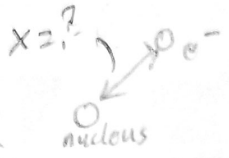


# Lecture 7

How big are molecules?

$$V(x) = \frac{-Ze^2}{4\pi\epsilon_0 x}$$



$$K = \frac{p^2}{2m_e} \leftarrow 9.1 \times 10^{-31} \text{ Kg (mass of electron)}$$

As particles move around, their K and V (Kinetic & potential energy)

exchange, while the total E is conserved.

$$\Delta V \approx \Delta K \approx \frac{E}{2} \quad (\Delta \text{ means range of variation})$$

$$\Delta V \approx \frac{-Ze^2}{4\pi\epsilon_0 \Delta x} \approx \Delta K \approx \frac{\Delta p^2}{2m_e} \quad \Delta x \cdot \Delta p \approx \frac{\hbar}{2}$$

$$\Delta x \approx \frac{\pi \epsilon_0 \hbar^2}{2m_e Z^2 e^2} \approx 0.06 \text{ \AA} \text{ for H atom}$$

In actuality,  $\Delta x \approx 0.7 \text{ \AA}$ . But this gets fairly close, and shows that atoms & molecules are small.

## Molecule as a spring

$M \gg m$  (for now, assume one mass is much higher.)



We will see later that  $e^-$  pairs between nuclei act like springs holding nuclei together.

$$F = -kx \quad \rightarrow \text{plug into Schrodinger}$$

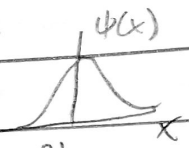
$$V(x) = \frac{1}{2} kx^2 \quad \rightarrow \text{Schrodinger}$$

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \right) \psi_n(x) = E_n \psi_n(x)$$

n subscript gives more than 1 solution may be possible. In this case, there are countably infinite solutions.

$$\text{try } \psi_0 = e^{-ax^2}$$

$$\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_0 = \frac{-\hbar^2}{2m} \frac{d}{dx} (-2ax e^{-ax^2}) =$$



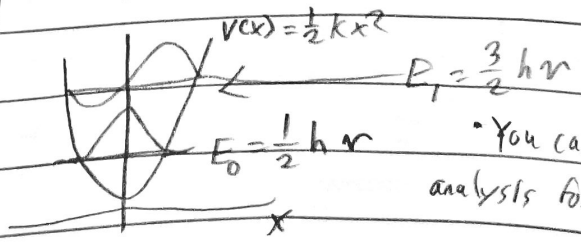
$$= \frac{\hbar^2}{2m} (2a - 4a^2 x^2) e^{-ax^2}$$

$$\frac{\hbar^2}{2m} (2a - 4a^2 x^2) e^{-ax^2} + \frac{1}{2} kx^2 e^{-ax^2} = E_0 \psi_0$$

$$\text{We want } \frac{\hbar^2}{2m} (-4a^2 x^2) + \frac{1}{2} kx^2 = 0$$

$$\Rightarrow a = \frac{\sqrt{km}}{2\hbar} \quad \text{This cancels the } x^2 \text{ terms.}$$

$$E_0 = \frac{\hbar^2}{2m} 2a = \frac{\hbar}{2} \sqrt{\frac{k}{m}} = \frac{\hbar}{2} \nu \leftarrow \sqrt{\frac{k}{m}} = 2\pi\nu$$



You can repeat this analysis for higher n.