QM 115B Lec 2

Schrödinger Eq in 3D

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = H \Psi(\vec{r},t)$$

$$H_{classical} = \frac{1}{2} m v^2 + V = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V$$

$$p_x \longrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad p_y \Rightarrow \frac{\hbar}{i}\frac{\partial}{\partial y} \qquad p_z \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial z}$$

$$i\hbar \frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2 \Psi + V\Psi$$

$$\nabla^2 = \frac{\partial}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\frac{\text{prob}}{\text{Vol}} = |\Psi(\vec{r},t)|^2 = \Psi^*(\vec{r},t)\,\Psi(\vec{r},t)$$

normalization $\displaystyle\int_{\text{all space}} |\Psi|^2 d^3r = 1$

time indpendent potential

sep. of variables $\Psi(\vec{r},t) = \phi(t)\,\psi(\vec{r})$

$$i\hbar \frac{\partial \phi}{\partial t}\psi = \phi\left(-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right)$$

③

$$\frac{i\hbar}{\phi}\frac{\partial \phi}{\partial t} = \frac{1}{\psi}\left(-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right)$$

indep. of $\vec{r}$ $\qquad$ independent of t

$$i\hbar\frac{\partial\phi}{\partial t} = E\phi \qquad E\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

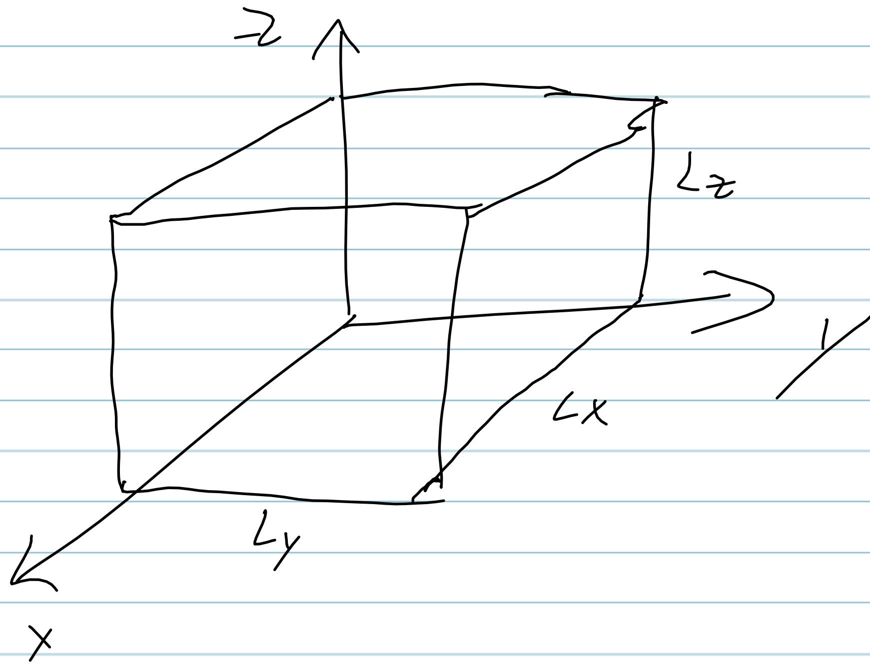
$$\phi = c\, e^{-iEt/\hbar}$$

time independent Sch. eq.

in general $\quad \Psi(\vec{r},t) = \sum_n c_n e^{-\frac{iE_n t}{\hbar}} \psi_n(\vec{r})$

3D Infinite Well (Box) (1D pg 30)

$$V(\vec{r}) = \begin{cases} 0 & 0<x<L_x,\ 0<y<L_y,\ 0<z<L_z \\ \infty & \text{otherwise} \end{cases}$$



seperation of variables

$$\psi(\vec{r}) = X(x)\,Y(y)\,Z(z)$$

$$EXYZ = -\frac{\hbar^2}{2m}\left(YZ\frac{\partial^2 X}{\partial x^2} + XZ\frac{\partial^2 Y}{\partial y^2} + XY\frac{\partial^2 Z}{\partial z^2}\right)$$

$$+ VXYZ$$

$$E = -\frac{\hbar^2}{2m}\left(\underbrace{\frac{1}{X}\frac{\partial^2 X}{\partial x^2}}_{-k_x^2} + \underbrace{\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}}_{-k_y^2} + \underbrace{\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}}_{-k_z^2}\right)$$

$$\frac{\partial^2 X}{\partial x^2} = -k_x^2 X \qquad X = 0 \text{ at } x = 0,\ x = L_x$$

$$X = c_1 \sin x k_x$$

$$\sin L_x k_x = 0 \qquad k_x L_x = n_x \pi$$

$$k_x = \frac{n_x \pi}{L_x}$$

$$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z}\right)$$

$$\psi_{n_x n_y n_z}(x,y,z) = c\sin\left(\frac{n_x \pi x}{L_x}\right)\sin\left(\frac{n_y \pi y}{L_y}\right)\sin\left(\frac{n_z \pi z}{L_z}\right)$$

Lowest energy state $(n_x, n_y, n_z) = (1,1,1)$

(5)

$L_x = L_y = L_z = L$

$E_{111} = (1^2+1^2+1^2)\dfrac{\pi^2\hbar^2}{2mL^2} = 3E_1$

		# states
3 integer	the same	1
2	the same	3
	different	6

$E_{333} = (3^2+3^2+3^2)E_1 = 27E_1$

$E_{511} = (5^2+1^2+1^2)E_1 = 27E_1$

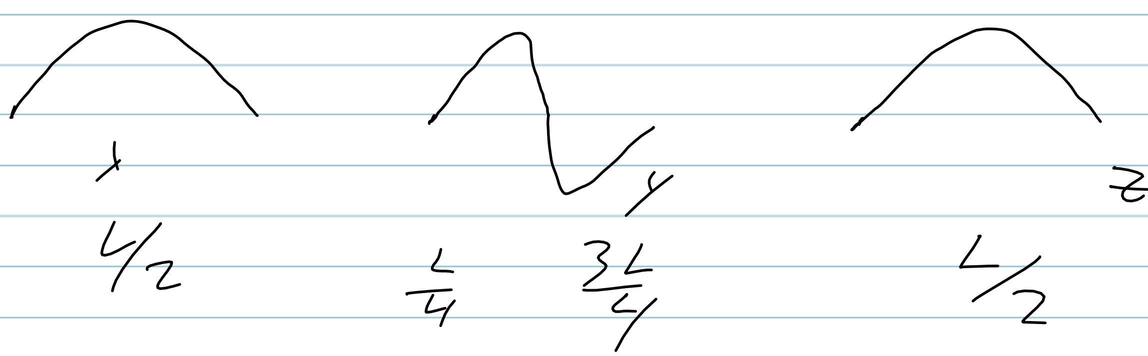
electron 1nm cube

$E_{111} = \dfrac{3\pi^2\hbar^2}{2mL^2} = \dfrac{3\cdot(3,14)^2(1,055\times10^{-34}\,Js)^2}{2\; 9,11\times10^{-31}\,kg\,(10^{-9}\,m)^2}$

$= 1,81\times10^{-19}\,J \quad \dfrac{1eV}{1,6\times10^{-19}\,J}$

$= 1,13\,eV$

$(n_x, n_y, n_z) = (1, 2, 1)$



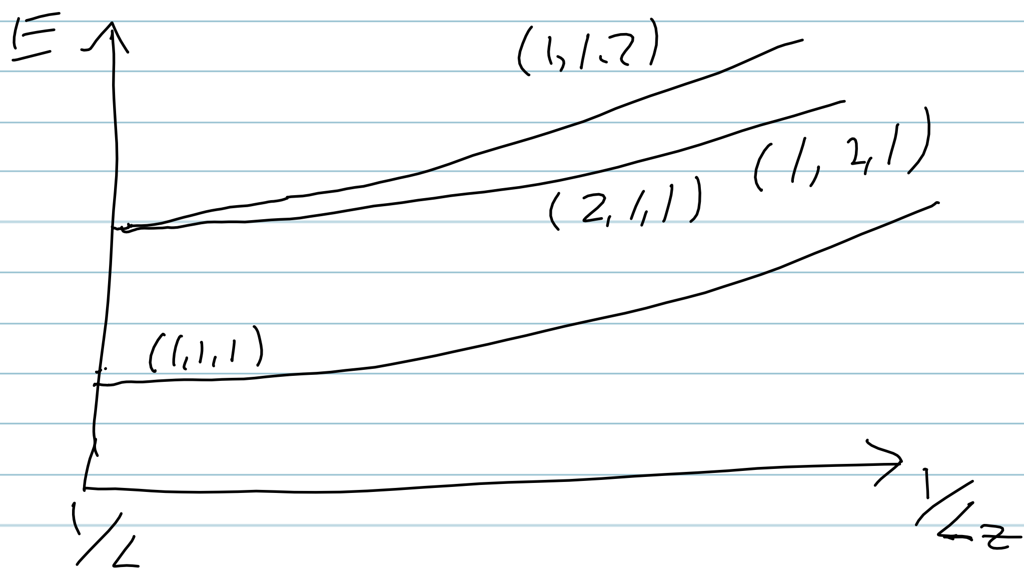
reduced symmetry $\leftrightarrow$ split degeneracies

$L_x = L_y = L \qquad L_z = 0.9L$

$$\frac{2^2}{L^2} + \frac{1^2}{L^2} + \frac{1^2}{(0.9L)^2} = \frac{1^2}{L^2} + \frac{2^2}{L^2} + \frac{1^2}{(0.9L)^2}$$

$$< \frac{1^2}{L^2} + \frac{1^2}{L^2} + \frac{2^2}{(0.9L)^2}$$

$$E_{211} = E_{121} < E_{112}$$



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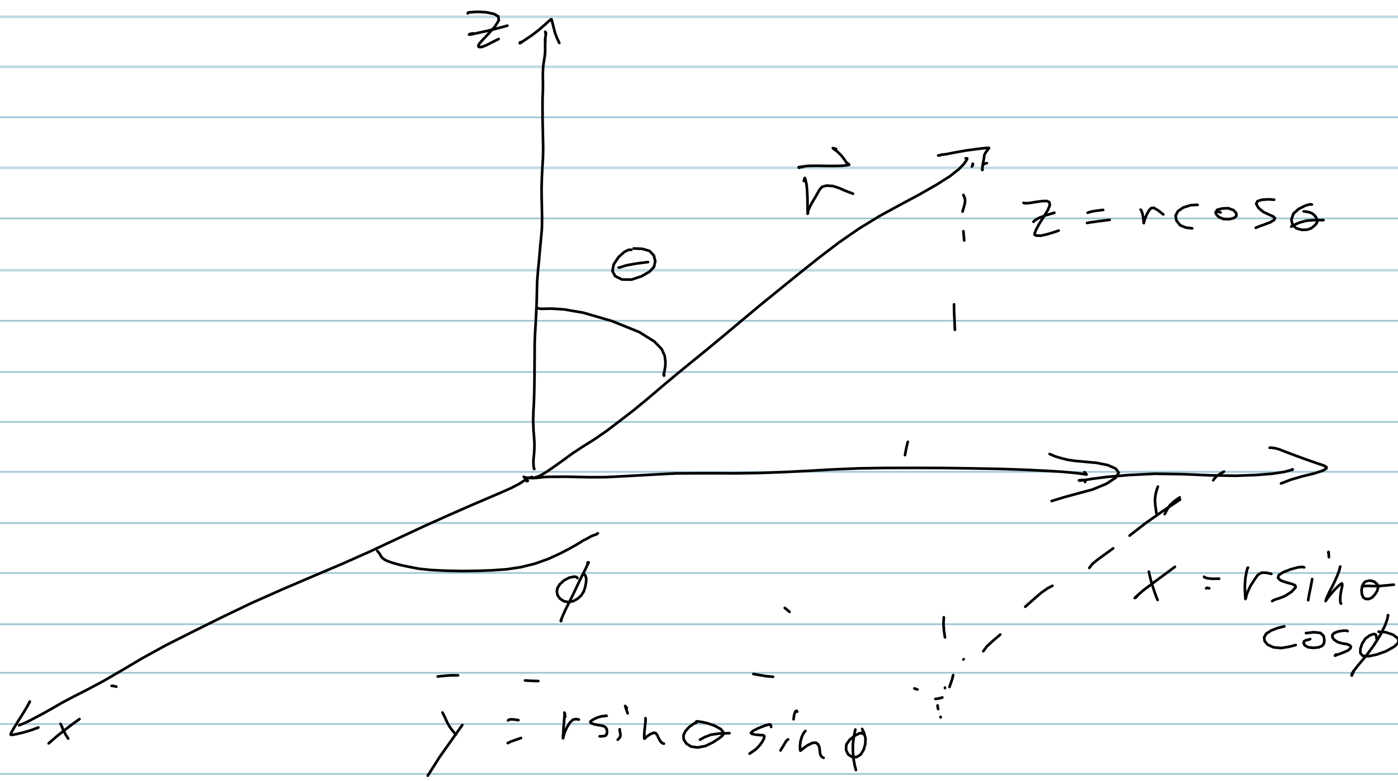
Spherical Coordinates

$$V(\vec{r}) = V(|\vec{r}|)$$



$$\nabla^2 = \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

$$dV = dx\,dy\,dz = r^2 dr \sin\theta\, d\theta\, d\phi$$

$$\psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$$

$$\nabla^2\psi = -\frac{2\mu}{\hbar^2}\left(E - V(r)\right)\psi$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\frac{1}{r^2}\left(\Theta\Phi\frac{\partial}{\partial r}\left(r^2\frac{dR}{dr}\right)+\frac{R\Phi}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\frac{R\Theta}{\sin^2\theta}\frac{d^2\Phi}{d\phi^2}\right)$$

$$= -\frac{2\mu}{\hbar^2}\left(E-V(r)\right) R\Theta\Phi$$

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\phi^2}$$

$$= -\frac{2\mu r^2}{\hbar^2}\left(E-V(r)\right)$$

$$\frac{d^2\Phi}{d\phi} = C_\phi\Phi$$

solutions: $C_\phi > 0$ exp

$C_\phi < 0$ sin, cos

$$C_\phi = -m^2$$

$$\Phi(\phi) = Ae^{im\phi}$$

$$\Phi(\phi) = \Phi(\phi+2\pi)$$

$$e^{i2\pi m} = 1$$

m integer

$m = 0, \pm 1, \pm 2, \ldots$

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m is a quantum number of what?