible – the transition will never be accepted in the computational scheme. This is ensured as $A_{old\to new} = 0$ in this case, which is never *larger* than the acceptance threshold $h \in [0, 1]$. The calculations of the derivative will therefore assume that $r_{ij} \leq a$.

1. The Gradients of the One-Body Wave Function

To calculate the gradient of the one-body wave function, the gradient of $\phi(\mathbf{r})$. The gradient of $\phi(\mathbf{r})$ with respect to the k^{th} boson is

$$\nabla_k \phi(\mathbf{r}_k) = -2\alpha(x_k\mathbf{e}_x + y_k\mathbf{e}_y + \beta z_k\mathbf{e}_z)\phi(\mathbf{r}_k), \tag{42}$$

where $\mathbf{e}_x$, $\mathbf{e}_y$ and $\mathbf{e}_z$ are the unit vectors of the three spatial dimensions.

The gradient of the one-body wave function with respect to the k^{th} boson is

$$\begin{aligned}\nabla_k \Psi_{OB}(\mathbf{R}) =& \nabla_k \prod_{i=1}^{N} \phi(\mathbf{r}_i) = \nabla_k \phi(\mathbf{r}_k) \prod_{i\neq k} \phi(\mathbf{r}_i) \\ =& \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \prod_{i=1}^{N} \phi(\mathbf{r}_i) = \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \Psi_{OB}(\mathbf{R}),\end{aligned} \tag{43}$$

where we have used the shorthand notation

$$\prod_{i\neq k} \phi(\mathbf{r}_i) = \left[\prod_{i=1}^{k-1} \phi(\mathbf{r}_i)\right]\left[\prod_{i=k+1}^{N} \phi(\mathbf{r}_i)\right].$$

Moving on to the Laplacian, we start with the Laplacian of $\phi(\mathbf{r}_k)$; this is given by

$$\begin{aligned}\nabla_k^2 \phi(\mathbf{r}_k) =& 4\alpha^2(x_k\mathbf{e}_x + y_k\mathbf{e}_y + \beta z_k\mathbf{e}_z)^2\phi(\mathbf{r}_k) \\ & - 2\alpha(\mathbf{e}_x^2 + \mathbf{e}_y^2 + \beta\mathbf{e}_z^2)\phi(\mathbf{r}_k) \\ =& \left[4\alpha^2(x_k^2 + y_k^2 + \beta^2 z_k^2) - 2\alpha(2+\beta)\right]\phi(\mathbf{r}_k),\end{aligned} \tag{44}$$

where the unit vectors are *orthonormal*.

Letting the Laplacian of the k^{th} boson act on the one-body wave function we get

$$\nabla_k^2 \Psi_{OB}(\mathbf{R}) = \nabla_k^2 \prod_{i=1}^{N} \phi(\mathbf{r}_i) = \frac{\nabla_k^2 \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \Psi_{OB}(\mathbf{R}), \tag{45}$$

where same trick as for the gradient was used.

Lastly, we will look at the derivative with respect to the variational parameter α. We start by finding the expression for $\phi(\mathbf{r})$, given by

$$\frac{\partial \phi(\mathbf{r}_k)}{\partial \alpha} = -(x_k^2 + y_k^2 + \beta z_k^2)\phi(\mathbf{r}_k), \tag{46}$$

which shows that the derivative of the one-body wave function with respect to α must be

$$\frac{\partial \Psi_{OB}(\mathbf{R})}{\partial \alpha} = -\Psi_{OB}(\mathbf{R}) \sum_{k=0}^{N} (x_k^2 + y_k^2 + \beta z_k^2). \tag{47}$$

Next we move on to the correlation factor of the wave function.

2. The Gradients of the Correlation Factor

Before tackling the full correlation factor, we will introduce some useful expressions. Starting with the gradient of the relative distance between two bosons given by

$$\hat{\mathbf{r}}_{ij} \equiv \nabla_i r_{ij} = \frac{\mathbf{r}_i - \mathbf{r}_j}{r_{ij}}. \tag{48}$$

Note the symmetry $r_{ij} = r_{ji}$, which also implies that $\nabla_i r_{ij} = \nabla_j r_{ij}$. We also have that $\nabla_k r_{ij} = 0$ if $k \neq i, j$.

Next we take the gradient of $f(\mathbf{r})$ as given in Eq. 10. By using the chain rule we see that $\nabla_i f(r_{ij}) = f'(r_{ij}) \cdot \nabla_i r_{ij}$, where we have defined

$$f'(r_{ij}) \equiv \frac{\partial f(r_{ij})}{\partial r_{ij}} = \frac{a}{r_{ij}^2}. \tag{49}$$

Using this result we see that the gradient of $f(r_{ij})$ with respect to the i^{th} is given by

$$\nabla_i f(r_{ij}) = \frac{a}{r_{ij}^2} \hat{\mathbf{r}}_{ij}. \tag{50}$$

Lastly, we need the gradient of $u(r_{ij}) = \ln(f(r_{ij}))$. We again use the chain rule to rewrite $\nabla_i u(r_{ij}) = u'(r_{ij}) \cdot \nabla_i r_{ij}$, where we have equivalently defined

$$u'(r_{ij}) \equiv \frac{\partial \ln(f(r_{ij}))}{\partial r_{ij}} = \frac{1}{f(r_{ij})} f'(r_{ij}) = \frac{a}{r_{ij}^2 - a r_{ij}}. \tag{51}$$

We can then easily see that the gradient of $u(r_{ij})$ can be written as

$$\nabla_i u(r_{ij}) = u'(r_{ij}) \cdot \hat{\mathbf{r}}_{ij} = \frac{a}{r_{ij}^2 - a r_{ij}} \hat{\mathbf{r}}_{ij}. \tag{52}$$

We can clearly see that $\nabla_k u(r_{ij}) = 0$ if $k \neq i, j$. Note the symmetry $u(r_{ij}) = u(r_{ji})$ and $\nabla_i u(r_{ij}) = \nabla_j u(r_{ij})$, these will be used shortly.

The gradient of the correlation factor of the wave function with respect to the k^{th} boson is

$$\begin{aligned}
\nabla_k \Psi_C(\mathbf{R}) =& \nabla_k \exp\left(\sum_{i<j} u(r_{ij})\right) \\
=& \left[\nabla_k \sum_{i<j} u(r_{ij})\right] \exp\left(\sum_{i<j} u(r_{ij})\right) \\
=& \left[\sum_{i\neq k} \nabla_k u(r_{ki})\right] \Psi_C(\mathbf{R}) \\
=& \left[a \sum_{i\neq k} \frac{\hat{\mathbf{r}}_{ki}}{r_{ki}(r_{ki} - a)}\right] \Psi_C(\mathbf{R}),
\end{aligned} \tag{53}$$

where the double sum over $i < j$ is reduced to a single sum over i by removing all trivial terms $\nabla_k u(r_{ij})$ when $k \neq i, j$. Included in this leap, the property $\nabla_i u(r_{ij}) = \nabla_j u(r_{ij})$ is also needed. Note the shorthand notation

$$\sum_{i\neq k} u(r_{ki}) = \sum_{i=1}^{k-1} u(r_{ki}) + \sum_{i=k+1}^{N} u(r_{ki}).$$

We then turn our attention to the Laplacian of a single boson. Staring by calculating the Laplacian of the relative distance

$$\nabla_i^2 r_{ij} = \nabla_i \cdot \frac{\mathbf{r}_i - \mathbf{r}_j}{r_{ij}} = \frac{d_r}{r_{ij}} - \frac{r_{ij}^2}{r_{ij}^3} = \frac{d_r - 1}{r_{ij}}, \tag{54}$$

where it bears repeating that d_r is the number of dimensions the coordinates are given in. This means that $\nabla_i^2 r_{ij} = \frac{2}{r_{ij}}$ when $\mathbf{r}$ is given in three dimensions.

Another property that we will need is doubly differentiated $u(r_{ij})$ with respect to r_{ij} which is given by

$$\begin{aligned}
u''(r_{ij}) \equiv& \frac{\partial^2 u(r_{ij})}{\partial r_{ij}^2} = \frac{-a(2r_{ij} - a)}{r_{ij}^2 (r_{ij} - a)^2} \\
=& -u'(r_{ij}) \left(\frac{1}{r_{ij}} + \frac{1}{r_{ij} - a}\right),
\end{aligned} \tag{55}$$

which will be useful when finding the Laplacian of $u(r_{ij})$. The expression for the Laplacian of $u(r_{ij})$ is given by

$$\begin{aligned}
\nabla_i^2 u(r_{ij}) &= \hat{\mathbf{r}}_{ij} \cdot \nabla_i u'(r_{ij}) + u'(r_{ij}) \cdot \nabla_i^2 r_{ij} \\
&= \hat{\mathbf{r}}_{ij} \cdot u''(r_{ij}) \cdot \hat{\mathbf{r}}_{ij} + u'(r_{ij}) \cdot \nabla_i^2 r_{ij} \\
&= u''(r_{ij}) + \frac{d_r - 1}{r_{ij}} u'(r_{ij}),
\end{aligned} \tag{56}$$

where we have used that $\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{r}}_{ij} = 1$ and an excessive amount of the product rule. With this result we are ready to move on to the full correlation factor.

Letting the Laplacian of the k^{th} boson act on the correlation factor of the wave function we get

$$\begin{aligned}
\nabla_k^2 \Psi_C(\mathbf{R}) =& \nabla_k^2 \exp\left(\sum_{i<j} u(r_{ij})\right) \\
=& \left[\left(\sum_{i\neq k} \nabla_k u(r_{ki})\right)^2 + \sum_{i\neq k} \nabla_k^2 u(r_{ki})\right] \Psi_C(\mathbf{R}) \\
=& \left[\sum_{i\neq k} \sum_{j\neq k} \nabla_k u(r_{ki}) \cdot \nabla_k u(r_{kj})\right] \Psi_C(\mathbf{R}) \\
&+ \left[\sum_{i\neq k} \nabla_k^2 u(r_{ki})\right] \Psi_C(\mathbf{R}) \\
=& \left[\sum_{i\neq k} \sum_{j\neq k} u'(r_{ki}) u'(r_{kj}) (\hat{\mathbf{r}}_{ki} \cdot \hat{\mathbf{r}}_{kj})\right] \Psi_C(\mathbf{R}) \\
&+ \left[\sum_{i\neq k} \left(u''(r_{ki}) + \frac{d_r - 1}{r_{ki}} u'(r_{ki})\right)\right] \Psi_C(\mathbf{R}).
\end{aligned} \tag{57}$$

Lastly, we will look at the derivative with respect to the variational parameter α. This is quite trivial as the correlation factor contains no α. We then get

$$\frac{\partial \Psi_C(\mathbf{R})}{\partial \alpha} = 0. \tag{58}$$

We are now ready to take on the gradients of the full wave function.

3. *The Gradients of the Trial Wave Function*

The gradient of the trial wave function becomes trivial to calculate given the gradient of the one-body wave function found in Eq. 43 and the gradient of the correlation factor found in Eq. 53. The gradient with respect to the k^{th} particle is

$$\begin{aligned}
\nabla_k \Psi_T(\mathbf{R}) =& \Psi_{OB}(\mathbf{R}) \nabla_k \Psi_C(\mathbf{R}) + \Psi_C(\mathbf{R}) \nabla_k \Psi_{OB}(\mathbf{R}) \\
=& \left[\sum_{i\neq k} (u'(r_{ki}) \cdot \hat{\mathbf{r}}_{ki}) + \frac{\nabla_k \phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\right] \Psi_T(\mathbf{R}).
\end{aligned} \tag{59}$$

The Laplacian, with respect to the k^{th} boson, of the trial wave function can be found by using the Laplacian of the one-body wave function in Eq. 45 and Laplacian of the correlation factor found in Eq. 57. Using the product rule we get

$$\begin{aligned}\nabla_k^2\Psi_T(\mathbf{R}) =&\Psi_C(\mathbf{R})\nabla_k^2\Psi_{OB}(\mathbf{R}) + \Psi_{OB}(\mathbf{R})\nabla_k^2\Psi_C(\mathbf{R})\\ &+ 2\nabla_k\Psi_{OB}(\mathbf{R})\cdot\nabla_k\Psi_C(\mathbf{R})\\ =&\frac{\nabla_k^2\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\Psi_T(\mathbf{R})\\ &+\left[\sum_{i\neq k}\sum_{j\neq k}u'(r_{ki})u'(r_{kj})(\hat{\mathbf{r}}_{ki}\cdot\hat{\mathbf{r}}_{kj})\right.\\ &\left.+\sum_{i\neq k}\left(u''(r_{ki})+\frac{d_r-1}{r_{ki}}u'(r_{ki})\right)\right]\Psi_T(\mathbf{R})\\ &+2\frac{\nabla_k\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\left[\sum_{i\neq k}u'(r_{ki})\cdot\hat{\mathbf{r}}_{ki}\right]\Psi_T(\mathbf{R}).\end{aligned} \tag{60}$$

Again we end by finding the derivative with respect to the variational parameter α. Using the results from the derivative of the one-body wave function in Eq. 47 and the derivative of the correlation factor in Eq. 58 we get

$$\begin{aligned}\frac{\partial\Psi_T(\mathbf{R})}{\partial\alpha} &= \Psi_C(\mathbf{R})\frac{\partial\Psi_{OB}(\mathbf{R})}{\partial\alpha} + \Psi_{OB}(\mathbf{R})\frac{\partial\Psi_C(\mathbf{R})}{\partial\alpha}\\ &= -\Psi_T(\mathbf{R})\sum_{k=0}^{N}(x_k^2+y_k^2+\beta z_k^2).\end{aligned} \tag{61}$$

Now that the gradients are in place, we turn our attention to the specific case of non-interacting bosons in a spherical trap.

B. Non-Interacting Bosons in a Sperical Trap

For the non-interacting Hamiltonian, $\hat{H}_0$, the corresponding wave function will be $\Psi_{OB}(\mathbf{R})$. Considering only the case of a spherical trap we get $\phi^{\beta=1}(\mathbf{r}_i) \equiv \phi(\alpha,\beta=1,\mathbf{r}) = \exp\{-\alpha r^2\}$, which gives us the wave function

$$\Psi_{OB}^{\beta=1}(\mathbf{R}) \equiv \Psi_{OB}(\alpha,\beta=1,\mathbf{R}) = \prod_{i=1}^{N}\exp\left(-\alpha r_i^2\right).$$

The Hamiltonian for this system will be given by

$$\hat{H}_0 = \frac{1}{2}\sum_{i=1}^{N}\left(-\nabla_i^2 + r_i^2\right), \tag{62}$$

as $\gamma = 1$ in a spherical potential.

1. The Local Energy

The general expression for the local energy is given in Eq. 15. For the calculation of the local energy of the system om non-interaction bosons in a spherical potential, we will need the Laplacian of $\phi^{\beta=1}(\mathbf{r}_i)$, which is given by

$$\nabla_i^2\phi^{\beta=1}(\mathbf{r}_i) = (4\alpha^2 r_i^2 - 2\alpha d_r)\phi^{\beta=1}(\mathbf{r}_i). \tag{63}$$

The local energy of the given system is then

$$\begin{aligned}E_L =&\frac{1}{\Psi_{OB}^{\beta=1}(\mathbf{R})}\hat{H}_0\Psi_{OB}^{\beta=1}(\mathbf{R})\\ =&\frac{1}{2\Psi_{OB}^{\beta=1}(\mathbf{R})}\sum_{i=1}^{N}\left(-\nabla_i^2+r_i^2\right)\Psi_{OB}^{\beta=1}(\mathbf{R})\\ =&\frac{-1}{2\Psi_{OB}^{\beta=1}(\mathbf{R})}\sum_{i=1}^{N}\frac{\nabla_i^2\phi(\mathbf{r}_i)}{\phi(\mathbf{r}_i)}\Psi_{OB}^{\beta=1}(\mathbf{R}) + \frac{1}{2}\sum_{i=1}^{N}r_i^2\\ =&\sum_{i=1}^{N}(\alpha d_r - 2\alpha^2 r_i^2) + \frac{1}{2}\sum_{i=1}^{N}r_i^2\\ =&N\alpha d_r + \left(\frac{1}{2}-2\alpha^2\right)\sum_{i=1}^{N}r_i^2.\end{aligned} \tag{64}$$

In the exact solution of this Schrödinger equation, we have that $\alpha = 1/2$. We then get $E_L = \frac{Nd_r}{2}$.

2. The Drift Force

Additionally, the *drift force* on an arbitrary particle in the given system is defined as the eigenvalue $\mathbf{F}_i$ in the eigenvalue problem

$$\mathbf{F}_i\Psi_{OB}^{\beta=1}(\mathbf{R}) = 2\nabla_i\Psi_{OB}^{\beta=1}(\mathbf{R}). \tag{65}$$

The result from this can be extracted from our earlier calculations of the gradient of the one-body wave function, as given in Eq. 43 combined with the expression for $\nabla_i^2\phi^{\beta=1}(\mathbf{r}_i)$, which is given by

$$\nabla_i\phi^{\beta=1}(\mathbf{r}_i) = -2\alpha\mathbf{r}_i\cdot\phi^{\beta=1}(\mathbf{r}_i). \tag{66}$$

The drift force of the i^{th} particle in a system of non-interacting particles in a spherical potential is then

$$\mathbf{F}_i = -4\alpha\mathbf{r}_i. \tag{67}$$

In the exact solution of this Schrödinger equation, we have that $\alpha = 1/2$. We then get $\mathbf{F}_i = -2\mathbf{r}_i$.

We will now allow interaction between the bosons.

C. Interacting Bosons

Now considering a system of interacting bosons, we will move over to the full Hamiltonian $\hat{H}$ as given in Eq. 7 and use the trial wave function $\Psi_T(\mathbf{R})$. As in the case on non-interacting bosons, we will find the expressions for the local energy and the drift force.

1. The Local Energy

We will start by dividing the Hamiltonian into three parts in the equation for the local energy, such that the local energy is expressed as

$$\begin{aligned}\frac{1}{\Psi_T(\mathbf{R})}\hat{H}\Psi_T(\mathbf{R}) = &\frac{-1}{2\Psi_T(\mathbf{R})}\sum_{i=1}^{N}\nabla_i^2\Psi_T(\mathbf{R}) \\ &+ \frac{1}{\Psi_T(\mathbf{R})}\sum_{i=1}^{N}V_{ext}(\mathbf{r}_i)\Psi_T(\mathbf{R}) \\ &+ \frac{1}{\Psi_T(\mathbf{R})}\sum_{i<j}V_{int}(r_{ij})\Psi_T(\mathbf{R}),\end{aligned} \tag{68}$$

This will allow us to calculate the local energy in a less cluttered fashion.

First is the expression for the second derivative

$$\begin{aligned}\frac{1}{\Psi_T(\mathbf{R})}\nabla_k^2\Psi_T(\mathbf{R}) = &\frac{\nabla_k^2\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} \\ &+ \sum_{i\neq k}\sum_{j\neq k}\frac{(\mathbf{r}_k-\mathbf{r}_i)\cdot(\mathbf{r}_k-\mathbf{r}_j)}{r_{ki}r_{kj}}u'(r_{ki})u'(r_{kj}) \\ &+ \sum_{i\neq k}\left(u''(r_{ki})+\frac{d_r-1}{r_{ki}}u'(r_{ki})\right) \\ &+ 2\frac{\nabla_k\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)}\sum_{i\neq k}\frac{\mathbf{r}_k-\mathbf{r}_i}{r_{ki}}u'(r_{ki}),\end{aligned} \tag{69}$$

where we have taken the result from Eq. 60 where we found the results of the Laplacian of the k^{th} boson acting on the trial wave function, which was a meritorious effort.

The two next terms are quite simple, as both $V_{ext}(\mathbf{r}_i)$ and $V_{int}(r_{ij})$ commute with the wave function. We then get

$$\frac{1}{\Psi_T(\mathbf{R})}V_{ext}(\mathbf{r}_i)\Psi_T(\mathbf{R}) = V_{ext}(\mathbf{r}_i) \tag{70}$$

$$\frac{1}{\Psi_T(\mathbf{R})}V_{int}(r_{ij})\Psi_T(\mathbf{R}) = V_{int}(r_{ij}). \tag{71}$$

So finally, we have our energy eigenvalue for the interacting bosons

$$\begin{aligned}E_L = &\frac{1}{2}\sum_{i=1}^{N}\left[-\frac{1}{\Psi_T(\mathbf{R})}\nabla_i^2\Psi_T(\mathbf{R}) + x_i^2+y_i^2+\gamma^2z_i^2\right] \\ &+ \sum_{i<j}V_{int}(r_{ij}).\end{aligned} \tag{72}$$

Next, we will show the expression for the drift force.

2. The Drift Force

We will now find the drift force of an arbitrary boson, as given in Eq. 25. The drift force of the i^{th} particle in a system of interaction bosons will be

$$\begin{aligned}\mathbf{F}_i = &\frac{2}{\Psi_T(\mathbf{R})}\nabla_i\Psi_T(\mathbf{R}) \\ = &2\frac{\nabla_k\phi(\mathbf{r}_k)}{\phi(\mathbf{r}_k)} + 2\sum_{i\neq k}\left(u'(r_{ki})\cdot\hat{\mathbf{r}}_{ki}\right),\end{aligned} \tag{73}$$

where we have used the results from Eq. 59.