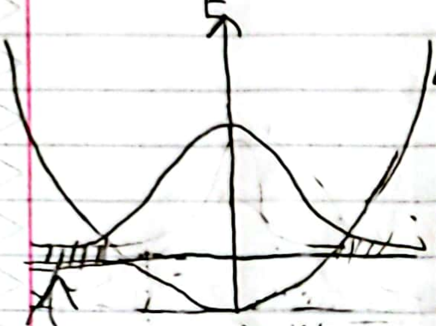
Lecture 9

06-Feb 2023

Last time: quantum Spring $\approx$ Vibrating molecule



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

$E_0 = \frac{1}{2}h\nu$ "Zero point energy"

Classical particle can be at rest, not allowed in QM since $\Delta x \Delta p = \frac{\hbar}{2}$

Classically forbidden region

Proved: $E_{photon} = \Delta E = h\nu$ "Planck's Law"

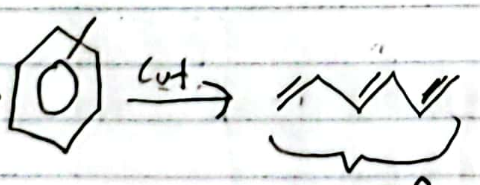
Spectroscopy: remote sensing of molecules "no touch", even light years away

---

Today: another simple model for a molecule: the box of electrons

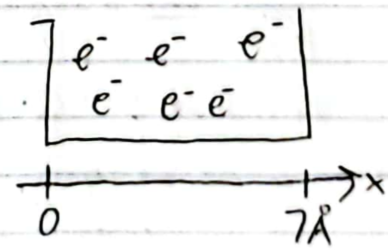
ex: Benzene - colored or transparent?

6π electrons



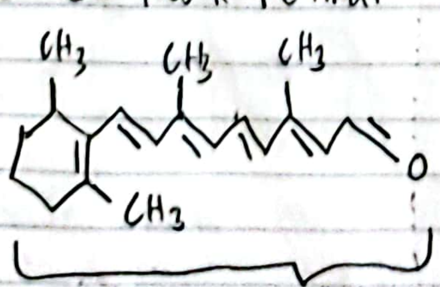
$L \approx 7Å$

$\equiv$

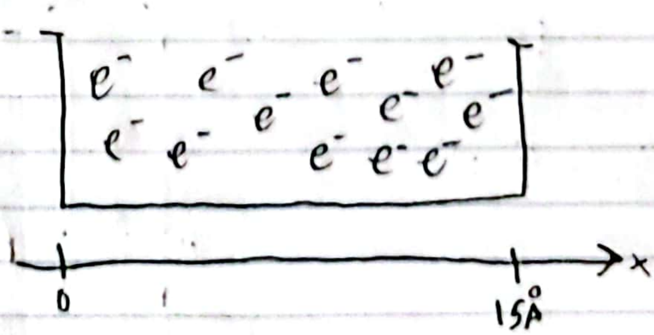


box filled with 6π e⁻

Other ex: Hawk retinal

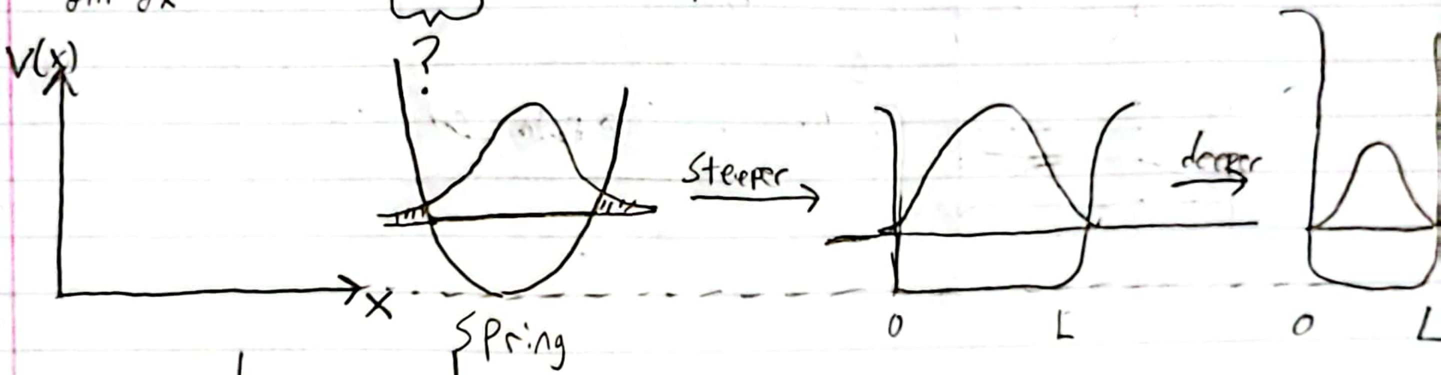


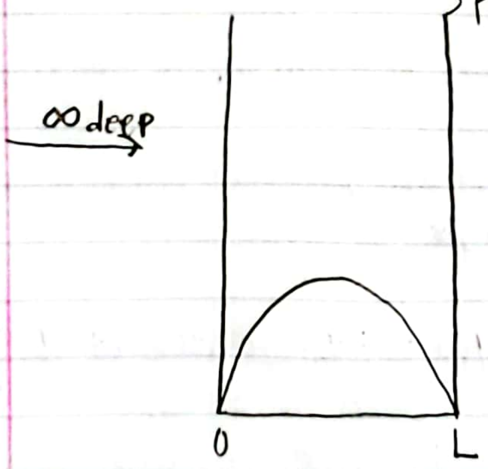
$L = 15Å$



Schrödinger eq. for box

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_n(x) + \underbrace{V(x)}_{?}\psi_n(x) = E_n \cdot \psi_n(x)$$



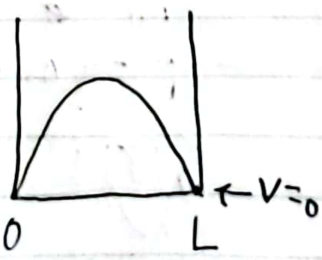


$\boxed{\text{V=0 inside the box; V very large outside the box}}$

(potential V)

As the box gets deeper and deeper, we expect $\psi(x) \to 0$ at $x=0$ or

Guess a Solution:



Sin or ~~cos~~

Sin starts at 0 ✓

$\boxed{\sin(n\pi \frac{x}{L})}$

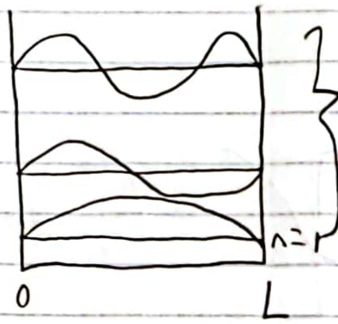
- Second derivative of $\psi \sim \psi$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\sin\left(n\pi\frac{x}{L}\right) + 0 \cdot \sin\left(n\pi\frac{x}{L}\right) = E_n \sin\left(n\pi\frac{x}{L}\right)$$

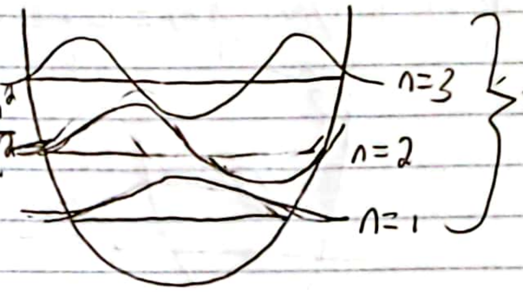
$$= +\frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 \sin\left(n\pi\frac{x}{L}\right) = E_n \cdot \sin\left(n\pi\frac{x}{L}\right)$$

$$= \frac{h^2 n^2}{8mL^2}\sin\left(n\pi\frac{x}{L}\right) = E_n \sin\left(n\pi\frac{x}{L}\right) \Rightarrow \therefore \boxed{E_n = \frac{h^2 n^2}{8mL^2}}$$

Do a plot of E-Levels $n = 1, 2, 3, 4, 5, \ldots$ ($n=0$ gives $\psi = 0$)



$E_n = \frac{h^2 n^2}{8mL^2}$

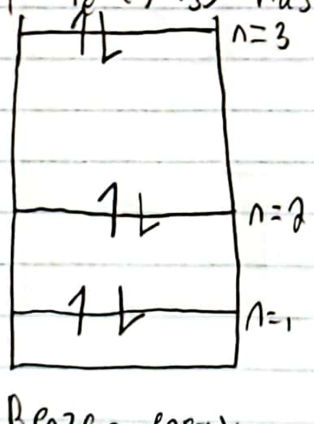


$E_n = h\nu(n - \frac{1}{2})$

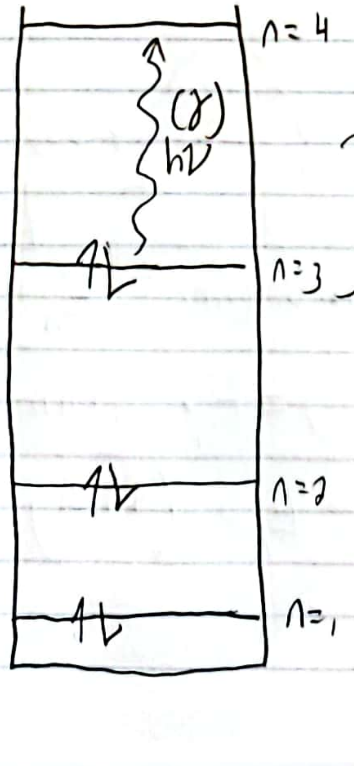
Before we fill in the $6e^-$ for benzene, a word about spin (no proof!)

- Spin is the "angular momentum" intrinsic to the particle and has conjugate variable φ_s, the spin angle
- the direction in which the spin points is quantized in steps of "1"
  ex: $S = \frac{1}{2}$ $\uparrow m_s = +\frac{1}{2}$ and $\downarrow m_s = -\frac{1}{2}$ (difference of 1)
  "spin up" $\Delta m_s = 1$ "spin down" (don't worry too much about this)

If $\psi_{e^-}(x, \varphi_s)$ has all q.n. identical $\psi(1, 2) \to 0$



Benzene energy Levels



$\frac{E_4 - E_3}{h} = \nu \approx 1.3 \times 10^{15}$ Hz

$\downarrow$

$\lambda = 230$ nm (UV)