Last Time.

$$\left\{\frac{\hat{p}^2}{2m} + V(x)\right\}\psi(x) = i\hbar\frac{\partial}{\partial t}\psi \quad \text{or} \quad H\psi = E\psi$$

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \quad \text{and} \quad \hat{E} = -\frac{\hbar}{i}\frac{\partial}{\partial t}$$

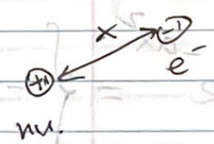
Put together $\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right\}\psi(x)$

$$= \hat{E}\psi \quad \text{or} \quad H\psi = E\psi$$

kinetic energy (more curvature, more kinetic energy "k")

Today: How big are atoms and molecules?

$$V(x) = \frac{Ze^2}{4\pi\varepsilon_0 x} \qquad k = \frac{p^2}{2m_e}$$



$\Delta V \simeq \Delta K \simeq \frac{E}{2}$

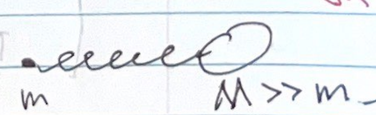
As the e^- moves around, energy goes back and forth between potential and kinetic energy.

$$\Delta V = \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{\Delta x} \simeq \Delta K \simeq \frac{\Delta p^2}{2m_e} \qquad \Delta p = \frac{\hbar}{2\Delta x}\langle p \rangle$$

$$\Rightarrow \Delta x \simeq \frac{4\pi\varepsilon_0\hbar^2}{2m_e Z e} \simeq 0.06\ \text{Å}$$

$F = -kx = -\frac{\partial V}{\partial x}$

Vibrating molecules



As we'll see later, e^- pair act as a spring holding the molecules together

$n = 0, 1, 2,$

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

Q2.1

$$\psi_0(x) \sim e^{-ax^2}$$

$$\frac{d^2}{dx^2} e^{-ax^2} = \frac{d}{dx}\left(\frac{d}{dx} e^{-ax^2}\right)$$

$$= \frac{d}{dx}\left(-2ax\, e^{-ax^2}\right)$$

$$= -2ae^{-ax^2} + 4a^2x^2e^{-ax^2}$$

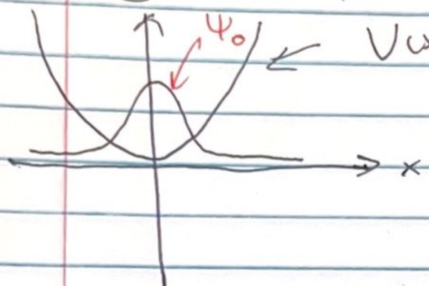
$$E_0 e^{-ax^2} = \left\{ -\frac{\hbar^2}{2m}\left(-2a + 4a^2x^2\right)e^{-ax^2} + \frac{1}{2}kx^2e^{-ax^2} \right\}$$

This can only be ~~ture~~ true eigenfunction if two x^2 terms cancel.

$$\Rightarrow -\frac{\hbar^2}{2m}4a^2x^2 + \frac{1}{2}kx^2 = 0$$

$$\Rightarrow \begin{cases} a = \dfrac{\sqrt{km}}{2\hbar} \\[2ex] E_0 = \dfrac{\hbar^2 a}{m} = \dfrac{\hbar\sqrt{km}}{2m} = \dfrac{\hbar}{2}\sqrt{\dfrac{k}{m}} \end{cases}$$

Diagram of the solution.



$V(x) = \frac{1}{2}kx^2$

$$E_0 = \cancel{\frac{\hbar}{2}} \frac{h}{2} \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

$$= \frac{h}{2} \cdot \nu$$

where $\nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$.

Q. Why the energy not be zero like a classical spring ?

A. Heisenberg principle $\Delta x \Delta p \neq 0$

$\Rightarrow$ The energy for Ψ_0 is called zero point energy.

O2.1

$\Psi_1 \propto xe^{-ax^2}$ is also a solution.