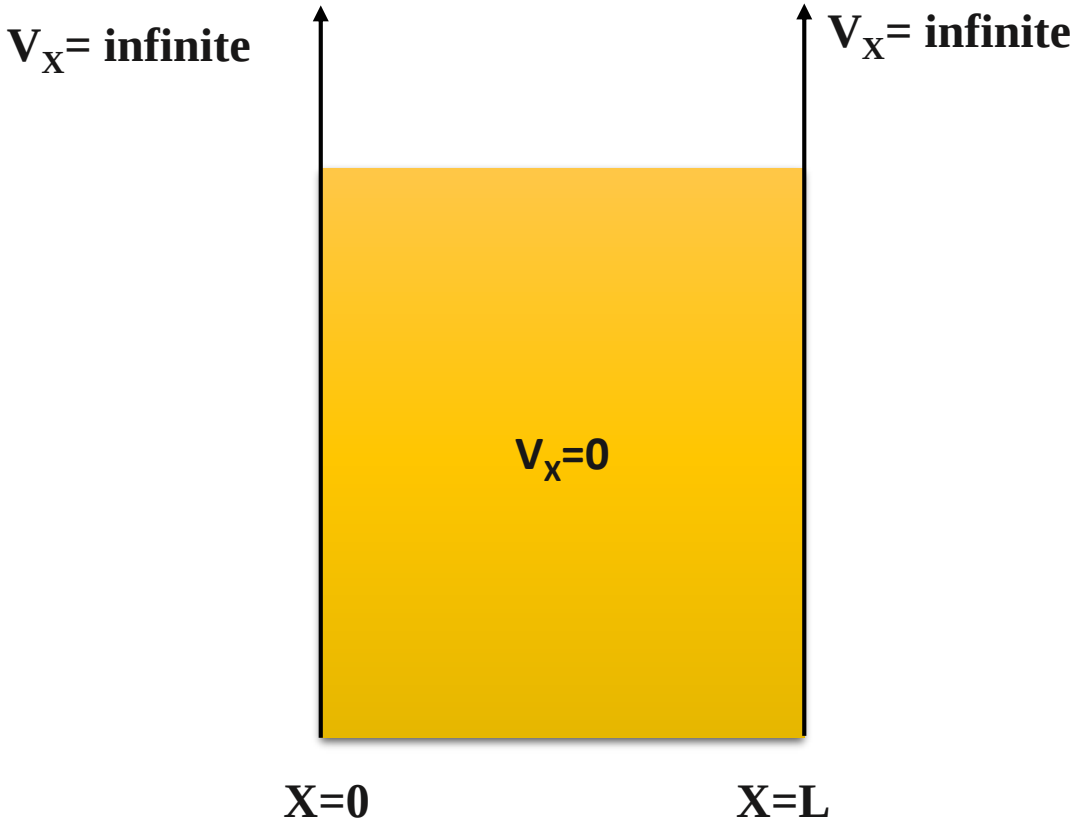
Materials Chemistry III

Day 7

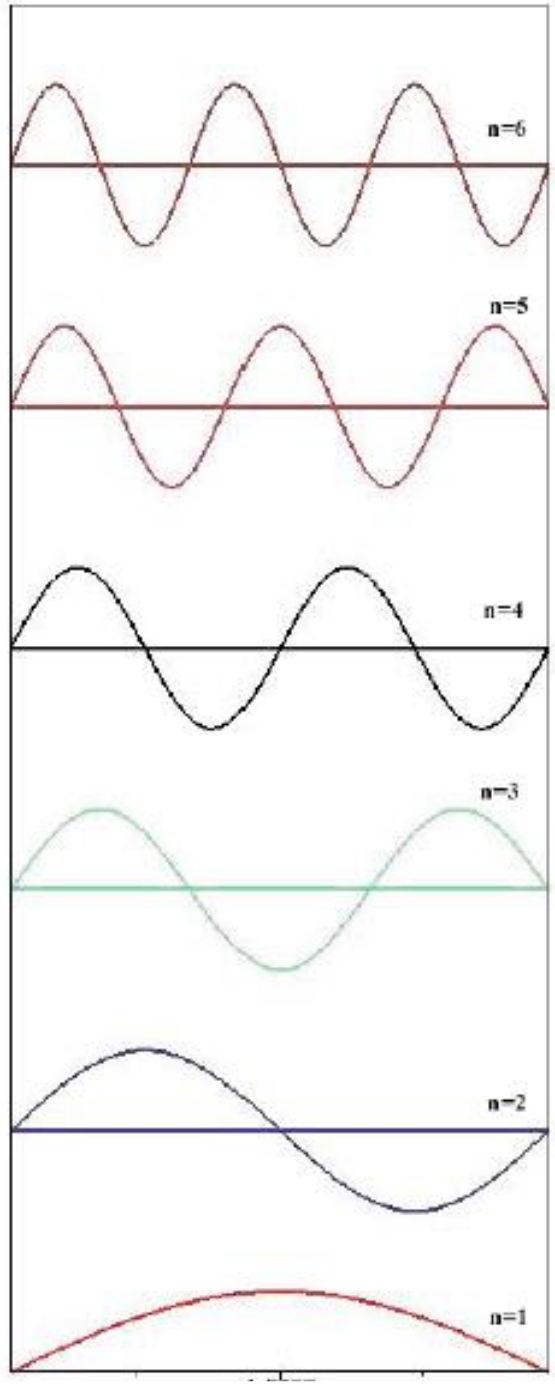
Summary of Lecture 5 and Tutorial 3

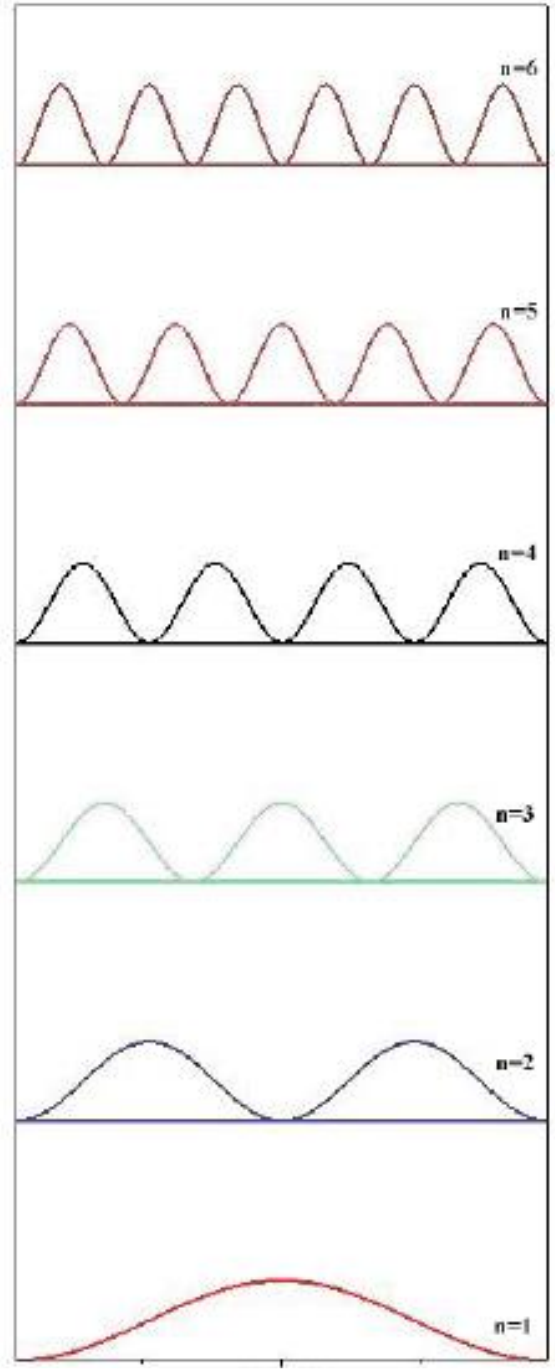
"Particle in 1D/2D box"



1) Energy level variation and relationships for 1D box.
2) Orthogonality
3) Relation ship between de Broglie wavelength (λ) and Length (L) of the box for a particle confined in a box.

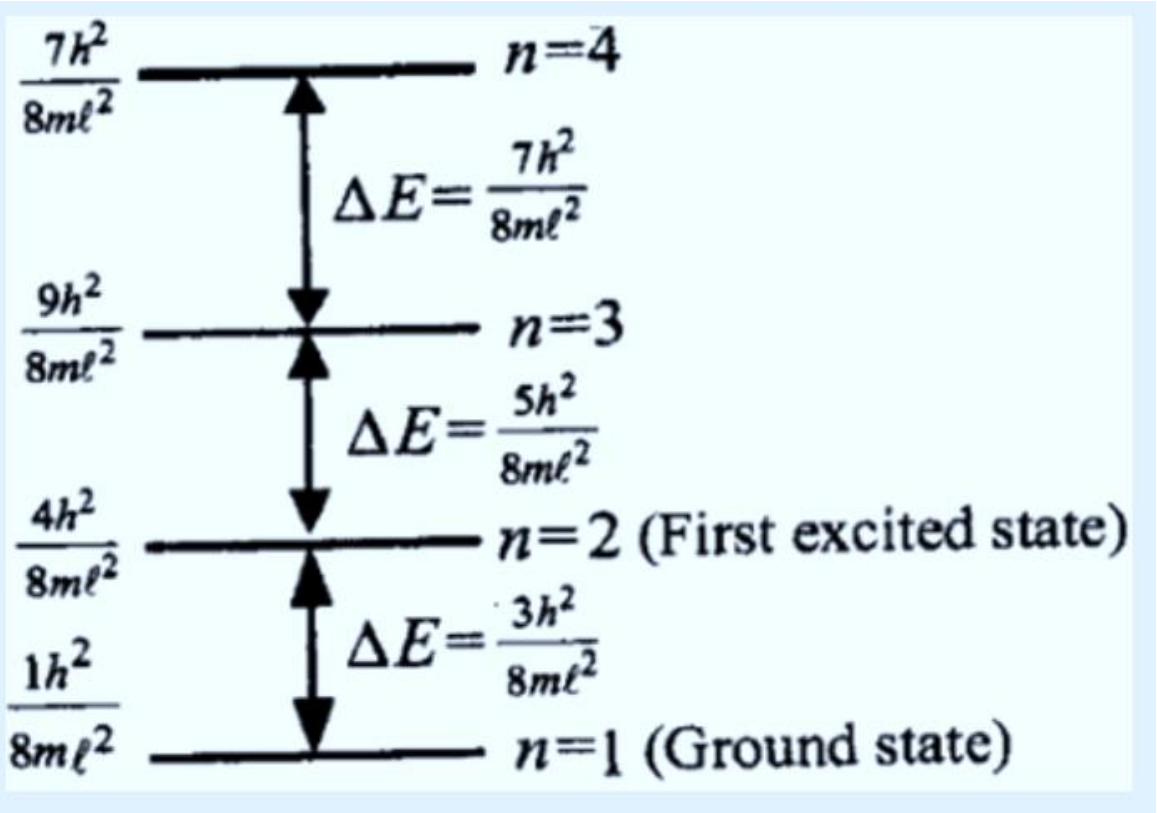
$$\lambda = 2L/n$$


n=6
n=5
n=4
n=3
n=2
n=1


n=6
n=5
n=4
n=3
n=2
n=1

For immediate transition to next higher state:

$$\Delta E_{general} = (2n+1)h^2/8mL^2$$



For n=1 to n=2; $\Delta E = 3h^2/(8mL^2)$

Particle in 2D Box-Concept of Degeneracy

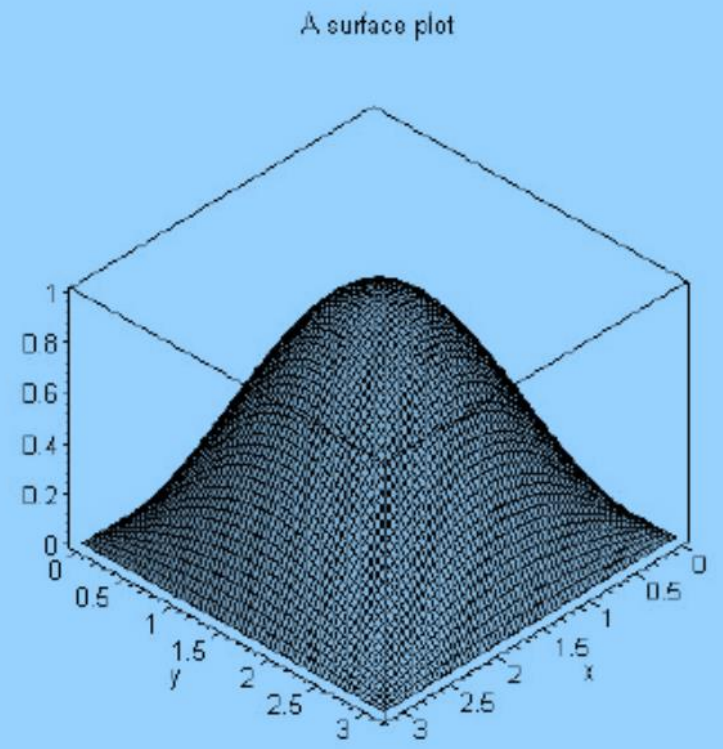
$$X_{n_1}(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n_1 \pi x}{L}\right), \quad E_{n_1} = \frac{h^2 n_1^2}{8mL^2}$$

$$Y_{n_2}(y) = \sqrt{\frac{2}{L}} \sin\left(\frac{n_2 \pi y}{L}\right), \quad E_{n_2} = \frac{h^2 n_2^2}{8mL^2}$$

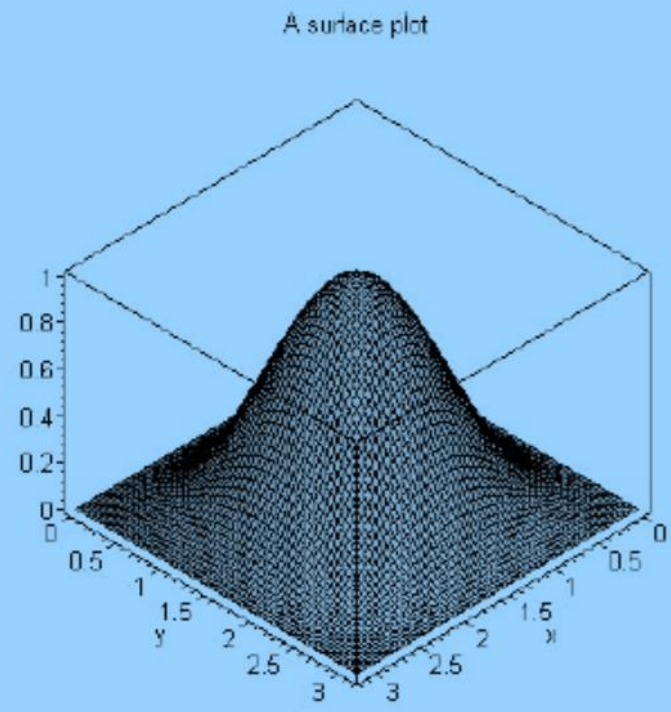
$$E_{n_1} + E_{n_2} = \frac{h^2}{8mL^2}\left(n_1^2 + n_2^2\right) = E_{n_1 n_2}$$

$n_1 = 1, n_2 = 1$	$\psi_{11}(x,y) = \frac{2}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)$	$E_{11} = \frac{h^2}{8mL^2}(1^2+1^2) = \frac{h^2}{4mL^2}$
$n_1 = 2, n_2 = 1$	$\psi_{21}(x,y) = \frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)$	$E_{21} = \frac{h^2}{8mL^2}(2^2+1^2) = \frac{5h^2}{8mL^2}$
$n_1 = 1, n_2 = 2$	$\psi_{12}(x,y) = \frac{2}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)$	$E_{12} = \frac{h^2}{8mL^2}(1^2+2^2) = \frac{5h^2}{8mL^2}$
$n_1 = 2, n_2 = 2$	$\psi_{22}(x,y) = \frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)$	$E_{22} = \frac{h^2}{8mL^2}(2^2+2^2) = \frac{h^2}{mL^2}$

$$\psi_{11}(x,y) = \frac{2}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)$$



$$\psi_{11}^2(x,y) = \frac{4}{L^2}\sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{\pi y}{L}\right)$$



Particle in 3D Box?