

Project 1 a)

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

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

where

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

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

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

and

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

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

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

Differentiating once with respect to the x_i -coordinate.

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

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

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

The Hamiltonian is given by

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

The local energy is thus

$$\begin{aligned}
E_L(\mathbf{R}) &= \frac{1}{\psi_T(\mathbf{R})} H \psi_T(\mathbf{R}) = \sum_i^N \left\{ -\frac{\hbar^2}{2m} \left[-6\alpha + 4\alpha^2 (x_i^2 + y_i^2 + z_i^2) \right] + \frac{1}{2} m \omega_{\text{ho}}^2 (x_i^2 + y_i^2) + \frac{1}{2} m \omega_z^2 z^2 \right\} \\
&= \sum_i^N \left[\frac{3\hbar^2 \alpha}{m} - \frac{2\hbar^2 \alpha^2}{m} (x_i^2 + y_i^2 + z_i^2) + \frac{1}{2} m \omega_{\text{ho}}^2 (x_i^2 + y_i^2) + \frac{1}{2} m \omega_z^2 z^2 \right]
\end{aligned}$$

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

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