Chapter 9 - 2, 3, 4, 5, 6, 7, 13, 16, 23a

Chapter 8 - Suggested Chapter problems
1-7, 9, 10a-d, 12, 13, 14, 16, 18, 19, 21a, 22, 25

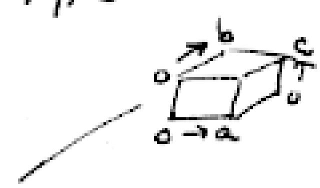
Chapter 9 Reading - Skip "Tunneling" pp 463-464
DO Read "Harmonic Osc" pp 465-467
Skip "Rigid Rotater" pp 468-469
DO Read "Hydrogen Atom" and sections following
ie pp. 469-476
Skip "Many Electron Atoms" pp. 476-478
Read ligtly 479-490. Skip 491-513
Read 514-517

Review past ~~3~~ 2 lectures - Chapter 9

Wave-particle duality - small particles show wave-like prop's

Describe wave behavior by wave function: $\Psi(x, y, z)$

$\Psi^2(x,y,z) \rightarrow \Psi^2 \propto$ Probability of finding $e^{\ominus}$ at x, y, z

Finite Probability $= \int_0^a \int_0^b \int_0^c \Psi^2 \, dz \, dy \, dx \longrightarrow$ 

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Psi^2 \, dx \, dy \, dz = 1$$

Operator <=> Expectation Value

$$\bar{z} = \int \Psi_n \, z \, \Psi_n \, dv$$

$$E = \int \Psi_n \mathcal{H} \Psi_n \, dv$$

ONE-DIMENSION

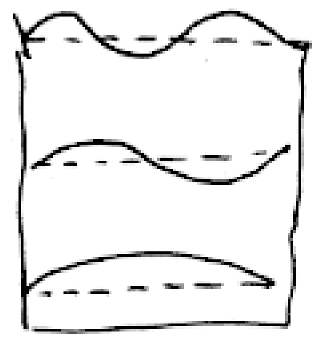
$$\mathcal{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)$$

One Dimensional

Particle in a Box - A really simple atom

Use $\int_{-\infty}^{\infty} \psi^2 \, dv = 1$ and Boundary Conditions to yield

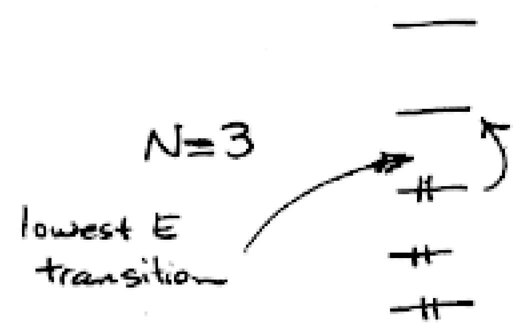
$$\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$$



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

$$\lambda_{N \to N+1} = \frac{8mca^2}{h(2N+1)}$$

N = Quantum number of the highest filled orbital
(For simple atom, N = ½ (# electrons))



Particle in a Box had a very simple $U(x)$.

Fancier Version Harmonic Oscillator Elaborate why

Bonding Orbital

$$\mathcal{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$$

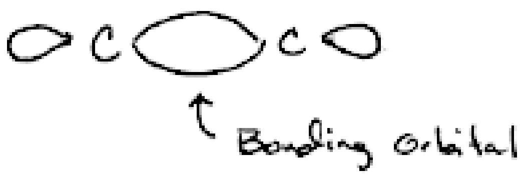
$F = -kx$

$U = \frac{1}{2}kx^2$

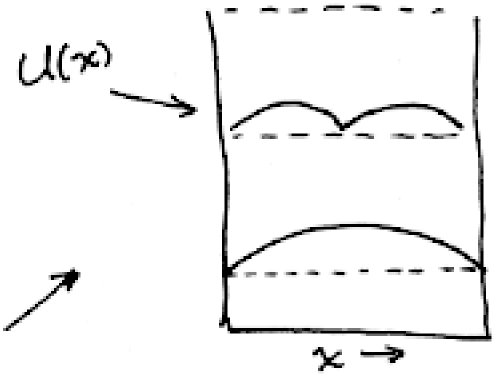
x = deviation from lowest E length

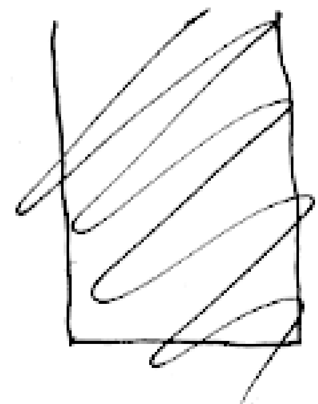
⇒

Again, <u>one-dimensional</u>

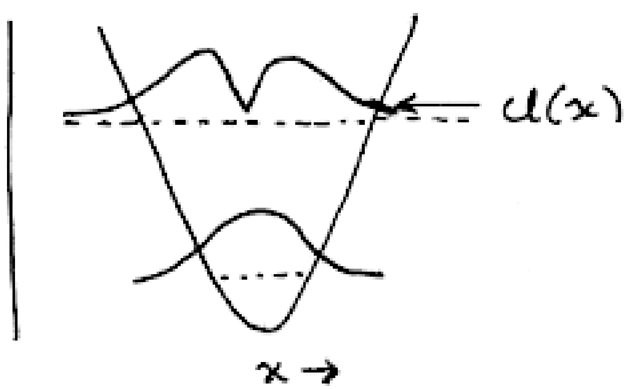


$$-\frac{\hbar^2}{2m}\frac{d^2\psi_v}{dx^2} + \frac{1}{2}kx^2\psi_v = E_v\psi_v$$





Note similarities



see p. 465

Good descriptor for <u>BOND</u> wavefunctions

<u>Quant</u>ized energy levels ⇒ $n = 1, 2, 3, 4, \ldots$

Harmonic oscillator is used as a wavefunction for many molecular dynamics and molecular mechanics calculations. NOT BAD

H Atom – 3 Dimensions

move from x, y, z to polar Coords.

$$\mathcal{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{-e^2}{4\pi\varepsilon_0 r}$$

radius of $e^{\ominus}$ from center (nucleus)

3 QUANTUM NUMBERS – POLAR COORDS

n, $\underbrace{l, m}_{\text{angular}}$

radial

Back to General Chemistry

Reduced mass ↳ "m"

↳ Related to moment of inertia

$$E_n = -\frac{\mu e^4}{2\hbar^2 n^2}$$

$n = 1, 2, 3, \ldots$

TAKE HOME

Quantized Values for energy

$$\boxed{\text{READ pp 469-476 H-atom}}$$

Read lightly pp. 479-490 and relate it back to your General and Organic Chemistry

Skip 491-513. Read 514-517

Heisenberg Uncertainty Principle

$$\Delta p \; \Delta x \geq \frac{1}{2}\left(\frac{h}{2\pi}\right) = \frac{1}{2}\hbar$$

WAVE: mv ↓ relates to $\lambda = \frac{h}{mv}$

PARTICLE: position

CANNOT KNOW BOTH TO HIGH ACCURACY