Project 1 a)

The (position representation of the) Hamiltonian of this problem is given by

$$H = \sum_{i}^{N}\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2 + V_{\text{ext}}(\mathbf{r}_i)\right] + \sum_{j<k}^{N} V_{\text{int}}(|\mathbf{r}_j - \mathbf{r}_k|)$$

where

$$V_{\text{ext}}(\mathbf{r}_i) = \begin{cases} \frac{1}{2}m\omega_{\text{ho}}^2 r_i^2 & (S) \\ \frac{1}{2}m\omega_{\text{ho}}^2\left(x_i^2 + y_i^2\right) + \frac{1}{2}m\omega_z^2 z^2 & (E) \end{cases}$$

and

$$V_{\text{int}}(|\mathbf{r}_j - \mathbf{r}_k|) = \begin{cases} \infty & |\mathbf{r}_j - \mathbf{r}_k| \leq a \\ 0 & |\mathbf{r}_j - \mathbf{r}_k| > a \end{cases}$$

The trial wavefunction is

$$\psi_T(\mathbf{R}) \propto \left[\prod_{l}^{N} g(\alpha, \beta, \mathbf{r}_l)\right]\left[\prod_{m<n}^{N} f(a, |\mathbf{r}_m - \mathbf{r}_n|)\right]$$

where

$$g(\alpha, \beta, \mathbf{r}_l) = \exp\left\{-\alpha\left(x_l^2 + y_l^2 + \beta z_l^2\right)\right\}$$

and

$$f(a, |\mathbf{r}_m - \mathbf{r}_n|) = \begin{cases} 0 & |\mathbf{r}_m - \mathbf{r}_n| \leq a \\ 1 - \dfrac{a}{|\mathbf{r}_m - \mathbf{r}_n|} & |\mathbf{r}_m - \mathbf{r}_n| > a \end{cases}$$

Task: Set $a = 0,\ \beta = 1$ and find the local energy

$$E_L(\mathbf{R}) = \frac{1}{\psi_T(\mathbf{R})} H\psi_T(\mathbf{R})$$

Solution:

Setting $a = 0$ results in $f = 1$ and $V_{\text{int}} = 0$. The trial wave function is given by

$$\psi_T(\mathbf{R}) \propto \left[\prod_l^N g(\alpha, \beta, \mathbf{r}_l)\right] = \prod_l^N \exp\left\{-\alpha\left(x_l^2 + y_l^2 + z_l^2\right)\right\}$$

Differentiating once with respect to the x_i-coordinate.

$$\frac{\partial}{\partial x_i}\psi_T(\mathbf{R}) \propto -2\alpha x_i \prod_l^N \exp\left\{-\alpha\left(x_l^2 + y_l^2 + z_l^2\right)\right\} = -2\alpha x_i \psi_T(\mathbf{R})$$

And once more

$$\frac{\partial^2}{\partial x_i^2}\psi_T(\mathbf{R}) \propto -2\alpha\psi_T(\mathbf{R}) + 4\alpha^2 x_i^2 \psi_T(\mathbf{R})$$

The Laplacian of $\psi_T(\mathbf{R})$ with respect to the coordinates of the i-th particle is thus given by

$$\nabla_i^2 \psi_T(\mathbf{R}) \propto -6\alpha\psi_T(\mathbf{R}) + 4\alpha^2\left(x_i^2 + y_i^2 + z_i^2\right)\psi_T(\mathbf{R})$$

The Hamiltonian is given by

$$H = \sum_i^N \left[-\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}m\omega_{\text{ho}}^2\left(x_i^2 + y_i^2\right) + \frac{1}{2}m\omega_z^2 z^2\right]$$

The local energy is thus

$$E_L(\mathbf{R}) = \frac{1}{\psi_T(\mathbf{R})} H\psi_T(\mathbf{R}) = \sum_i^N \left\{ -\frac{\hbar^2}{2m}\left[-6\alpha + 4\alpha^2\left(x_i^2 + y_i^2 + z_i^2\right)\right] + \frac{1}{2}m\omega_{\text{ho}}^2\left(x_i^2 + y_i^2\right) + \frac{1}{2}m\omega_z^2 z^2 \right\}$$

$$= \sum_i^N \left[\frac{3\hbar^2\alpha}{m} - \frac{2\hbar^2\alpha^2}{m}\left(x_i^2 + y_i^2 + z_i^2\right) + \frac{1}{2}m\omega_{\text{ho}}^2\left(x_i^2 + y_i^2\right) + \frac{1}{2}m\omega_z^2 z^2\right]$$

In the special (spherical) case where $\omega_z = \omega_{\text{ho}}$ we have

$$E_L(\mathbf{R}) = \sum_i^N \left[\frac{3\hbar^2\alpha}{m} - \frac{2\hbar^2\alpha^2}{m} r_i^2 + \frac{1}{2}m\omega_{\text{ho}}^2 r_i^2\right]$$

Verification: The energy eigenvalues of the 3-dimensional harmonic oscillator Hamiltonian is

$$E_{n_x,n_y,n_z} = \hbar\omega_{\text{ho}}\left(n_x + \frac{1}{2}\right) + \hbar\omega_{\text{ho}}\left(n_y + \frac{1}{2}\right) + \hbar\omega_{\text{ho}}\left(n_z + \frac{1}{2}\right)$$

The ground state is thus

$$E_0 = \frac{3}{2}\hbar\omega_{\text{ho}}$$

The correct value of the parameter α is given in the project text as $\alpha = 1 \,/\, 2a_{\text{ho}}^2$ with $a_{\text{ho}}^2 = \hbar \,/\, m\omega_{\text{ho}}$. Inserting this into the expression for the local energy:

$$E_L(\mathbf{R}) = \sum_i^N \left[\frac{3\hbar^2}{m} \cdot \frac{1}{2a_{\text{ho}}^2} - \frac{2\hbar^2}{m} \cdot \frac{1}{4a_{\text{ho}}^4} \cdot r_i^2 + \frac{1}{2}m\omega_{\text{ho}}^2 r_i^2\right]$$

$$= \sum_i^N \left[\frac{3\hbar^2}{m} \cdot \frac{m\omega_{\text{ho}}}{2\hbar} - \frac{2\hbar^2}{m} \cdot \frac{m^2\omega_{\text{ho}}^2}{4\hbar^2} \cdot r_i^2 + \frac{1}{2}m\omega_{\text{ho}}^2 r_i^2\right] = \sum_i^N \left[\frac{3\hbar\omega_{\text{ho}}}{2} - \frac{m\omega_{\text{ho}}^2}{2} r_i^2 + \frac{1}{2}m\omega_{\text{ho}}^2 r_i^2\right]$$

$$= \sum_{i}^{N} \frac{3\hbar\omega_{\mathrm{ho}}}{2} = NE_0$$