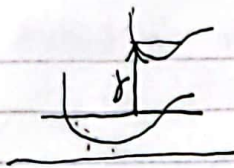


# Lecture 16

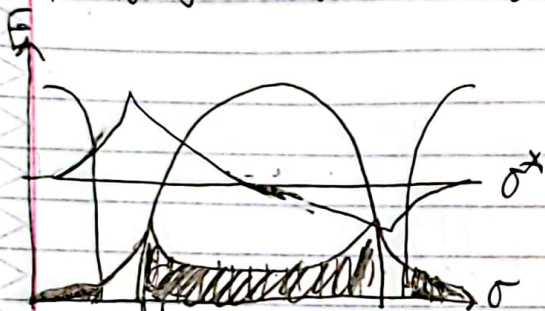
Last time:  
Spectroscopy



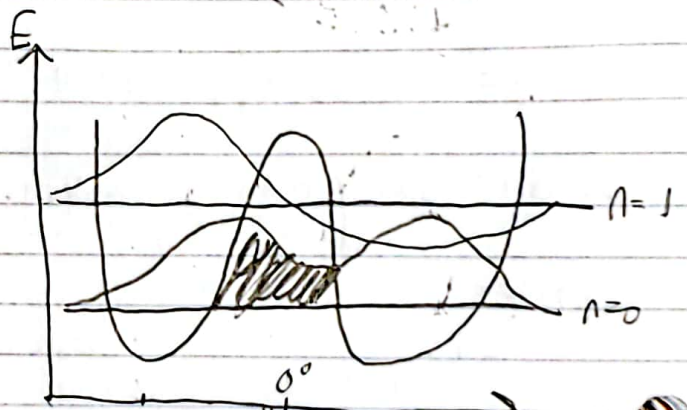
water and microwaves

Fourier principle: telescopes and spectroscopy  $\Delta\theta \cdot \Delta d = \frac{\lambda}{4\pi}$

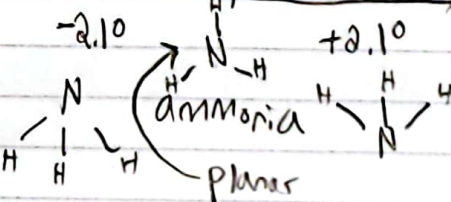
Tunneling: (well, we didn't get to this)



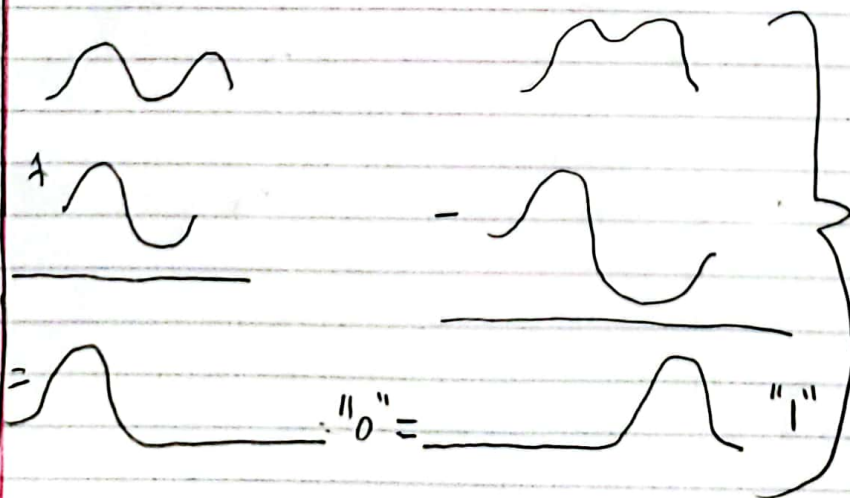
Molecular bond



$$n=0 \left. \begin{array}{l} \\ \\ \\ \end{array} \right\} \frac{\Delta E}{h} = \nu \approx 306 \text{ Hz (microwaves again)}$$



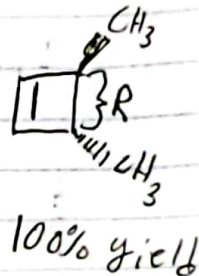
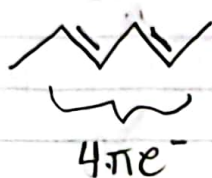
## Quantum Superposition



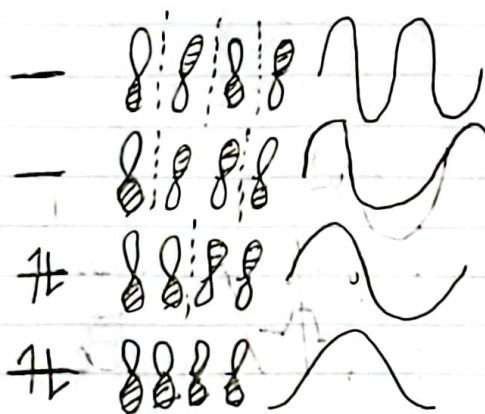
qubits in a  
Quantum computer

Today: How reactions go over (or through) barriers:

ex: 2,4-hexadiene



$E_{\text{orbitals}}$

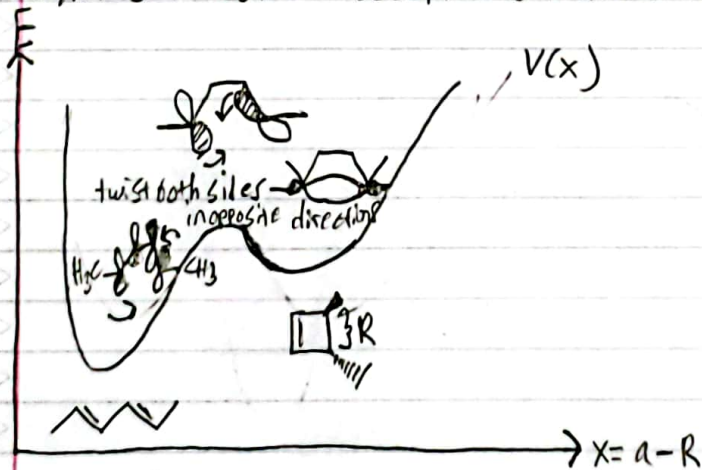


Lumo (lowest unoccupied molecular orbital)

Homo (highest occupied molecular orbital)

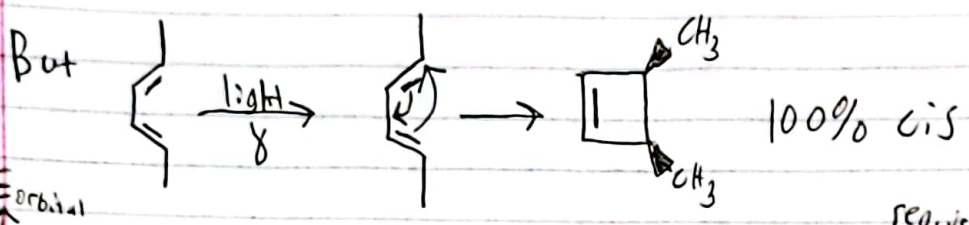
Why 100% yield?

Hypothesis: Highest-occupied orbital controls the reaction



Reaction coordinate

twist for  $\pi$  or  $\pi$ - $\pi$  overlap (bonding), do not want  $\pi$ - $\sigma$  or  $\pi$  (antibonding)  
 The molecule twists (rotates) for bonding character for new  $\sigma$  bond,



$E_{orbital}$

