1 Method

The Hamiltonian for the we are using has the following 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 given by the boson trap

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

and a repulsive potential due to bosons interaction given by

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

As for the trial wavefunction for the ground state with N atoms

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

with α, β as variational parameters. The correlation function $f(a, |\mathbf{r}_i - \mathbf{r}_j|)$ is given by

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

Analytical local energy E_L Using natural units and setting the interaction potential to zero and $\beta = 1$, Ψ_T becomes $exp[-\alpha r^2]$. The second derivative will then be

$$\nabla^2 \Psi_T = \nabla^2 e^{-\alpha r^2} = \nabla - \alpha 2 r e^{-\alpha r^2} = \alpha e^{-\alpha r^2} (1 - 2\alpha r^2) \tag{6}$$

Giving us the expression for the local energy

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

A Benchmarks

Benchmarking for 10^6 cycles for analytical and numerical solutions

A.1 Brute force Metropolis algorithm

A.1.1 Analytical

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

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

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.1.2 Numerical

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

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

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

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

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

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

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

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

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