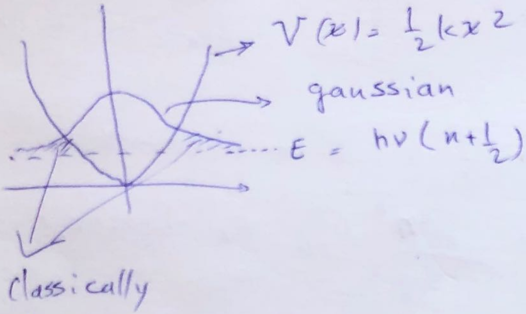
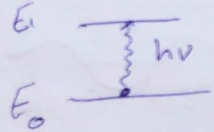
L9: review

quantum spring (vibrating molecule)



Proved:



$\Delta E = h\nu$

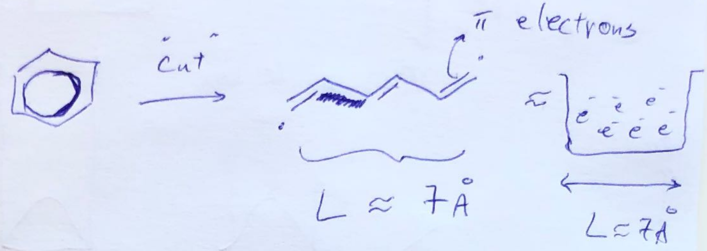
Planck's law

$\Delta x \, \Delta p = \frac{\hbar}{2}$: Heisenberg principle (conjugate principles)

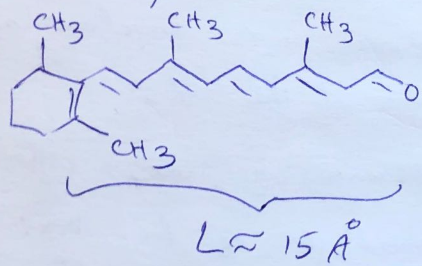
we also discussed how spectroscopy can facilitate remote-sensing of molecules

Today: ch3 "other molecules"

"Benzene: colored or transparent"



another famous molecule with extended π system is retinal, the molecule responsible for vision (light absorption) in eye:

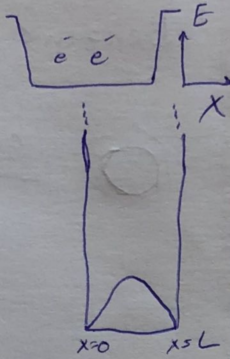


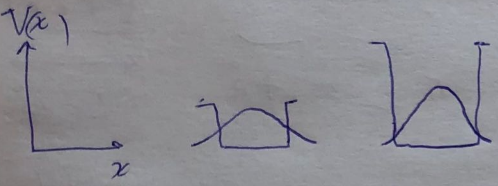
Schrödinger eq. for "box"

$$\left\{-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2}+0\right\}\psi_n=E_n\,\psi_n$$

$\downarrow$

V(x) inside box





* as the potential wall increases the wing of the wave function outside the box decreases. In the extreame of $V(x@\text{wall}) \to \infty$: wavefunction goes to zero at the walls.

* trigonal functions, e.g. $\sin x$, will solve the schrödinger eq. for box:

$\sin(x)=0$ at $x=0$

$\sin\left(\frac{n\pi}{L}x\right)=0$ @ $x=L$

plug in our guess:

$$-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2}\sin\left(\frac{n\pi}{L}x\right)=\frac{h^2\pi^2}{8m_eL^2}\sin\left(\frac{n\pi}{L}x\right)$$

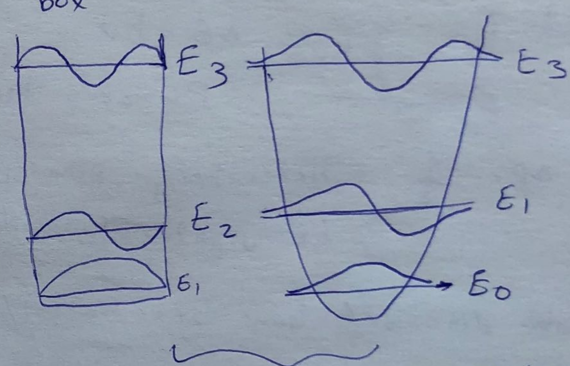
$\hbar=\frac{h}{2\pi}$

$\Rightarrow$ $\sin\left(\frac{n\pi}{L}x\right)$ is an eigenfunction

and $\frac{h^2\pi^2}{8m_eL^2}$ is the eigenvalue.

$(n=1,2,3,\cdots)$

box

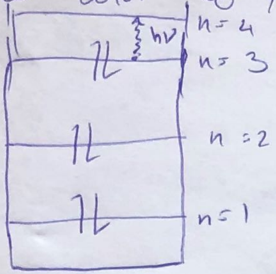


note the similarity between the wave function of box and spring.

The main difference is that

$\psi(x)_{box}=0, \quad x\geq L$ or $x\leq 0$

now, let's use the box function to find the color of the conjugated molecules:



6 π electrons

* note that electron has spin of $\frac{1}{2}$ ($s_e = \frac{1}{2}$); $m_s = -\frac{1}{2}$ or $m_s = +\frac{1}{2}$.

Therefore Pauli exclusion dictates that only two electrons can occupy each orbital. For six electrons, we need three orbitals. (The highest occupied orbital is n=3)

$$h\nu = \Delta E = E_4 - E_3 = \frac{h^2 4^2}{8 m_e L^2} - \frac{h^2 3^2}{8 m_e L^2} \Rightarrow \nu \approx 1.3 \times 10^{15}\ Hz$$

$$\nu \cdot \lambda = c \Rightarrow \lambda \approx 230\ nm$$