1 Introduction

Since it has been shown that Bose-Einstein condensation occur in gases of alkali atoms confined in magnetic traps, understanding the confined Bose systems has become a popular field. In this project I have tried to calculate the ground state energy of various number of trapped bosons using Variational Monte Carlo calculations with a specific trial wavefunction. Firstly using the spherical harmonic oscillator as a trap with no interaction between the particles, then swtiching to an elliptical trap. Where in both cases I calculate both the analytical and numerical solution. Also running the calculations with and without a repulsive potential due to the fact that bosons have a size.

2 Method

2.1 System

A two-body Hamiltonian of this system is on the form

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

where the external potential for the trap is for the spherical and elliptical part given by

$$V_{ext}(\boldsymbol{r}) = \begin{cases} \frac{1}{2} m\omega^2 r^2 & \text{Spherical} \\ \frac{1}{2} m[\omega^2(x^2+y^2) + \gamma^2 z^2] & \text{Elliptical} \end{cases} \tag{2}$$

where ω is the trap potential strength, and in the elliptical trap γ is the strength in z-direction. The internal potential which represents the repulsion when two boson gets close is

$$V_{int}(|\boldsymbol{r}_i - \boldsymbol{r}_j|) = \begin{cases} \infty & |\boldsymbol{r}_i - \boldsymbol{r}_j| \leq a \\ 0 & |\boldsymbol{r}_i - \boldsymbol{r}_j| > a \end{cases} \tag{3}$$

with a as the hard-core diamater of the bosons. Setting up the system with a trial wavefunction Ψ_T for the ground state of the form

$$\Psi_T(\mathbf{R}) = \Psi_T(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N, \alpha, \beta) = \prod_i g(\alpha, \beta, \mathbf{r}_i) \prod_{i<j} f(a, |\mathbf{r}_i - \mathbf{r}_j|), \tag{4}$$

using α and β as variational parameters, and

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

and

$$f(a, |\mathbf{r}_i - \mathbf{r}_j|) = \begin{cases} 0 & |\mathbf{r}_i - \mathbf{r}_j| \leq a \\ (1 - \frac{a}{|\mathbf{r}_i - \mathbf{r}_j|}) & |\mathbf{r}_i - \mathbf{r}_j| > a. \end{cases} \tag{5}$$

For the simplest cases where I set the boson size $a = 0$ and $\beta = 1$ the trial wavefunction becomes

$$\Psi_T(\boldsymbol{R}) = e^{-\alpha r^2} \tag{6}$$

Calculating the double derivative of the wavefunction returns

$$\nabla^2 \Psi_T = \nabla^2 e^{-\alpha r^2} = \nabla - \alpha 2 r e^{-\alpha r^2} = 2\alpha e^{-\alpha r^2}(2\alpha r^2 - 1) \tag{7}$$

then inserting this result into the expression for the local energy yields

$$E_L(\boldsymbol{R}) = \frac{1}{\Psi_T(\boldsymbol{R})} H \Psi_T(\boldsymbol{R}) = 2\alpha(2\alpha r^2 - 1) \tag{8}$$

which is the analytical experssion for the local energy in a spherical trap without interaction.

2.2 Numerical method

2.2.1 Brute force Metropolis

For the first part I use a Variational Monte Carlo program with a brute force Metropolis sampling to calculate the ground state energy. The Metropolis algorithm compares the probability of being in the old position $A_{j\to i}$ against the probability of being in a position in a chosen direction $A_{i\to j}$.

$$\frac{A_{j\to i}}{A_{i\to j}} = \frac{p_i T_{i\to j}}{p_j T_{j\to i}} \tag{9}$$

where T is the transition probability and p is the probability distribution. Given that the transition probability is independent of direction we are left with the

$$\frac{A_{j\to i}}{A_{i\to j}} = \frac{p_i}{p_j} \tag{10}$$

The Metropolis choice is to maximize the A values so preferring

$$A_{j\to i} = \min\left(1, \frac{p_i}{p_j}\right) \tag{11}$$

This is done by first placing the system in a random, Gaussian distributed position around 0 with a $\sigma = 1/\sqrt{2}$. Evaluating the wavefunction according to equation 8. Then choosing a random particle and dimension, and moving it with a Gaussian distribution to a new position. Do the same evaluation for the new position and comparing

$$\frac{|\Psi_{New}|^2}{|\Psi_{Old}|^2}$$

Then by taking a random, uniformly distributed number between 0 and 1 and compare it to the ratio between the new and old wavefunction. If the ratio is larger I accept the new step, if not I revert back to the old position. Then lastly I sample the energy for the resulting system.

Listing 1: Brute force Metropolis

```
randomMove        = normalDistribution;
waveFunctionOld = my_waveFunction->evaluate();

my_particles[chosenParticle]->changePosition(chosenDimension, randomMove);

waveFunctionNew = my_waveFunction->evaluate();

waveFunctionsCompared = (waveFunctionNew*waveFunctionNew)/
                (waveFunctionOld*waveFunctionOld);

if (waveFunctionsCompared < uniformDistribution{
  my_particles[chosenParticle]->changePosition(chosenDimension, -randomMove);
  return false;
}
return true;
```

When using this method I get the result which is shown in table A.1.1. This result is in exact correspondence to the analytical solution.

2.2.2 Importance sampling

To make the choice of sampling more relevant I use importance sampling. Here there is a biased direction in the new step which is dependent on the trial wavefunction. The new position is given as the solutions to Langevin equation,

$$y = x + DF(x)\Delta t + \xi\sqrt{\Delta t} \tag{12}$$

Here x is the old position, D is the diffusion coefficient, $F(x)$ quantum force and ξ is a normal distributed random variable. The quantum force is given by

$$\mathbf{F} = 2\frac{1}{\Psi_T}\nabla\Psi_T \tag{13}$$

which gives the walker an incentive to go towards areas where the wavefunction is large. The new comparison is now

$$\frac{G(x,y,\Delta t)|\Psi_T(y)|^2}{G(y,x,\Delta t)|\Psi_T(x)|^2} \tag{14}$$

where

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

A Tables

A.1 Brute force Metropolis algorithm

All runs are with with 10^6 cycles and step length of 0.1.

A.1.1 Analytical 1D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	5.000000e-01	0.000000e+00	0.968346	473
10	5.000000e+00	0.000000e+00	0.968118	593
100	5.000000e+01	0.000000e+00	0.968481	1837
500	2.500000e+02	0.000000e+00	0.968320	7329

A.1.2 Analytical 2D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	1.000000e+00	0.000000e+00	0.968367	470
10	1.000000e+01	0.000000e+00	0.967963	711
100	1.000000e+02	0.000000e+00	0.968089	2808
500	5.000000e+02	0.000000e+00	0.968799	12433

A.1.3 Analytical 3D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	1.500000e+00	0.000000e+00	0.968941	484
10	1.500000e+01	0.000000e+00	0.967473	792
100	1.500000e+02	0.000000e+00	0.968197	3623
500	7.500000e+02	0.000000e+00	0.969128	16629

A.1.4 Numerical 1D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	5.000000e-01	3.122502e-14	0.968660	600
10	5.000000e+00	-3.304024e-13	0.968201	2433
100	5.000000e+01	6.593837e-11	0.967691	67993
500	2.500000e+02	3.885361e-09	0.968383	1390252

A.1.5 Numerical 2D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	9.999999e-01	6.494805e-14	0.968163	751
10	9.999999e+00	1.747935e-12	0.968789	5478
100	9.999999e+01	1.618901e-10	0.968061	235928
500	5.000000e+02	2.732850e-08	0.969589	5144598

A.1.6 Numerical 3D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	1.500000e+00	1.509903e-14	0.968088	917
100	1.500000e+02	2.619345e-10	0.967844	415179
100	1.500000e+02	-7.275958e-11	0.968416	413230
500	7.499999e+02	-3.352761e-08	0.969971	9641421

A.2 Metropolis algorithm with Importance sampling

All runs are with with 10^6 cycles and step length of 0.1.

A.2.1 Analytical 1D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	5.000000e-01	0.000000e+00	0.996284	723
10	5.000000e+00	0.000000e+00	0.996449	920
100	5.000000e+01	0.000000e+00	0.996320	2715
500	2.500000e+02	0.000000e+00	0.996494	10450

A.2.2 Analytical 2D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	1.000000e+00	0.000000e+00	0.996363	746
10	1.000000e+01	0.000000e+00	0.996489	1090
100	1.000000e+02	0.000000e+00	0.996347	4204
500	5.000000e+02	0.000000e+00	0.996431	18594

A.2.3 Analytical 3D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	1.500000e+00	0.000000e+00	0.996373	780
10	1.500000e+01	0.000000e+00	0.996321	1198
100	1.500000e+02	0.000000e+00	0.996450	5396
500	7.500000e+02	0.000000e+00	0.996357	24110

A.2.4 Numerical 1D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	4.999999e-01	1.915135e-15	0.996353	839
10	4.999999e+00	-2.351896e-12	0.996342	2724
100	4.999999e+01	3.310561e-10	0.996470	68701
500	2.500000e+02	5.456968e-10	0.996473	1410677

A.2.5 Numerical 2D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	9.999999e-01	2.009504e-14	0.996349	1026
10	9.999999e+00	4.661160e-12	0.996371	6074
100	9.999999e+01	-7.275958e-12	0.996320	228597
500	4.999999e+02	-1.082662e-08	0.996328	5160175

A.2.6 Numerical 3D

N particles	$< E >$	Variance	Accepted	Time [ms]
1	1.500000e+00	1.243450e-13	0.996377	1198
10	1.500000e+01	6.025402e-12	0.996434	9108
100	1.500000e+02	1.615263e-09	0.996397	429843
500	7.499999e+02	-9.709038e-08	0.996334	9671595