FYS- - Project 1

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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

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

The Hamiltonian operator H for the system is given by

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

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

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

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

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

2.2 Trial wave function with two-body potential

The trial wave function with two-body potential is given by

$$\Psi_T(r) = \left(\prod_i g(\alpha,\beta,\boldsymbol{r_i})\right)\prod_{j<k} f(a,|\boldsymbol{r_j}-\boldsymbol{r_k}|). \tag{7}$$

Defining the quantities

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

we rewrite the trial wave function as

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

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

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

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

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

Dividing this expression with the trial wave function, we get

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

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

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

$$= \frac{\boldsymbol{\nabla}^2 \o(\boldsymbol{r_k})}{\o(\boldsymbol{r_k})} + 2 \frac{\boldsymbol{\nabla}_k \o(\boldsymbol{r_k})}{\o(\boldsymbol{r}_k)} \sum_{l \neq k} \boldsymbol{\nabla}_k u(r_{kl})$$