


* the quantum oscillator matches the
Correspondence Principle

EXpectation values

$$\bar{X} = \sum x P_x$$

$$\langle X \rangle = \int_{-\infty}^{\infty} x |\psi(x,t)|^2 dx$$


Expectation
value.

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x,t)|^2 dx$$

Uncertainty

$$\text{S.D.E} = \sigma = \sqrt{\frac{\sum (x_i - \bar{x})^2}{N}}$$

$$\sum_i \frac{x_i^2 - 2\bar{x}x_i + \bar{x}^2}{N}$$

$$\sum_i \frac{x_i^2}{N} - 2\bar{x} \sum_i \frac{x_i}{N} + \bar{x}^2 \sum_i \frac{1}{N}$$

↓

$$\overline{x^2} - 2\bar{x}\bar{x} + \bar{x}^2$$

$$\overline{x^2} - 2\bar{x}^2 + \bar{x}^2$$

$$\overline{x^2} - \bar{x}^2$$

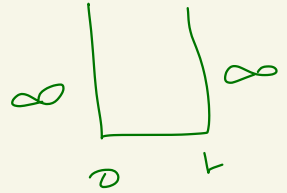
→ the uncertainty in position

$$\sigma = \sqrt{\overline{x^2} - \bar{x}^2} \quad \text{Q.M.}$$

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$\Delta P = \sqrt{\langle P^2 \rangle - \langle P \rangle^2}$$

Ex. Particle in a Box



$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$n=1 \quad \psi(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$$

$$\frac{2}{L} \int_0^L x \left(\frac{1}{2} - \frac{1}{2} \cos \frac{2\pi x}{L} \right) dx$$

$$\frac{2}{L} \left[\frac{L^2}{4} - \frac{1}{2} \int_0^L x \cos \frac{2\pi x}{L} dx \right]$$

$$-\frac{1}{2} \left[x \frac{\sin 2\pi x/L}{2\pi/L} + \frac{\cos 2\pi x/L}{2\pi^2/L^2} \right]_0^L$$

$$x \quad \cos \frac{2\pi x}{L}$$

$$1 \quad \frac{\sin \frac{2\pi x}{L}}{2\pi/L}$$

$$0 \quad \frac{-\cos \frac{2\pi x}{L}}{2\pi^2/L^2}$$

$$\frac{2}{L} \left[\frac{L^2}{4} - \cancel{\frac{1}{2} \left[0 + \frac{1}{\frac{2^2 \pi^2}{L^2}} - \frac{1}{\frac{2^2 \pi^2}{L^2}} \right]} \right]$$

$$= \frac{L}{2} = \langle x \rangle$$

What is Δx ?

$$\langle x^2 \rangle = \int_0^L x^2 |\psi|^2 dx = \frac{2}{L} \int_0^L x^2 \sin^2 \frac{\pi x}{L} dx$$

$$= \frac{2}{L} \int_0^L x^2 \left[\frac{1}{2} - \cos \frac{2\pi x}{L} \right] dx$$

$$= \frac{1}{L} \int_0^L x^2 - x^2 \cos \frac{2\pi x}{L}$$

$$\frac{1}{L} \left[\frac{x^3}{3} - \left[\cancel{\frac{x^2 \sin 2\pi x/L}{2\pi/L}} + 2x \frac{\cos 2\pi x/L}{4\pi^2/L^2} - 2 \frac{\sin 2\pi x/L}{8\pi^3/L^3} \right] \right]_0^L$$

$$\langle X^2 \rangle = \frac{X^3}{3} - 2X \frac{\cos 2\pi X/L}{4\pi^2/L^2} \Big|_0^L$$

$$\langle X^2 \rangle = \frac{L^3}{3} - \frac{2L}{4\pi^2/L^2}$$

$$\langle X^2 \rangle = \frac{1}{L} \left[\frac{L^3}{3} - \frac{L^3}{2\pi^2} \right]$$

$$\langle X^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2\pi^2}$$

$$\langle X \rangle^2 = \frac{L^2}{4}$$

$$\Delta X = \sqrt{\langle X^2 \rangle - \langle X \rangle^2} = \sqrt{\frac{L^2}{3} - \frac{L^2}{2\pi^2} - \frac{L^2}{4}}$$

$$\Delta X = 0.181L$$

$$\frac{L}{2} \pm \frac{L}{5}$$

$$\begin{array}{l} X^2 \quad \cos \frac{2\pi X}{L} \\ \quad \quad \quad + \\ 2X \quad \frac{\sin 2\pi X/L}{2\pi X/L} \\ \quad \quad \quad - \\ 2 \quad - \frac{\cos 2\pi X/L}{4\pi^2 X^2/L^2} \\ \quad \quad \quad + \\ 0 \quad - \frac{\sin 2\pi X/L}{8\pi^3 X^3/L^3} \end{array}$$

$$\langle P \rangle = \int_{-\infty}^{\infty} p |\psi|^2 dx = \int_{-\infty}^{\infty} \psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \psi dx$$

x-space

$$p = \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)$$

$$\langle P \rangle = \frac{2}{L} \frac{\hbar}{i} \int_0^L \sin \frac{\pi x}{L} \left(\frac{d}{dx} \sin \frac{\pi x}{L} \right) dx$$

$$= \frac{2\hbar}{iL} \int_0^L \sin \frac{\pi x}{L} \cos \frac{\pi x}{L} dx$$

$$= \frac{2\hbar}{iL} \int_0^L \frac{\sin \frac{2\pi x}{L}}{2} = 0$$

$$\langle p^2 \rangle = \frac{2}{L} \int_0^L \sin \frac{\pi x}{L} \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^2 \sin \frac{\pi x}{L} dx$$

$$\langle p^2 \rangle = -\frac{2}{L} (-\hbar^2) \frac{\pi}{L} \int_0^L \sin \frac{\pi x}{L} \sin \frac{\pi x}{L} dx$$

$$= \frac{2\hbar^2}{L} \frac{\pi^2}{L^2} \left(\frac{L}{2} \right) = \frac{\hbar^2 \pi^2}{L^2}$$

$$\Delta p = \frac{\pi \hbar}{L}$$

$$\Delta x \Delta p = (0.181 L) \left(\frac{\pi \hbar}{2} \right) \approx \frac{\hbar}{2} !$$

you can prove it in any case !

$\langle L \rangle, \langle K \rangle, \langle U \rangle, \langle E \rangle$

Observable Values

$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ you need them to find

the Values

Table 6.2 Common Observables and Associated Operators

Observable	Symbol	Associated Operator
Position	x	x
Momentum	p	$\frac{\hbar}{i} \frac{\partial}{\partial x}$
Potential energy	U	$U(x)$
Kinetic energy	K	$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
Hamiltonian	H	$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x)$
Total energy	E	$i\hbar \frac{\partial}{\partial t}$

$$\langle \hat{L} \rangle = \int \psi^* \hat{L} \psi dx$$

$$\psi_1 = A e^{ikx} + B e^{-ikx}$$

$$E < U$$

$$\psi_2 = C e^{-\alpha x}$$

$$\alpha = \sqrt{\frac{2m}{\hbar^2} (U - E)}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

ψ and ψ' are cont

$A \rightarrow$ incident
Reflected $\leftarrow B$

$$\text{at } x=0, \psi_1 = A + B = C$$

$$\psi_1' = A i k e^{ikx} - i k B e^{-ikx}$$

$$\psi_2' = -C \alpha e^{\alpha x}$$

$$x=0, \psi_1' = \psi_2'$$

$$i k (A - B) = -\alpha C$$

$$A + B = C$$

$$i k (A - B) = -\alpha (A + B)$$

$$i k A - B i k = -\alpha A - \alpha B$$

$$(i k + \alpha) A = (i k - \alpha) B$$

$$\frac{B}{A} = \frac{i k + \alpha}{i k - \alpha}$$

$$R = \frac{B}{A} * \left(\frac{B}{A} \right)^* = \frac{ik + \alpha}{ik - \alpha} \cdot \frac{-ik + \alpha}{-ik - \alpha}$$

Reflection
coeff

$$\frac{-ik + \alpha}{-ik - \alpha} = 1$$

classical

100% will be Reflected

C, A

$$ik(A - B) = -\alpha C$$

$$ik \cdot A + B = C \cdot ik$$

$$2ikA = C(ik - \alpha)$$

$$\frac{C}{A} = \frac{2ik}{ik - \alpha}$$

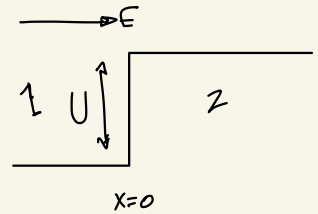
$$T = \frac{C}{A} \cdot \frac{C^*}{A} = \frac{2ik}{ik - \alpha} \cdot \frac{-2ik}{-ik - \alpha} = \frac{4k^2}{\alpha^2 + k^2} > 0$$

↓

Transmission rate

What if $E > U$?

C.M : $T = 100\%$, $R = 0\%$.



$$\frac{d^2 \psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad 0 < x$$

→ k^2

$$\psi_I = A e^{ikx} + B e^{-ikx}$$

$$x > 0$$

$$\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - U) \psi = 0$$

$$\psi = C e^{ik'x} + D e^{-ik'x}$$

$$k' = \frac{2m}{\hbar^2} (E - U)$$

$$\psi(0) \rightarrow A + B = C$$

$$\psi'(0) = \psi'_r = ik(A - B) = ik'C$$

$$ik'C = ik(A + B)$$

$$(k - k')A = (k + k')B$$

$$\frac{B}{A} = \frac{k - k'}{k + k'} =$$

$$R = \frac{(k - k')^2}{(k + k')^2} > 0$$

there is a value

$$T = \frac{4kk'}{(k+k')^2}$$

$$k' = \sqrt{\frac{2m}{\hbar} (E - U)}$$

if $E \gg U$

$$E - U = E$$

$$k \sim k'$$

$$R = 0$$

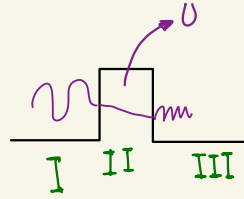
$$T = 1$$

$$E \ll U$$

$$R = 1, T = 0$$

$E \text{ high} \rightarrow T \text{ higher}$

$$U(x) \begin{cases} 0 & x < 0 & \psi_I \\ U & 0 < x < L & \psi_{II} \\ 0 & x > L & \psi_{III} \end{cases}$$



$$\psi_I = A e^{ikx} + B e^{-ikx}$$

incident Ref

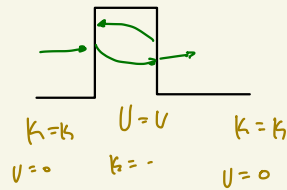
$$\psi_{III} = F e^{ikx} + \cancel{G e^{-ikx}}$$

$$\frac{d^2 \psi}{dx^2} - \frac{2m}{\hbar^2} (U - E) \psi = 0$$

$$\psi_{II}(x) = C e^{-\alpha x} + D e^{+\alpha x}$$

$$I = III$$

has the
Same E



because of the conservation of E but A is diff

Bondry conditions

$$U < E$$

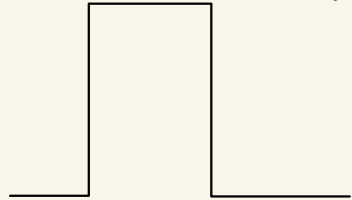
$$T = \left| \frac{F}{A} \right|^2$$

$$T = \left[1 + \frac{1}{4} \left[\frac{U^2}{E(U-E)} \right] \sinh^2 \alpha L \right]^{-1}$$

$$\alpha = \sqrt{\frac{2m}{\hbar}} (U-E)$$

$$E \gg U$$

only
solution



$$E > U$$

$$\psi_{II} = C e^{ik'x} + D e^{-ik'y}$$

ψ_I the same

ψ_{III} the same

Boundary conditions

$$T = \left[1 + \frac{1}{4} \left[\frac{U^2}{E(E-U)} \right] \sin^2 k' L \right]^{-1}$$

$$E_n = U + \frac{n^2 \pi^2 \hbar^2}{2m L^2} \longrightarrow T = 100\%$$

How at $n=1, 2, \dots$ is $R = \text{zero}$?

Constructive and destructive

U has two

central U

Coulomb $U \rightarrow U = \frac{2kZe^2}{r}$ daughter

$$T = \exp \left[-4\pi Z \sqrt{\frac{F_0}{E}} + 8 \sqrt{\frac{ZR}{r_0}} \right] \rightarrow \text{radius of}$$

$R = 1.3 A^{1/3}$
↳ mass

half life time Energy of α Particle

$$N_t \rightarrow \frac{N_0}{2}$$

$$r_0 = \text{Boh radius } \alpha = \frac{h^2}{m\alpha k e^2} = \frac{1}{7295} \approx 0.0524 \text{ nm}$$

$7.25 \times 10^{-15} \text{ m}$

$$E_0 = R$$

$$\frac{ke^2}{2r_0} = \left(\frac{a_0}{r_1}\right) \left(\frac{ke^2}{2a_0}\right) = 7245 \text{ (13.6 eV)}$$

$$= 0.0993 \text{ MeV}$$

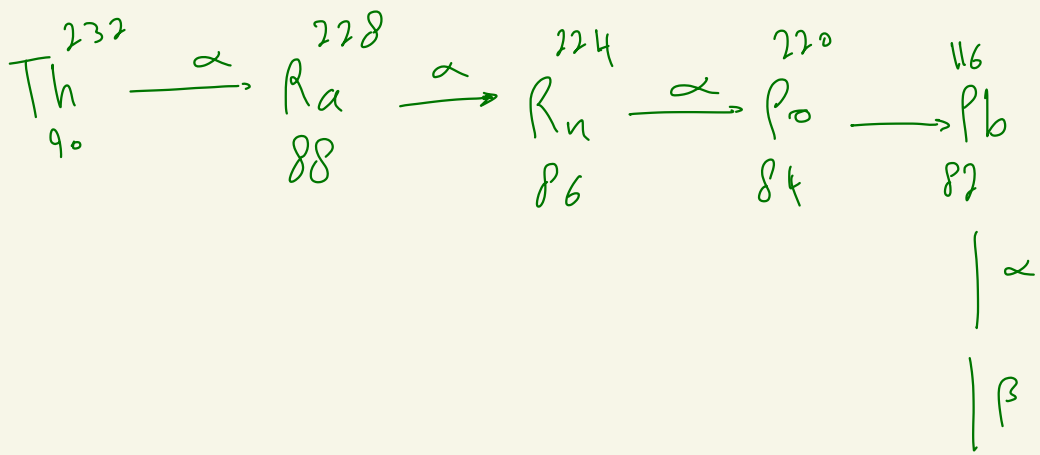
$$\lambda = \text{decay rate}$$

$$\lambda = f T = 10^{21} T$$

↓

frequency =

$$t_{1/2} = \frac{\ln 2}{\lambda} = \frac{\ln 2}{10^{21} T}$$



CH 8

A Particle in a Box

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t) + V(x) \Psi(x,t) = i\hbar \frac{\partial}{\partial t} \Psi(x,t)$$

$$V(x) \longrightarrow V(x,y,z) ; \Psi(x,t) \longrightarrow \Psi(x,y,z,t)$$

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

$$\frac{-\hbar^2}{2m} \nabla^2 \Psi(\vec{r},t) + V(\vec{r}) \Psi(\vec{r},t) = i\hbar \frac{\partial}{\partial t} \Psi(\vec{r},t)$$

if U does not

$$\text{depend on } t \implies \Psi(\vec{r},t) = \Psi(\vec{r}) \phi(t)$$

$$\frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(r) \psi(\vec{r}) = E \psi(\vec{r}) \quad \text{time-independent}$$

$$P(\vec{r}, t) = |\psi(\vec{r}, t)|^2 = |\psi(\vec{r})|^2 \quad \phi(t) = 1$$

Stationary states E

$$U = \begin{cases} 0 & 0 < x, y, z < L \\ \infty & \text{otherwise} \end{cases}$$

x, y, z are independent coordinates

$$\frac{-\hbar^2}{2m} \nabla^2 \psi(x, y, z) = E \psi(x, y, z)$$

$$\psi(x, y, z) = \psi_1(x) \psi_2(y) \psi_3(z)$$

$$\frac{-\hbar^2}{2m} \psi(x, y, z) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} \psi(x, y, z) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \psi(x, y, z) = E \psi(x, y, z)$$

$$\frac{-\hbar^2}{2m} \left[\psi_2 \psi_3 \frac{d^2 \psi_1}{dx^2} + \psi_1 \psi_3 \frac{d^2 \psi_2}{dy^2} + \psi_1 \psi_2 \frac{d^2 \psi_3}{dz^2} \right] = E \psi_1 \psi_2 \psi_3$$

$$\psi_1 \psi_2 \psi_3$$



$$\left[\frac{-\hbar^2}{2m} \frac{1}{\psi_1} \frac{d^2 \psi_1}{dx^2} \right] - \left[\frac{-\hbar^2}{2m} \frac{1}{\psi_2} \frac{d^2 \psi_2}{dy^2} \right] - \left[\frac{-\hbar^2}{2m} \frac{1}{\psi_3} \frac{d^2 \psi_3}{dz^2} \right] = E$$

$$E_1 + E_2 + E_3 = E$$

$$\frac{-\hbar^2}{2m} \frac{d^2 \psi_1}{dx^2} = E_1 \psi_1 \Rightarrow \frac{d^2 \psi_1}{dx^2} + \frac{2m E_1}{\hbar^2} \psi_1 = 0$$

$$\psi_1 = A \sin k_1 x + B \cos k_1 x$$

$$\psi_1 = A \sin k_1 x = A \sin \frac{n_1 \pi}{L} x$$

$$\psi_2 = A' \sin \frac{n_2 \pi}{L} y$$

$$\psi_3 = A'' \sin \frac{n_3 \pi}{L} z$$

$$n_1, n_2, n_3 = 1, 2, 3, \dots$$

$$\psi = \psi_1 \psi_2 \psi_3$$

$$\psi(x, y, z) = A \sin \frac{n_1 \pi x}{L} \sin \frac{n_2 \pi y}{L} \sin \frac{n_3 \pi z}{L}$$

$$1 = \iiint |\psi|^2 dx dy dz =$$

$$A^2 \int_0^L \sin^2 \frac{n_1 \pi x}{L} dx \int_0^L \sin^2 \frac{n_2 \pi y}{L} dy \int_0^L \sin^2 \frac{n_3 \pi z}{L} dz = 1$$

$$A^2 \int_0^L \left[\frac{1}{2} - \frac{1}{2} \cos \frac{2n_1 \pi x}{L} \right] dx \dots \dots$$

$$A^2 \cdot \frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{2} = 1$$

$$A^2 \left(\frac{L}{2} \right)^3 = 1$$

$$A = \left(\frac{2}{L} \right)^{3/2}$$

$$E = E_1 + E_2 + E_3$$



$$\Psi(L) = 0$$

$$p = \frac{h}{\lambda}$$

$$\Psi_1 = A \sin k_1 L = 0$$

$$k_1 L = n\pi \implies k_1 = \frac{n\pi}{L}, \quad k_1 = \frac{2\pi}{\lambda} \rightarrow \frac{p}{\hbar}$$

$$\rightarrow k_1 = \frac{p}{\hbar} \rightarrow p = \hbar k_1 \rightarrow p = \frac{n\pi \hbar}{L}$$

$$E_1 = \frac{p^2}{2m} = \frac{n_1^2 \pi^2 \hbar^2}{2L^2 m}$$

$$E_2 = \frac{n_2^2 \pi^2 \hbar^2}{2L^2 m}$$

$$E = E_1 + E_2 + E_3 = \frac{\hbar^2 \pi^2}{2mL^2} \overbrace{(n_1^2 + n_2^2 + n_3^2)}^{n^2}$$

$$E_3 = \frac{n_3 \pi^2 \hbar^2}{2L^2 m}$$

total

$$\Psi_{n_1, n_2, n_3} = \left(\frac{2}{L}\right)^{3/2} \sin \frac{n_1 \pi x}{L} \sin \left(\frac{n_2 \pi y}{L}\right) \sin \left(\frac{n_3 \pi z}{L}\right) e^{-i E_{n_1, n_2, n_3} t / \hbar}$$

$$\Psi = \Psi(\vec{r}) e^{-i E t / \hbar} \quad v = \frac{E}{\hbar}$$

$$E_{n_1, n_2, n_3} = \frac{\pi^2 \hbar^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2)$$

* Ψ_{21} and Ψ_{12} have the same Energy

but different wavefunction "called degenerate, degeneracy"

$$\Psi_{221} = A \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right) e^{-iE_{221}t/\hbar}$$

$$\Psi_{212} = A \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{2\pi z}{L}\right) e^{-iE_{212}t/\hbar}$$

$$\Psi_{122} = A \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \sin\left(\frac{2\pi z}{L}\right) e^{-iE_{122}t/\hbar}$$

$$E_{221} = E_{212} = E_{122} = \frac{9\pi^2\hbar^2}{2mL^2}$$

Table 8.1 Quantum Numbers and Degeneracies of the Energy Levels for a Particle Confined to a Cubic Box*

n_1	n_2	n_3	n^2	Degeneracy
1	1	1	3	None
1	1	2	6	Threefold
1	2	1	6	
2	1	1	6	
1	2	2	9	Threefold
2	1	2	9	
2	2	1	9	
1	1	3	11	Threefold
1	3	1	11	
3	1	1	11	
2	2	2	12	None

*Note: $n^2 = n_1^2 + n_2^2 + n_3^2$.

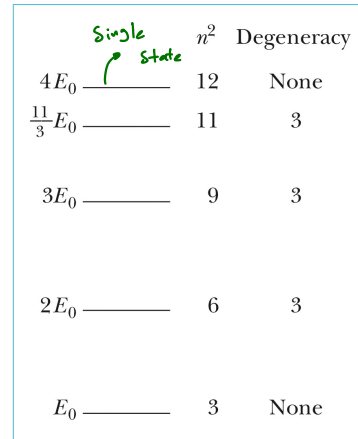


Figure 8.3 An energy-level diagram for a particle confined to a cubic box. The ground-state energy is $E_0 = 3\pi^2\hbar^2/2mL^2$, and $n^2 = n_1^2 + n_2^2 + n_3^2$. Note that most of the levels are degenerate.

I will see the difference
if I apply m or E field force

if it is not cube:

$$E_{n_1, n_2, n_3} = \frac{\pi^2 \hbar^2}{2m} \left[\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right]$$

Real case H atom

$$U(r) = - \frac{Z k e^2}{r}$$

r : the radius

θ = the angle
between z and r

ϕ = is the projection
for x, y plane

$$\frac{-\hbar^2}{2m_e} \nabla^2 \Psi(\vec{r}) + U(r) \Psi(\vec{r}) = E \Psi(\vec{r})$$

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

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

$$\frac{\partial^2 \phi}{\partial \phi^2} + m_l^2 \phi(\phi) = 0$$

m_l : magnetic quantum number = integer

$$\Phi(\phi) = \exp(im_l \phi)$$

$$e^{im_l \phi} = e^{im_l(\phi + 2\pi)} = e^{im_l \phi} e^{im_l 2\pi}$$

↑
1
integer

m_l
 P_l

Orbital quantum number

$$m_l = 0, \pm 1, \pm 2, \dots, \pm l$$

$$l = 0, 1, 2, 3, \dots, \text{max}$$

↓
+ only

$$\psi_l^{m_l} = \Theta(\theta) \Phi_l^{m_l}(\phi) e^{im_l \phi}$$

$$\begin{aligned} P_0^0 &= 1 \\ P_1^0 &= 2 \cos \theta \\ P_1^1 &= \sin \theta \\ P_2^0 &= 4(3 \cos^2 \theta - 1) \\ P_2^1 &= 4 \sin \theta \cos \theta \\ P_2^2 &= \sin^2 \theta \\ P_3^0 &= 24(5 \cos^3 \theta - 3 \cos \theta) \\ P_3^1 &= 6 \sin \theta (5 \cos^2 \theta - 1) \\ P_3^2 &= 6 \sin^2 \theta \cos \theta \\ P_3^3 &= \sin^3 \theta \end{aligned}$$

Table 8.3 The Spherical Harmonics $Y_l^{m_l}(\theta, \phi)$

$$\begin{aligned} Y_0^0 &= \frac{1}{2\sqrt{\pi}} \\ Y_1^0 &= \frac{1}{2} \sqrt{\frac{3}{\pi}} \cdot \cos \theta \\ Y_1^{\pm 1} &= \pm \frac{1}{2} \sqrt{\frac{3}{2\pi}} \cdot \sin \theta \cdot e^{\pm i\phi} \\ Y_2^0 &= \frac{1}{4} \sqrt{\frac{5}{\pi}} \cdot (3 \cos^2 \theta - 1) \\ Y_2^{\pm 1} &= \pm \frac{1}{2} \sqrt{\frac{15}{2\pi}} \cdot \sin \theta \cdot \cos \theta \cdot e^{\pm i\phi} \\ Y_2^{\pm 2} &= \frac{1}{4} \sqrt{\frac{15}{2\pi}} \cdot \sin^2 \theta \cdot e^{\pm 2i\phi} \\ Y_3^0 &= \frac{1}{4} \sqrt{\frac{7}{\pi}} \cdot (5 \cos^3 \theta - 3 \cos \theta) \\ Y_3^{\pm 1} &= \pm \frac{1}{8} \sqrt{\frac{21}{\pi}} \cdot \sin \theta \cdot (5 \cos^2 \theta - 1) \cdot e^{\pm i\phi} \\ Y_3^{\pm 2} &= \frac{1}{4} \sqrt{\frac{105}{2\pi}} \cdot \sin^2 \theta \cdot \cos \theta \cdot e^{\pm 2i\phi} \\ Y_3^{\pm 3} &= \pm \frac{1}{8} \sqrt{\frac{35}{\pi}} \cdot \sin^3 \theta \cdot e^{\pm 3i\phi} \end{aligned}$$

it lefts $R!$

$\Psi = Y_{\ell}^{m_{\ell}}(\theta, \phi)$

 spherical harmonics

 the same for all the atoms

$E_{n, \ell}$

quantized

$L = \sqrt{\ell(\ell+1)} \hbar$ for $\ell = 0, 1, 2, \dots$

total angular momentum orbital

for the same $r \rightarrow$ different ℓ

$\vec{L} = L_x, L_y, L_z$

 Changing

 constant

quantized

$L_z = m_{\ell} \hbar$ for $m_{\ell} = 0, \pm 1, \pm 2, \dots, \pm \ell$

quantized!

$\cos \theta = \frac{L_z}{|L|} = \frac{m_{\ell} \hbar}{\sqrt{\ell(\ell+1)} \hbar}$

* E does not depend on m_{ℓ}

* Ψ depends on m_{ℓ}

Different solutions with the same E . ("degeneracy")

$2\ell + 1 \Rightarrow$ degree of degeneracy

How many states with the same E ?

$L_x, L_y =$ can not be calculated

Table 8.5 Spectroscopic Notation for Atomic Shells and Subshells

n	Shell Symbol	ℓ	Shell Symbol
1	K	0	s
2	L	1	p
3	M	2	d
4	N	3	f
5	O	4	g
6	P	5	h
...		...	

it lefts $R!$

only for H and H like atom (one e^- only)

$$E_n = \left(\frac{ke^2}{2a_0} \right) \left(\frac{Z^2}{n^2} \right) \quad n = 1, 2, 3, \dots \quad E_n = -\frac{13.6 \text{ eV}}{n^2}$$

$Z = 1$ for H

n = Principal quantum number $1, 2, 3, \dots$

L = angular momentum quantum number $0, 1, 2, 3, \dots, n-1$

m_l = magnetic quantum number $0, \pm 1, \pm 2, \dots, \pm l$

l = orbital quantum number

the degree of degeneracy is $= n^2$

Table 8.4 The Radial Wavefunctions $R_{n\ell}(r)$ of Hydrogen-like Atoms for $n = 1, 2$, and 3

n	ℓ	$R_{n\ell}(r)$
1	0	$\left(\frac{Z}{a_0}\right)^{3/2} 2e^{-Zr/a_0}$
2	0	$\left(\frac{Z}{2a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$
2	1	$\left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{\sqrt{3}a_0} e^{-Zr/2a_0}$
3	0	$\left(\frac{Z}{3a_0}\right)^{3/2} 2 \left[1 - \frac{2Zr}{3a_0} + \frac{2}{27} \left(\frac{Zr}{a_0}\right)^2\right] e^{-Zr/3a_0}$
3	1	$\left(\frac{Z}{3a_0}\right)^{3/2} \frac{4\sqrt{2}}{3} \frac{Zr}{a_0} \left(1 - \frac{Zr}{6a_0}\right) e^{-Zr/3a_0}$
3	2	$\left(\frac{Z}{3a_0}\right)^{3/2} \frac{2\sqrt{2}}{27\sqrt{5}} \left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$

Selection Rules

forbidden = impossible

$$\Delta \ell = \pm 1 \quad |\Delta \ell| = 1$$

$$\Delta n > 1$$

Probability density for r

$$P(r) = r^2 |R_{n,l}(r)|^2$$

$$P(\theta, \phi) = |\Theta_{l,m_l}(\theta) \Phi_{m_l}(\phi)|^2$$