Quiz 7.5 – Vibrational Motion

Name: Key

Harmonic Oscillator

O_2 vibrations can me modeled as a quantum mechanical harmonic oscillator with reduced mass equal to $8.0\ AMU$ and a force constant of $1138\frac{N}{m}$. Give the fundamental angular frequency (ω), fundamental linear frequency (ν), and zero-point energy for oxygen vibrations.

$$\omega = \sqrt{\frac{k_f}{m}} = \sqrt{\frac{1138\ \frac{N}{m}}{8.0\ AMU\ \frac{1g}{6.022 \cdot 10^{23}\ AMU}\ \frac{1\ kg}{1000g}}} = 2.93 \cdot 10^{14}\ s^{-1}$$

$$\nu = \frac{\omega}{2\pi} = 4.66 \cdot 10^{13}\ s^{-1}$$

$$ZPE = \frac{1}{2}\hbar\omega = \frac{1}{2} \cdot 1.05 \cdot 10^{-34}\ J{\cdot}s \cdot 2.93 \cdot 10^{14}\ s^{-1} = 1.54 \cdot 10^{-20}\ J$$

Write the wavefunction for the first three states of a harmonic oscillator. You may use generic symbols for N and α, but you must expand the Hermite polynomials.

$$\psi_0 = N_0 e^{-\frac{x^2}{2\alpha^2}}$$

$$\psi_1 = N_1 \frac{2x}{\alpha} e^{-\frac{x^2}{2\alpha^2}}$$

$$\psi_2 = N_2 \left(4\frac{x^2}{\alpha^2} - 2\right) e^{-\frac{x^2}{2\alpha^2}}$$

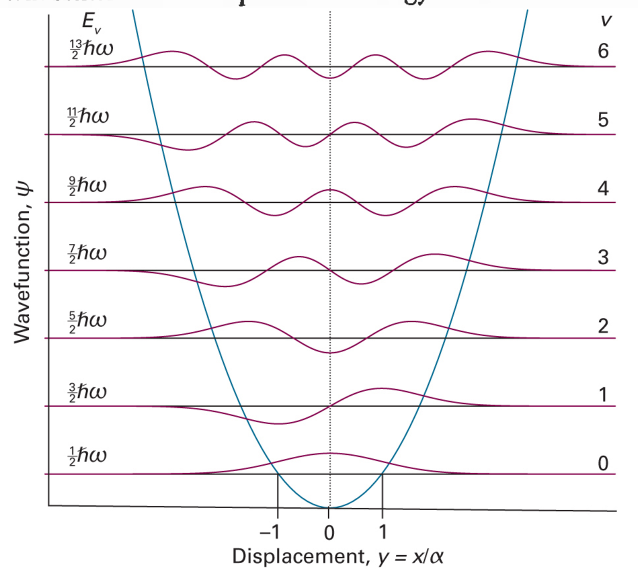
Give the energies of these three states, and sketch their wavefunctions on a potential energy curve.

$$E_v = (v+\tfrac{1}{2})\hbar\omega \quad \text{-or-} \quad E_v = (v+\tfrac{1}{2})h\nu$$

$$E_0 = \tfrac{1}{2}\hbar\omega = 1.54\cdot 10^{-20}\ J$$

$$E_1 = \tfrac{3}{2}\hbar\omega = 4.61\cdot 10^{-20}\ J$$

$$E_2 = \tfrac{5}{2}\hbar\omega = 7.69\cdot 10^{-20}\ J$$



Give the classical maximum displacement for each of these three states, both in pm and in % of the equilibrium O_2 bond length (121 pm)

Max displacement when $E = V(x) = \frac{1}{2}kx^2 \rightarrow x = \sqrt{\frac{2E}{k}}$

$$x_0 = \sqrt{\frac{2\cdot 1.54\cdot 10^{-20}\ J}{1138\ N/m}} = 5.20\cdot 10^{-12}\ m \quad (\text{FYI, this} = \alpha)$$

$$\frac{x_0}{121\ pm}\cdot 100\% = 4.30\%$$

$$x_1 = \sqrt{\frac{2\cdot 4.61\cdot 10^{-20}\ J}{1138\ N/m}} = 9.01\cdot 10^{-12}\ m \rightarrow 7.45\%$$

$$x_2 = \sqrt{\frac{2\cdot 7.69\cdot 10^{-20}\ J}{1138\ N/m}} = 1.16\cdot 10^{-11}\ m \rightarrow 9.61\%$$

Vibrations are quite small!