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 we 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 we 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

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

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 we 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

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

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 we 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 6. 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 we accept the new step, if not we revert back to the old position. Then lastly we 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 we get the result which is shown in table **??**. This result is in exact correspondence to the analytical solution.

2.2.2 Importance sampling

To make the choice of sampling more relevant we 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

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

2.2.3 Interacting

3 Results

With the brute force Metropolis method and analytical calculation of the wavefunction the results are exactly right, as seen in table for 1 dimension, 10^5 cycles and steplength of 1.7. This gives an accpetance rate of about 50%. With lower step length the acceptance rate would go up, but then the energies would be sampled at a more narrow range and we could not be sure if it is the acutal ground state.

N particles	$< E >$	Variance	Accepted	Time [s]
1	5.000000e-01	0.000000e+00	0.553895	0.018
10	5.000000e+00	0.000000e+00	0.548784	0.024
100	5.000000e+01	0.000000e+00	0.550417	0.075
500	2.500000e+02	0.000000e+00	0.550962	0.312

In table A.1.1 and A.1.2 the runs have been done with the same parameters but with 2 and 3 dimensions. The result is the same with only a slight increase in time for the highest number of particles.

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 2D

N particles	$< E >$	Variance	Accepted	Time [s]
1	1.000000e+00	0.000000e+00	0.548395	0.019
10	1.000000e+01	0.000000e+00	0.549895	0.029
100	1.000000e+02	0.000000e+00	0.551184	0.121
500	5.000000e+02	0.000000e+00	0.551195	0.555

A.1.2 Analytical 3D

N particles	$< E >$	Variance	Accepted	Time [s]
1	1.500000e+00	0.000000e+00	0.550362	0.019
10	1.500000e+01	0.000000e+00	0.553095	0.034
100	1.500000e+02	0.000000e+00	0.549951	0.17
500	7.500000e+02	0.000000e+00	0.543150	0.8

A.1.3 Numerical 1D

N particles	$< E >$	Variance	Accepted	Time [s]
1	5.000000e-01	-9.436896e-16	0.550639	0.023
10	5.000000e+00	-5.115908e-13	0.548139	0.099
100	5.000000e+01	3.092282e-11	0.551551	2.868
500	2.500000e+02	3.419700e-10	0.550273	61.191

A.1.4 Numerical 2D

N particles	$< E >$	Variance	Accepted	Time [s]
1	9.999999e-01	-1.576517e-14	0.549651	0.029
10	9.999999e+00	1.961098e-12	0.551617	0.208
100	9.999999e+01	1.509761e-10	0.552251	10.063
500	5.000000e+02	-5.675247e-09	0.551295	232.441

A.1.5 Numerical 3D

N particles	$< E >$	Variance	Accepted	Time [s]
1	1.500000e+00	6.394885e-14	0.553662	0.035
10	1.500000e+01	3.097966e-12	0.552217	0.364
100	1.500000e+02	-6.184564e-11	0.550728	21.808
500	7.499999e+02	-2.328306e-10	0.546217	517.259

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 [s]
1	5.000000e-01	0.000000e+00	0.998522	0.03
10	5.000000e+00	0.000000e+00	0.998700	0.038
100	5.000000e+01	0.000000e+00	0.998644	0.111
500	2.500000e+02	0.000000e+00	0.998922	0.451

A.2.2 Analytical 2D

N particles	$< E >$	Variance	Accepted	Time [s]
1	1.000000e+00	0.000000e+00	0.998744	0.03
10	1.000000e+01	0.000000e+00	0.998644	0.044
100	1.000000e+02	0.000000e+00	0.998689	0.181
500	5.000000e+02	0.000000e+00	0.998800	0.817

A.2.3 Analytical 3D

N particles	$< E >$	Variance	Accepted	Time [s]
1	1.500000e+00	0.000000e+00	0.998756	0.031
10	1.500000e+01	0.000000e+00	0.998767	0.051
100	1.500000e+02	0.000000e+00	0.998967	0.254
500	7.500000e+02	0.000000e+00	0.998833	1.176

A.2.4 Numerical 1D

N particles	$< E >$	Variance	Accepted	Time [s]
1	4.999999e-01	1.337819e-14	0.998844	0.035
10	4.999999e+00	2.948752e-13	0.998800	0.111
100	4.999999e+01	-2.273737e-11	0.998711	2.907
500	2.500000e+02	1.455192e-10	0.998767	61.364

A.2.5 Numerical 2D

N particles	$< E >$	Variance	Accepted	Time [s]
1	9.999999e-01	1.099121e-14	0.998756	0.041
10	9.999999e+00	6.963319e-13	0.998767	0.223
100	9.999999e+01	2.546585e-11	0.998711	10.117
500	4.999999e+02	-5.587935e-09	0.998789	232.673

A.2.6 Numerical 3D

N particles	$< E >$	Variance	Accepted	Time [s]
1	1.500000e+00	1.332268e-15	0.998767	0.046
10	1.500000e+01	2.131628e-12	0.998833	0.38
100	1.500000e+02	-5.456968e-11	0.998611	21.95
500	7.499999e+02	1.012813e-08	0.998667	517.499