Lecture 7

Last Time:

$$\left(\frac{\hat{p}}{2m} + V(x)\right)\Psi = i\hbar \frac{\partial}{\partial t}\Psi \qquad (P2)$$

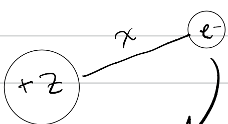
(P1) $\hat{p} = -i\hbar \frac{\partial}{\partial x}$ $\qquad$ $E = i\hbar \frac{\partial}{\partial t}$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi = E\Psi$$

$$\hat{H}\Psi = E\Psi$$

How big are atoms and molecules?

$$V(x) = \frac{Z e^2}{4\pi \varepsilon_0 x} \qquad KE = \frac{p^2}{2m_e}$$



as e^- moves:

$$\Delta V \approx \Delta KE$$

$$\Delta V \approx \Delta KE \approx \frac{E}{2}$$

(potential energy transfers to KE, and vice versa)

$$\Rightarrow \frac{Z e^2}{4\pi \varepsilon_0}\frac{1}{\Delta x} \approx \frac{\Delta p^2}{2m_e}$$

$$\Delta p = \frac{\hbar}{2\Delta x}$$

(heisenberg uncertainty principle)

$$\Delta x \approx \frac{\pi \varepsilon_0 \hbar^2}{2 m_e Z e^2}$$

Choose $Z = 1$ (like H), then

$$\Delta x = 0.06\ \text{Å} \quad \text{(Tiny!)}$$

Vibrating Molecules

m M

w/ M >> m

$F_{spring} = -kx$

$V_{spring}(x) = -\int -kx\,dx = \frac{1}{2}kx^2$

using this spring potential as our potential:

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2\right)\Psi_n = E_n\Psi_n \leftarrow \text{eigen-function}$$

$\uparrow$ eigenvalue

(many different solutions)

HW Q: Try $\Psi_0 \sim e^{-ax^2}$ as a solution.
(Check that this satisfies the above equation.)

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

$$-\frac{\hbar^2}{2m}\underbrace{\frac{\partial^2}{\partial x^2}e^{-ax^2}} + \frac{1}{2}k e^{-ax^2} = E_n e^{-ax^2}$$

chain rule reminder: $\frac{\partial}{\partial x} f(g(x)) = f'(g(x))\,g'(x)$

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

$$= -2ae^{-ax^2} + \left(-2ax\,e^{-ax^2}(-2ax)\right)$$

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

product rule reminder: $\frac{\partial}{\partial x}(f(x)g(x)) = f'(x)g(x) + f(x)g'(x)$

$$-\frac{\hbar^2}{2m}\left(-2ae^{-ax^2} + 4a^2x^2e^{-ax^2}\right) + \frac{1}{2}kx^2e^{-ax^2} = E_0e^{-ax^2}$$

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

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

x^2 on LHS but not on RHS $\Rightarrow 4a^2x^2 + \frac{1}{2}kx^2 = 0$

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

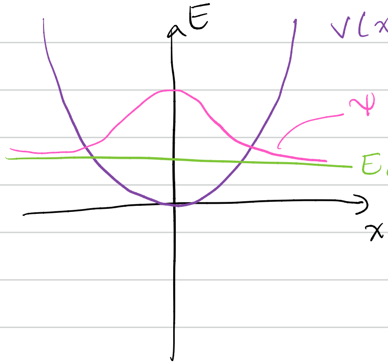
$$\frac{\hbar^2}{2m} 4a^2 = \frac{1}{2}k$$

$$a = \frac{\sqrt{mk}}{2\hbar}$$

sub in a and use $-\frac{\hbar^2}{2m} 4a^2x^2 + \frac{1}{2}kx^2 = 0$

$$-\frac{\hbar^2}{2m}\left(-2\frac{\sqrt{mk}}{2\hbar}\right) = E_0$$

$$E_0 = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$$



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

$\psi = e^{-ax^2}$

E_0 zero point energy (ZPE)

Q: Why is $E_0 \neq 0$?

In CM, lowest energy $= 0$.

Hint:

Heisenberg uncertainty: $\Delta x \Delta p \geq \frac{\hbar}{2}$

$\Rightarrow$ we must have some momentum

$\Rightarrow E > 0$.