Moving to 3D models

1) Solving $H\psi = i\hbar \frac{\partial}{\partial t}\psi$ and $H\psi = E\psi$ is equivalent (Fourier conjugates)

2) If 2 eigenfunction ψ_a and ψ_b are degenerate ($E_a = E_b$)
Then $\psi_a + \psi_b$, $\psi_a - \psi_b$, etc are also Eigen functions
(etc = any linear combination)

3) $\hat{H} = \hbar\omega(\hat{n} + 1/2) \Rightarrow$ harmonic oscillator | P/B: $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ | Ring: $\hat{H} = -\frac{\hbar^2}{2mR^2}\frac{\partial^2}{\partial \phi^2}$

$E_n = \hbar\omega(n + 1/2)$ | $E_n \frac{h^2 n^2}{8mL^2}$ | $E_m = \frac{(\hbar M)^2}{2mR^2}$

1D box: $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
$= H_x$

2D box: $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}$
$\hat{H}_x + \hat{H}_y$

3D box: sum of $\hat{H}_x, \hat{H}_y, \hat{H}_z$

If $H(x,y) = H_x(x) + H_y(y)$ what is $\psi(x,y)$

Either a sum or a product:
- $\psi_x(x) + \psi_y(y)$
- $\psi_x(x) \cdot \psi_y(y)$ → correct

$$\hat{H}\psi = (\hat{H}_x + \hat{H}_y)\psi_x \cdot \psi_y$$

$$= \psi_y \underbrace{\hat{H}_x \psi_x}_{E_x \psi_x} + \psi_x \underbrace{\hat{H}_y \psi_y}_{E_y \psi_y}$$

$$= (E_x + E_y)\psi_x \cdot \psi_y$$

$$= E\psi$$

Important

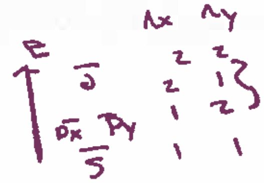
$E = E_x + E_y + \ldots$ sum

$\psi = \psi_x \cdot \psi_y \cdot \ldots$ Product

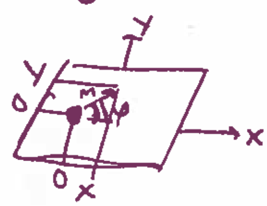
ex. PIB in 2D (square box)

$$E = \frac{h^2 n_x^2}{8mL_x^2} + \frac{h^2 n_y^2}{8mL_y^2} \quad n_x = 1,2,3\ldots \quad n_y = 1,2,3\ldots$$

$$\psi \sim \sin\left(\frac{n_x \pi}{L} x\right) \cdot \sin\left(\frac{n_y \pi}{L} y\right)$$



Rotating / Vibrating Molecule



$x = r\cos\varphi$
$y = r\sin\varphi$

$$\Rightarrow \hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}k(x^2+y^2)$$

move to polar coordinates

$$= \underbrace{-\frac{\hbar^2}{2mr^2}\frac{\partial^2}{\partial \varphi^2}}_{\hat{H}_{rot}} + \underbrace{-\frac{\hbar^2}{2m}\left\{\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right\} + \frac{1}{2}kr^2}_{\hat{H}_{vib}}$$

$\frac{1}{2}k(r-r_0)^2$ is more correct

$$\Rightarrow \psi(r,\varphi) = \psi(r) \cdot \psi(\varphi) = \frac{1}{\sqrt{2\pi}}\psi(r)e^{iM\varphi}$$

Energy is additive, wavefunction is multiplicative