FYS- - Project 1

Fredrik Junker Pedersen

March 13, 2023

Contents

1 Trapped hard sphere Bose gas setup **1**

2 Local energy **2**

2.1 Trial wave function without two-body potential 2

2.2 Trial wave function with two-body potential 3

1 Trapped hard sphere Bose gas setup

The trapped hard sphere Bose gas is a system of N bosons in a trap with a hard core repulsion. The trap we will use is either spherical (S) or elliptical (E) described by the potentials

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

The trial wave function is given by

$$\Psi_T(r) = \Psi_T(r_1, r_2, ..., r_N, \alpha, \beta) = \left[\prod_{i=1} g(\alpha, \beta, r_i)\right]\left[\prod_{j<k} f(a, |r_j - r_k|)\right], \tag{2}$$

where $g(\alpha, \beta, \boldsymbol{r_i})$ is the trial wave function for a single particle in the trap and $f(a, |\boldsymbol{r_j} - \boldsymbol{r_k}|)$ is the correlation wave function for the two-body potential

$$g(\alpha, \beta, \boldsymbol{r_i}) = \exp\big(-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\big), \quad f(a, |\boldsymbol{r_i} - \boldsymbol{r_j}|) = \begin{cases} 0 & \text{if } |\boldsymbol{r_i} - \boldsymbol{r_j}| \le a \\ (1 - \frac{a}{|\boldsymbol{r_i} - \boldsymbol{r_j}|} & \text{if } |\boldsymbol{r_i} - \boldsymbol{r_j}| > a. \end{cases} \tag{3}$$

The Hamiltonian operator H for the system is given by

$$H = \sum_{i=1}^{N}[\frac{-\hbar^2}{2m}\boldsymbol{\nabla}_{\boldsymbol{i}}^2 + V_{ext}(r_i)] + \sum_{i<j}^{N} V_{int}(r_i, r_j). \tag{4}$$

2 Local energy

The local energy is given by

$$E_L(r) = \frac{1}{\Psi_T(r)} H\Psi_T(r), \tag{5}$$

2.1 Trial wave function without two-body potential

The trial wave function without two-body potential is given by

$$\Psi_T(r) = \prod_i \exp\bigl(-\alpha(x_i^2 + y_i^2 + \beta z_i^2)\bigr). \tag{6}$$

Using Equation 5 we find the local energy of a single particle in the trap to be

$$\frac{1}{\exp(-\alpha(x^2 + y^2 + \beta z^2))}\left[\frac{-\hbar^2}{2m} + \boldsymbol{\nabla}^2 + V_{ext}(r)\right]\exp\bigl(-\alpha(x^2 + y^2 + \beta z^2)\bigr).$$

The laplace-operator $\Delta = \boldsymbol{\nabla}^2$ acting on our trial wave function gives

$$\Delta\exp\bigl(-\alpha(x^2 + y^2 + \beta z^2)\bigr) = \exp\bigl(-\alpha(x^2 + y^2 + \beta z^2)\bigr)\left(4\alpha^2(x^2 + y^2 + \beta^2 z^2) - 4\alpha - 2\alpha\beta\right).$$

With the spherical potential in Equation 1 we have

$$V_{ext}(r)\Psi_T(r) = \frac{1}{2}m\omega_{ho}^2(x^2 + y^2 + z^2)\exp\bigl(-\alpha(x^2 + y^2 + \beta z^2)\bigr).$$

The local energy for a single particle in the trap is then given by

$$\begin{aligned}
&\frac{1}{exp(-\alpha(x^2 + y^2 + \beta z^2))}\left[\frac{-\hbar^2}{2m}\nabla^2 + V_{ext}(r)\right]\exp\bigl(-\alpha(x^2 + y^2 + \beta z^2)\bigr) \\
&= \frac{1}{2}m\omega_{ho}^2(x^2 + y^2 + z^2) - \frac{\hbar^2}{4}\omega_{ho}^2\left(4\alpha^2(x^2 + y^2 + \beta^2 z^2) - 4\alpha - 2\alpha\beta\right).
\end{aligned}$$

For spherical traps we have $\beta = 1$ and for non-interacting bosons we have $\alpha = \frac{1}{2}a_{ho}^2$. Inserting these values we find the local energy to be

$$\begin{aligned}
E_L(r) &= \frac{1}{2}m\omega_{ho}^2(x^2 + y^2 + z^2) - \frac{\hbar^2}{4}\omega_{ho}^2\left(a_{ho}^4(x^2 + y^2 + z^2) - 2a_{ho}^2 - a_{ho}^2\right) \\
&= (x^2 + y^2 + z^2)\left(\frac{1}{2}m\omega_{ho}^2 - \frac{\hbar^2}{4}\omega_{ho}^2 a_{ho}^4\right) - 3a_{ho}^2 \\
&= r^2\left(\frac{1}{2}m\omega_{ho}^2 - \frac{\hbar^2}{4}\omega_{ho}^2 a_{ho}^4\right) - 3a_{ho}^2.
\end{aligned}$$

We observe the local energy to be symmetric around the origin such that it is only dependent on the length r of the position vector $\boldsymbol{r}$.

For N particles in the same potential, the trial wave function is given by Equation 6 with $\beta = 1$ and $\alpha = \frac{1}{2}a_{ho}^2$. This may be written as

$$\Psi_T(r) = \exp\left(-\alpha\sum_{i=1}^{N}(x_i^2 + y_i^2 + z_i^2)\right).$$

The laplace-operator acting on the new wavefunction gives

$$\sum_{i=1}^{N} \Delta_i \exp\big(-\alpha(x_i^2+y_i^2+z_i^2)\big) = \exp\left(-\alpha \sum_{i=1}^{N}(x_i^2+y_i^2+z_i^2)\right)\left(4\alpha^2 \sum_{i=1}^{N}(x_i^2+y_i^2+z_i^2) - 4\alpha N - 2\alpha N\right).$$

The drift force to be used in importance sampling is given by

$$F = \frac{2\nabla\Psi_T}{\Psi_T} = \frac{2\exp\big(-\alpha(x_i^2+y_i^2+z_i^2)\big)(-2\alpha\boldsymbol{r_i})}{\exp(-\alpha(x_i^2+y_i^2+z_i^2))} = -4\alpha\boldsymbol{r_i}.$$

2.2 Trial wave function with two-body potential

We will assume multiple bosons interact pairwise with each other in elastic collisions represented by the hard-sphere potential

$$V_{int}(|\boldsymbol{r_i}-\boldsymbol{r_j}|) = \begin{matrix} \infty & \text{if } |\boldsymbol{r_i}-\boldsymbol{r_j}| \le a \\ 0 & \text{else} \end{matrix} \tag{7}$$

The trial wave function of a system of bosons is given by

$$\Psi_T(r) = \left(\prod_i g(\alpha,\beta,\boldsymbol{r_i})\right)\prod_{j<k} f(a,|\boldsymbol{r_j}-\boldsymbol{r_k}|). \tag{8}$$

Defining the quantities

$$\begin{aligned} r_{ij} &= |\boldsymbol{r_i}-\boldsymbol{r_j}|, \\ ø(\boldsymbol{r_i}) &= \mathrm{g}(\alpha,\beta,\boldsymbol{r_i}) \quad \text{and} \\ u(r_{ij}) &= \ln(f(r_{ij})), \end{aligned} \tag{9}$$

we rewrite the trial wave function as

$$\Psi_T(r) = \left(\prod_i ø(\boldsymbol{r_i})\right)\exp\left(\sum_{j<k} u(r_{jk})\right),$$

where

$$\sum_{i<j}^{N} X_{ij} \equiv \sum_{i=1}^{N}\sum_{j=i+1}^{N} X_{ij}.$$

Using the product rule, we find the first derivative of particle k to be

$$\begin{aligned} \nabla_k\Psi_T(\boldsymbol{r}) &= \nabla_k ø(\boldsymbol{r_k})\prod_{i\neq k} ø(\boldsymbol{r_i})\exp\left(\sum_{j<m} u(r_{jm})\right) + \prod_i ø(\boldsymbol{r_i})\nabla_k \exp\left(\sum_{j<m} u(r_{jm})\right) \\ &= \nabla_k ø(\boldsymbol{r_k})\prod_{i\neq k} ø(\boldsymbol{r_i})\exp\left(\sum_{j<m} u(r_{jm})\right) + \prod_i ø(\boldsymbol{r_i})\exp\left(\sum_{j<m} u(r_{jm})\right)\nabla_k\sum_{j<m} u(r_{jm}) \\ &= \nabla_k ø(\boldsymbol{r_k})\prod_{i\neq k} ø(\boldsymbol{r_i})\exp\left(\sum_{j<m} u(r_{jm})\right) + \prod_i ø(\boldsymbol{r_i})\exp\left(\sum_{j<m} u(r_{jm})\right)\sum_{l\neq k}\nabla_k u(r_{kl}). \end{aligned}$$

Applying the gradient again using the product rule, we find the laplace-operator acting on the trial wave function to be

$$\Delta_k \Psi_T(\boldsymbol{r}) = \Delta_k \o(\boldsymbol{r_k}) \prod_{i\neq k} \o(\boldsymbol{r_i}) \exp\left(\sum_{j<m} u(r_{jm})\right) + \boldsymbol{\nabla}_k \o(\boldsymbol{r_k}) \prod_{i\neq k} \o(\boldsymbol{r_i}) \exp\left(\sum_{j<m} u(r_{jm})\right) \sum_{l\neq k} \boldsymbol{\nabla}_k u(r_{kl})$$

$$+\boldsymbol{\nabla}_k \o(\boldsymbol{r_k}) \prod_{i\neq k} \o(\boldsymbol{r_i}) \exp\left(\sum_{j<m} u(r_{jm})\right) \sum_{l\neq k} \boldsymbol{\nabla}_k u(r_{kl}) + \prod_{i} \o(\boldsymbol{r_i}) \exp\left(\sum_{j<m} u(r_{jm})\right) \sum_{j\neq k} \boldsymbol{\nabla}_k u(r_{kj}) \sum_{l\neq k} \boldsymbol{\nabla}_k u(r_{kl})$$

$$+ \prod_{i} \o(\boldsymbol{r_i}) \exp\left(\sum_{j<m} u(r_{jm})\right) \sum_{i\neq k} \boldsymbol{\nabla_k^2} u(r_{ki}).$$

Dividing this expression with the trial wave function, we get

$$\frac{\Delta_k \Psi_T(\boldsymbol{r})}{\Psi_T(\boldsymbol{r})}$$

$$= \Delta_k \o(\boldsymbol{r_k}) \frac{1}{\o(\boldsymbol{r_k})} + \boldsymbol{\nabla}_k \o(\boldsymbol{r_k}) \frac{1}{\o(\boldsymbol{r_k})} \sum_{l\neq k} \boldsymbol{\nabla}_k u(r_{kl})$$

$$+\boldsymbol{\nabla}_k \o(r_k) \frac{1}{\o(\boldsymbol{r_k})} \sum_{l\neq k} \boldsymbol{\nabla}_k u(r_{kl}) + \sum_{j\neq k} \boldsymbol{\nabla}_k u(r_{kj}) \sum_{l\neq k} \boldsymbol{\nabla}_k u(r_{kl}) + \sum_{i\neq k} \boldsymbol{\nabla}_k^2 u(r_{ki})$$

$$= \Delta_k \o(\boldsymbol{r_k}) \frac{1}{\o(\boldsymbol{r_k})} + \boldsymbol{\nabla}_k \o(\boldsymbol{r_k}) \frac{1}{\o(\boldsymbol{r_k})} \sum_{l\neq k} u'(r_{kl}) \boldsymbol{\nabla}_k r_{kl}$$

$$+\boldsymbol{\nabla}_k \o(r_k) \frac{1}{\o(\boldsymbol{r_k})} \sum_{l\neq k} u'(r_{kl}) \boldsymbol{\nabla}_k r_{kl} + \sum_{j\neq k} u'(r_{kj}) \boldsymbol{\nabla}_k r_{kj} \sum_{l\neq k} u'(r_{kl}) \boldsymbol{\nabla}_k r_{kl} + \sum_{i\neq k} \left(u''(r_{ki})(\boldsymbol{\nabla}_k r_{ki})^2 + u'(r_{ki}) \boldsymbol{\nabla}^2 r_{ki}\right).$$

By the definition of r_{ij} in Equation 9, we find

$$\sum_{l\neq k} \boldsymbol{\nabla}_k r_{kl} = \sum_{l\neq k} \boldsymbol{\nabla}_k |\boldsymbol{r_k} - \boldsymbol{r_l}| = \sum_{l\neq k} \frac{1}{2|\boldsymbol{r_k} - \boldsymbol{r_l}|} 2(\boldsymbol{r_k} - \boldsymbol{r_l})$$

$$= \sum_{l\neq k} \frac{\boldsymbol{r_k} - \boldsymbol{r_l}}{r_{kl}}, \quad \text{and}$$

$$\sum_{l\neq k} \boldsymbol{\nabla}_k^2 r_{kl} = \sum_{l\neq k} \left(\frac{3r_{kl} - (\boldsymbol{r_k} - \boldsymbol{r_l}) \frac{1}{2r_{kl}} 2(\boldsymbol{r_k} - \boldsymbol{r_l})}{r_{kl}^2}\right)$$

$$= \sum_{l\neq k} \frac{2}{r_{kl}},$$

such that

$$
\begin{aligned}
&\frac{\Delta_k \Psi_T(\boldsymbol{r})}{\Psi_T(\boldsymbol{r})} = \\
&= \frac{\boldsymbol{\nabla}^2 \o(\boldsymbol{r_k})}{\o(\boldsymbol{r_k})} + 2\frac{\boldsymbol{\nabla}_k \o(\boldsymbol{r_k})}{\o(\boldsymbol{r}_k)} \sum_{l\neq k} u'(r_{kl}) \frac{\boldsymbol{r_k} - \boldsymbol{r_l}}{r_{kl}} + \sum_{j\neq k} u'(r_{kj}) \frac{\boldsymbol{r_k} - \boldsymbol{r_j}}{r_{kj}} \sum_{l\neq k} u'(r_{kl}) \\
&\quad \frac{\boldsymbol{r_k} - \boldsymbol{r_l}}{r_{kl}} + \sum_{i\neq k} \left[u''(r_{kl}) \left(\frac{\boldsymbol{r_k} - \boldsymbol{r_l}}{r_{kl}} \right)^2 + \frac{2}{r_{kl}} u'(r_{kl}) \right] \\
&= \frac{\boldsymbol{\nabla}^2 \o(\boldsymbol{r_k})}{\o(\boldsymbol{r_k})} + 2\frac{\boldsymbol{\nabla}_k \o(\boldsymbol{r_k})}{\o(\boldsymbol{r}_k)} \sum_{l\neq k} u'(r_{kl}) \frac{\boldsymbol{r_k} - \boldsymbol{r_l}}{r_{kl}} + \sum_{j\neq k} \sum_{l\neq k} u'(r_{kl}) u'(r_{kj}) \frac{(\boldsymbol{r_k} - \boldsymbol{r_j})(\boldsymbol{r_k} - \boldsymbol{r_l})}{r_{kj} r_{kl}} \\
&\quad + \sum_{i\neq k} \left[u''(r_{ki}) + \frac{2}{r_{ki}} u'(r_{ki}) \right].
\end{aligned}
$$

Remembering the definitions from Equation 9 and Equation 3, we have

$$
\o(\boldsymbol{r_i}) = \exp\left(-\alpha \boldsymbol{r_i}^2\right), \quad \text{and} \quad u(r_{kl}) = \ln\left(1 - \frac{a}{r_{kl}}\right),
$$

such that

$$
\begin{aligned}
\boldsymbol{\nabla}_k \o(\boldsymbol{r_k}) &= -2\alpha \exp\left(-\alpha \boldsymbol{r_k}^2\right) \boldsymbol{r_k}, \\
\boldsymbol{\nabla}_k^2 \o(\boldsymbol{r}_k) &= 4\alpha^2 \exp\left(-\alpha \boldsymbol{r_k}^2\right) \boldsymbol{r_k}^2 - 2\alpha \exp\left(-\alpha \boldsymbol{r_k}^2\right) 3 = \exp\left(-\alpha \boldsymbol{r_k}^2\right)(4\alpha^2 \boldsymbol{r_k}^2 - 6\alpha), \\
u'(r_{kl}) &= \frac{\partial \ln(f(r_{kl}))}{\partial r_{kl}} = \frac{a}{r_{kl}^2 - a r_{kl}}, \\
u''(r_{kl}) &= \frac{a^2 - 2a r_{kl}}{(r_{kl}^2 - a r_{kl})^2}.
\end{aligned}
$$

Inserting these into the above equation, we find

$$
\begin{aligned}
\frac{\Delta_k \Psi_T(\boldsymbol{r})}{\Psi_T} &= \frac{\exp\left(-\alpha \boldsymbol{r_k}^2\right)(4\alpha^2 \boldsymbol{r_k}^2 - 6\alpha)}{\exp(-\alpha \boldsymbol{r_k}^2)} + 2\frac{-2\alpha \exp\left(-\alpha \boldsymbol{r_k}^2\right) \boldsymbol{r_k}}{\exp(-\alpha \boldsymbol{r_k}^2)} \sum_{l\neq k} \frac{a}{r_{kl}^2 - a r_{kl}} \frac{\boldsymbol{r_k} - \boldsymbol{r_l}}{r_{kl}} \\
&\quad + \sum_{j\neq k} \sum_{l\neq k} \frac{a}{r_{kl}^2 - a r_{kl}} \frac{a}{r_{kj}^2 - a r_{kj}} \frac{(\boldsymbol{r_k} - \boldsymbol{r_j})(\boldsymbol{r_k} - \boldsymbol{r_l})}{r_{kj} r_{kl}} \\
&\quad + \sum_{i\neq k} \left[\frac{a^2 - 2a r_{ki}}{(r_{ki}^2 - a r_{ki})^2} + \frac{2a}{r_{ki}^3 - a r_{ki}^2} \right] \\
&= 4\alpha^2 \boldsymbol{r_k}^2 - 6\alpha - 4\alpha \boldsymbol{r_k} \sum_{l\neq k} \frac{\boldsymbol{r_k} - \boldsymbol{r_l}}{\frac{r_{kl}^3}{a} - r_{kl}^2} + \sum_{j\neq k} \sum_{l\neq k} \frac{a^2 (\boldsymbol{r_k} - \boldsymbol{r_j})(\boldsymbol{r_k} - \boldsymbol{r_l})}{(r_{kl}^2 - a r_{kl})(r_{kj}^2 - a r_{kj})(r_{kl} r_{kj})} \\
&\quad + \sum_{i\neq k} \left[\frac{a^2 - 2a r_{ki}}{(r_{ki}^2 - a r_{ki})^2} + \frac{2a}{r_{ki}^3 - a r_{ki}^2} \right].
\end{aligned}
$$