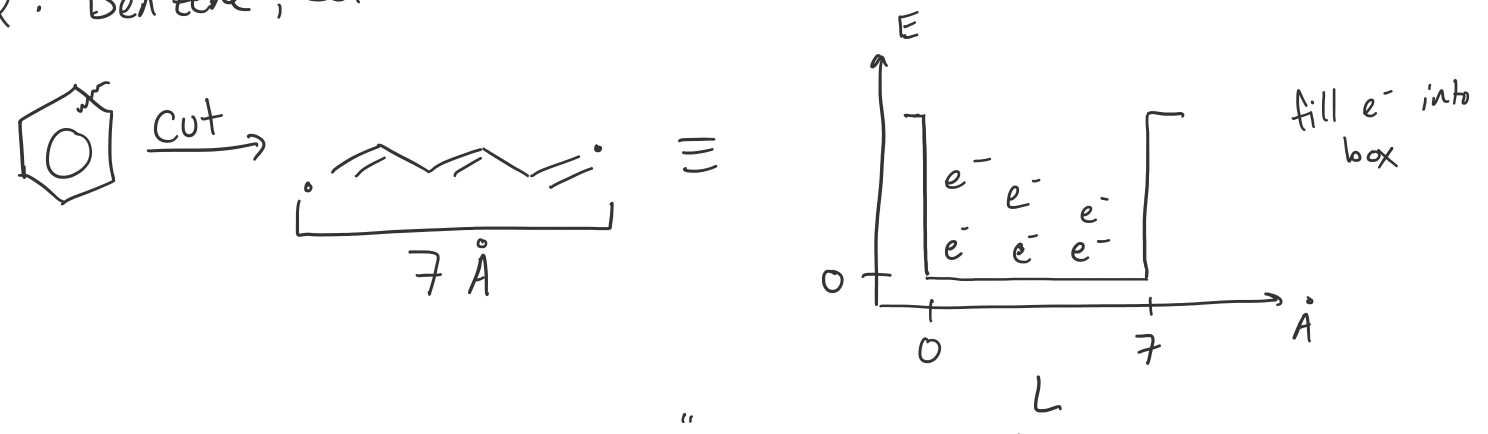
Lecture 9

Monday, September 11, 2023 10:03 AM

Molecule As a Box For Electrons :

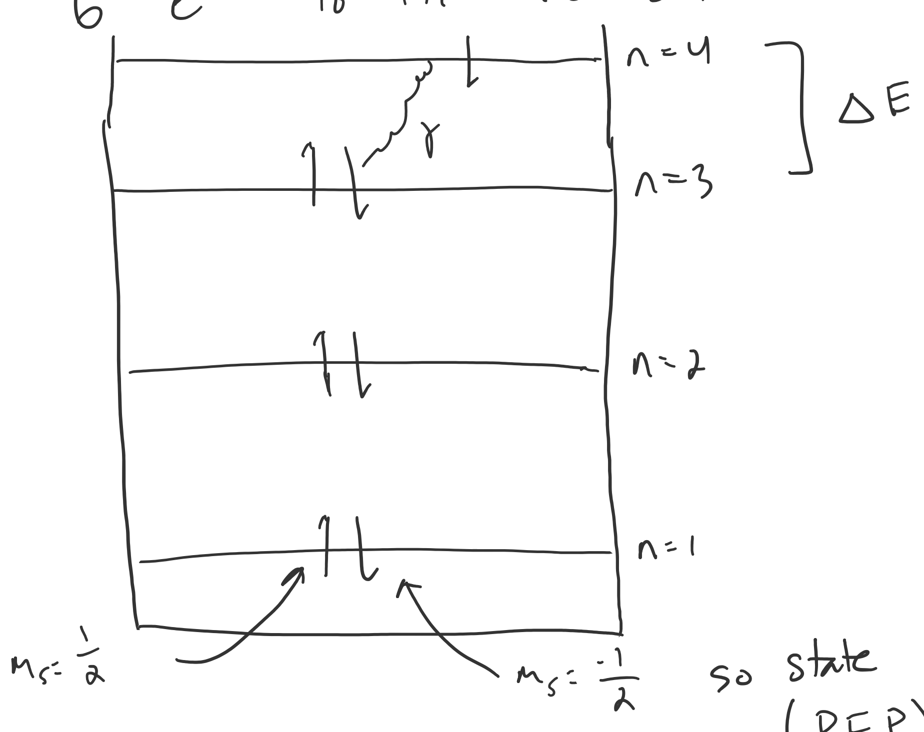
Q: Benzene, colored or transparent?



Before we fill e⁻ into the "benzene box" of $L = 7$ Å, a few words about Postulate 4 (spin):

- Spin is an angular momentum, in QM its conjugate variable is an angle $\varphi_s \Rightarrow \Delta S \cdot \Delta \varphi_s \geq \hbar/2$ & spin is quantized in integer steps
- e^- : $s = 1/2 \Rightarrow$ quantized in $m_s = \underbrace{-\frac{1}{2}, \frac{1}{2}}_{\Delta m_s = 1}$ — $-\frac{1}{2}$: e⁻ rotates CW; $\frac{1}{2}$: e rotates CCW
- γ : $S = 1 \Rightarrow$ quantized in $m_s = -1, 0, 1$

6 e⁻ to fill into box

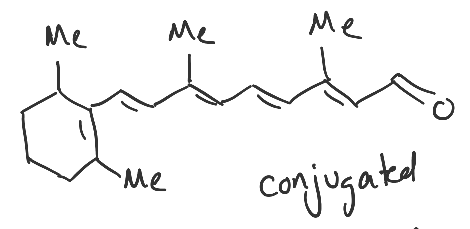


$\frac{E}{h} = \nu \approx 1.3 \times 10^{15}$ Hz

so state of e⁻ #1 ≠ state of e⁻ #2 (PEP)

Longer Molecule

retinol



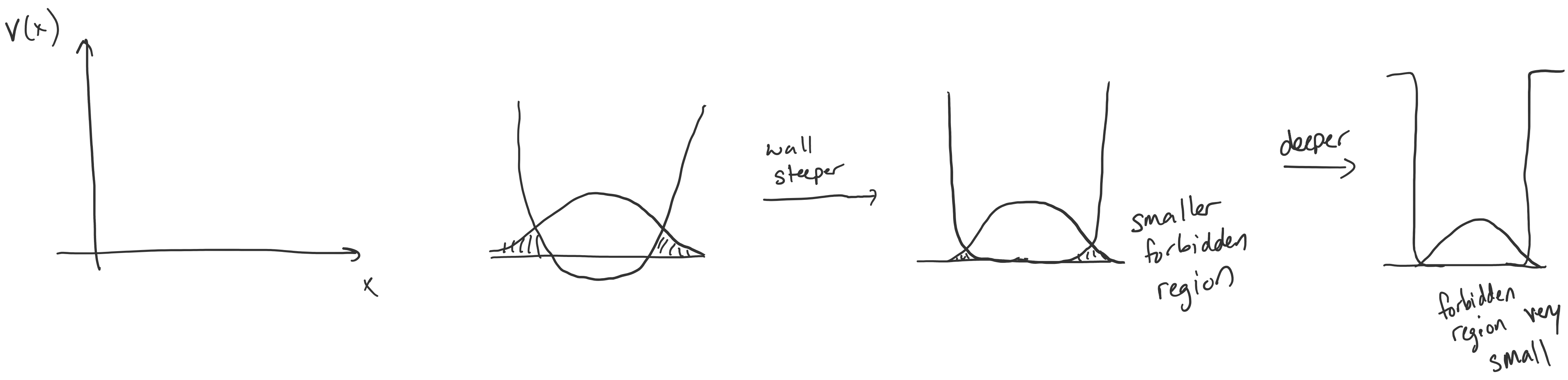
conjugated

$L \sim 15$ Å

Solve Schrödinger Eqn for "Particle in a Box"

$$\mathcal{H}\psi_n = E_n \psi_n \Rightarrow \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi_n = E_n \psi_n$$

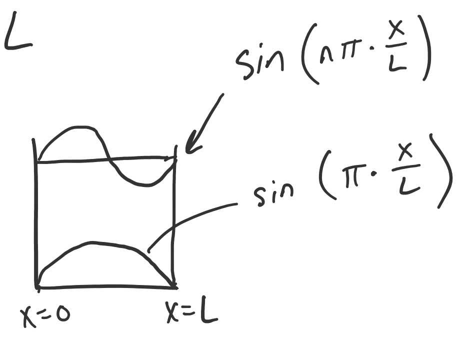
$V(x)$: 0 inside box



As we deform a spring (parabola as potential energy) into a box, $\psi \sim e^{-ax^2} \longrightarrow \sin(ax)$

Solution: a function equal to its 2nd derivative that is zero @ $x = 0$ & $x = L$

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_n(x) = E_n \psi_n(x)$$



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

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

$$\hbar = \frac{h}{2\pi}$$

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