

We know that the eigenstates of the 1D SHO are given by

$$\psi_n(x) = \left(\frac{1}{\pi x_0^2}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\frac{x}{x_0}\right) e^{-x^2/2x_0^2}, \text{ where } H_n = \text{polynomial of degree } n.$$

In 3D, separation of variables shows that the eigenstates of a 3D SHO

$$\text{are given by } \psi_{n_x n_y n_z}(x, y, z) = \psi_{n_x}(x) \psi_{n_y}(y) \psi_{n_z}(z) \text{ w/ energy } E_{n_x} + E_{n_y} + E_{n_z}.$$

Thus, the ground state of the SHO is given by

$$\psi_{000}(x, y, z) = \psi_0(x) \psi_0(y) \psi_0(z), \text{ w/ } \psi_0(x) = \left(\frac{1}{\pi x_0^2}\right)^{1/4} e^{-x^2/2x_0^2}$$

We need to calculate the first order correction due to  $\frac{U^2}{\hbar\omega} x^2 y^2 z^2$

and the first and second order corrections due to  $Uxyz$ . This will give us answers to 2nd order in  $U$ .

$$E_0^{(1)} = \langle \psi_{000} | Uxyz + \frac{U^2}{\hbar\omega} x^2 y^2 z^2 | \psi_{000} \rangle = U \langle \psi_{000} | xyz | \psi_{000} \rangle + \frac{U^2}{\hbar\omega} \langle \psi_{000} | x^2 y^2 z^2 | \psi_{000} \rangle$$

$$\textcircled{1} = \int dx \int dy \int dz \psi_0^*(x) \psi_0^*(y) \psi_0^*(z) xyz \psi_0(x) \psi_0(y) \psi_0(z)$$

$$= \int dx \psi_0^*(x) x \psi_0(x) \int dy \psi_0^*(y) y \psi_0(y) \int dz \psi_0^*(z) z \psi_0(z)$$

$$= \left( \int dx \psi_0^*(x) x \psi_0(x) \right)^3$$

$$= \left( \frac{1}{x_0 \sqrt{\pi}} \int_{-\infty}^{\infty} x e^{-x^2/x_0^2} dx \right)^3$$

$$= 0$$

$$\textcircled{2} = \int dx \psi_0^*(x) x^2 \psi_0(x) \int dy \psi_0^*(y) y^2 \psi_0(y) \int dz \psi_0^*(z) z^2 \psi_0(z)$$

$$= \left( \int dx \psi_0^*(x) x^2 \psi_0(x) \right)^3$$

$$= \left( \frac{1}{x_0 \sqrt{\pi}} \int_{-\infty}^{\infty} x^2 e^{-x^2/x_0^2} dx \right)^3$$

$$= \left( \frac{x_0^2}{2} \right)^3$$

$$\text{So } E_0^{(1)} = \frac{U^2}{\hbar\omega} \left( \frac{x_0^2}{2} \right)^3 = \frac{U^2 x_0^6}{8\hbar\omega}$$

The second-order piece is given by

$$E_{000}^{(2)} = \sum_{n_x n_y n_z > 0} \frac{|\langle \Psi_{n_x n_y n_z} | U_{xyz} | \Psi_{000} \rangle|^2}{E_{000} - E_{n_x n_y n_z}}$$

This seems bad. It looks like we have to do an infinite number of brackets. But actually, they are all zero except one.

Let's manipulate the expression for the bracket a little

$$\begin{aligned} \langle \Psi_{n_x n_y n_z} | xyz | \Psi_{000} \rangle &= \int \Psi_{n_x}^*(x) x \Psi_0(x) dx \int \Psi_{n_y}^*(y) y \Psi_0(y) dy \int \Psi_{n_z}^*(z) z \Psi_0(z) dz \\ &= \langle \Psi_{n_x} | \hat{x} | \Psi_0 \rangle \langle \Psi_{n_y} | \hat{x} | \Psi_0 \rangle \langle \Psi_{n_z} | \hat{x} | \Psi_0 \rangle \end{aligned}$$

We know that  $\Psi_0(x) = (\text{degree } 0 \text{ poly}) e^{-x^2/2x_0^2}$  and  $\Psi_1(x) = (\text{degree } 1 \text{ poly}) e^{-x^2/2x_0^2}$ .

Using linear combinations of  $\Psi_0$  and  $\Psi_1$ , then, we can form any function that looks like (degree 1 poly)  $e^{-x^2/2x_0^2}$ . In particular,  $x\Psi_0(x)$  can be written as a linear combination of  $\Psi_0$  &  $\Psi_1$ .

We know  $\Psi_0(x) = \left(\frac{1}{\pi x_0^2}\right)^{1/4} e^{-x^2/x_0^2}$ , and  $\Psi_1(x) = \left(\frac{1}{\pi x_0^2}\right)^{1/4} \frac{x}{x_0} e^{-x^2/x_0^2}$

Thus,  $x\Psi_0(x) = \frac{x_0}{\sqrt{2}} \Psi_1(x)$ . We then find

$$\begin{aligned} \langle \Psi_{n_x n_y n_z} | xyz | \Psi_{000} \rangle &= \langle \Psi_{n_x} | \hat{x} | \Psi_0 \rangle \langle \Psi_{n_y} | \hat{x} | \Psi_0 \rangle \langle \Psi_{n_z} | \hat{x} | \Psi_0 \rangle \\ &= \frac{x_0^3}{2^{3/2}} \langle \Psi_{n_x} | \Psi_1 \rangle \langle \Psi_{n_y} | \Psi_1 \rangle \langle \Psi_{n_z} | \Psi_1 \rangle \\ &= \begin{cases} x_0^3/2^{3/2} & \text{if } n_x = n_y = n_z = 1 \\ 0 & \text{else} \end{cases} \end{aligned}$$

Thus,  $E_{000}^{(2)} = \frac{|\langle \Psi_{111} | U_{xyz} | \Psi_{000} \rangle|^2}{E_{000} - E_{111}}$ . Note  $E_{000} = \frac{3}{2} \hbar \omega$ ,  $E_{111} = \frac{9}{2} \hbar \omega$

$$E_{000}^{(2)} = \frac{\frac{U^2 x_0^6}{-3 \hbar \omega}}{\frac{3}{2} \hbar \omega - \frac{9}{2} \hbar \omega} = \frac{U^2 x_0^6}{2^3} \frac{1}{\frac{3}{2} \hbar \omega - \frac{9}{2} \hbar \omega} = -\frac{U^2 x_0^6}{24 \hbar \omega}$$

Thus, in total, the change in energy is

$$\delta E = \frac{U^2 x_0^6}{\hbar \omega} \left( \frac{1}{8} - \frac{1}{24} \right) = \frac{U^2 x_0^6}{12 \hbar \omega}$$