Lecture 1

(One body) Central Force Problem
Three dimension

$$V(x, y, z) = V(r)$$

Schrodinger equation in spherical coordinate
(See Appendix A)

Seperation of variable

Time - dependent Schrodinger equation

$\downarrow$ V independent of time

time - independent Schrodinger equation

$$\hat{H}\psi_E = E\psi_E$$

$\downarrow$

eigenvalue problem

$V(r)$:

$$\psi(r, \theta, \phi) = R(r)\,Y(\theta, \phi)$$

Radial Equation $\longrightarrow$ dependent on $V(r)$

$$\left.\begin{array}{l}\theta \text{ equation}\\ \phi \text{ equation}\end{array}\right\} \text{independent of } V(r)$$

These equations are ordinary differential equations

Central force problem. $V(x,y,z) = V(r)$

$$r = \sqrt{x^2+y^2+z^2}$$

Obviously, it is more convenient to use the spherical coordinate

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right]$$

$$\mu \quad + V(r)\psi = E\psi$$

[$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$
are proved in various books on mathematical physics.
In the AppendixA]

Since $V(r)$ is a function of r only, we shall try to solve the problem using the method of seperation of variable

$\psi(r,\theta,\phi) \rightarrow$ time independent wave function

$$[\ \psi(r,\theta,\phi,t) = \psi_E(r,\theta,\phi)e^{-iEt/\hbar}\ ]$$

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$$

Substitute into the time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R^2}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]$$

$$+ V(r)RY = ERY$$

Divide by YR and rearrange. (multiple $-\frac{2mr^2}{\hbar^2}$)

$$\Rightarrow \left\{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}[V(r)-E]\right.$$

$$= -\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right.$$

Derivation of Some General Relations

The Cartesian coordinates (x, y, z) of a vector $\vec{r}$ are related to its spherical polar coordinates (r, θ, φ) by

$$x = r \sin\theta \cos\varphi, \qquad y = r \sin\theta \sin\varphi, \qquad z = r \cos\theta \tag{B.1}$$

The orthonormal Cartesian basis $(\hat{x}, \hat{y}, \hat{z})$ is related to its spherical counterpart $(\hat{r}, \hat{\theta}, \hat{\varphi})$ by

$$\hat{x} = \hat{r} \sin\theta \cos\varphi + \hat{\theta} \cos\theta \cos\varphi - \hat{\varphi} \sin\varphi \tag{B.2}$$

$$\hat{y} = \hat{r} \sin\theta \sin\varphi + \hat{\theta} \cos\theta \sin\varphi + \hat{\varphi} \cos\varphi, \tag{B.3}$$

$$\hat{z} = \hat{r} \cos\theta - \hat{\theta} \sin\theta. \tag{B.4}$$

Differentiating (B.1), we obtain

$$dx = \sin\theta \cos\varphi \, dr + r \cos\theta \cos\varphi \, d\theta - r \sin\theta \sin\varphi \, d\varphi \tag{B.5}$$

$$dy = \sin\theta \sin\varphi \, dr + r \cos\theta \sin\varphi \, d\theta + r \cos\varphi \, d\varphi, \tag{B.6}$$

$$dz = \cos\theta \, dr - r \sin\theta \, d\theta. \tag{B.7}$$

Solving these equations for dr, $d\theta$ and $d\varphi$, we obtain

$$dr = \sin\theta \cos\varphi \, dx + \sin\theta \sin\varphi \, dy + \cos\theta \, dz \tag{B.8}$$

$$d\theta = \frac{1}{r} \cos\theta \cos\varphi \, dx + \frac{1}{r} \cos\theta \sin\varphi \, dy - \frac{1}{r} \sin\theta \, dz, \tag{B.9}$$

$$d\varphi = -\frac{\sin\varphi}{r \sin\theta} dx + \frac{\cos\varphi}{r \sin\theta} dy. \tag{B.10}$$

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We can verify that (B.5) to (B.10) lead to

$$\frac{\partial r}{\partial x} = \sin\theta\cos\varphi, \qquad \frac{\partial \theta}{\partial x} = \frac{1}{r}\cos\varphi\cos\theta, \qquad \frac{\partial \varphi}{\partial x} = -\frac{\sin\varphi}{r\sin\theta}, \tag{B.11}$$

$$\frac{\partial r}{\partial y} = \sin\theta\sin\varphi, \qquad \frac{\partial \theta}{\partial y} = \frac{1}{r}\sin\varphi\cos\theta, \qquad \frac{\partial \varphi}{\partial y} = \frac{\cos\varphi}{r\sin\theta}, \tag{B.12}$$

$$\frac{\partial r}{\partial z} = \cos\theta, \qquad \frac{\partial \theta}{\partial z} = -\frac{1}{r}\sin\theta, \qquad \frac{\partial \varphi}{\partial z} = 0, \tag{B.13}$$

which, in turn, yield

$$\begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial x} \\ &= \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\varphi\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\theta}, \end{aligned} \tag{B.14}$$

$$\begin{aligned} \frac{\partial}{\partial y} &= \frac{\partial}{\partial r}\frac{\partial r}{\partial y} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial y} + \frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial y} \\ &= \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}, \end{aligned} \tag{B.15}$$

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial r}\frac{\partial r}{\partial z} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial z} + \frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{\partial r}\frac{\partial}{\partial\theta}. \tag{B.16}$$

B.2 Gradient and Laplacian in Spherical Coordinates

We can show that a combination of (B.14) to (B.16) allows us to express the operator $\vec{\nabla}$ in spherical coordinates:

$$\vec{\nabla} = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}, \tag{B.17}$$

and also the Laplacian operator ∇^2

$$\nabla^2 = \vec{\nabla}.\vec{\nabla} = \left(\hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial\theta} + \frac{\hat{\varphi}}{r\sin\varphi}\frac{\partial}{\partial\varphi}\right)\cdot\left(\hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial\theta} + \frac{\hat{\varphi}}{r\sin\theta}\frac{\partial}{\partial\varphi}\right). \tag{B.18}$$

Now, using the relations

$$\frac{\partial\hat{r}}{\partial r} = 0, \qquad \frac{\partial\hat{\theta}}{\partial r} = 0, \qquad \frac{\partial\hat{\varphi}}{\partial r} = 0, \tag{B.19}$$

$$\frac{\partial\hat{r}}{\partial \theta} = \hat{\theta}, \qquad \frac{\partial\hat{\theta}}{\partial \theta} = -\hat{r}, \qquad \frac{\partial\hat{\varphi}}{\partial \theta} = 0, \tag{B.20}$$

$$\frac{\partial\hat{r}}{\partial \varphi} = \hat{\varphi}\sin\theta, \qquad \frac{\partial\hat{\theta}}{\partial \varphi} = \hat{\varphi}\cos\theta, \qquad \frac{\partial\hat{\varphi}}{\partial \varphi} = -\hat{r}\sin\theta - \hat{\theta}\cos\theta, \tag{B.21}$$

we can show that the Laplacian operator reduces to

$$\nabla^2 = \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]. \tag{B.22}$$

LHS is function of r only

RHS is function of θ, ϕ

$\Rightarrow$ must be constant

For reasons that will appear in the due course, we shall choose the "seperation constant" to be $\ell(\ell+1)$

$$\Rightarrow \underbrace{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}[V(r)-E] = \ell(\ell+1)}_{\text{radial equation, depend on } V(r)}$$

$$\underbrace{\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = -\ell(\ell+1)}_{\text{angular equation, independent of } V(r)}$$

Multiply $Y\sin^2\theta$

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1)\sin^2\theta\, Y.$$

Again, try seperation of variables

Ansatz $\qquad Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$

Put it into above equation, divide through by $\Theta\Phi$, and rearrange

$$\Rightarrow \frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \ell(\ell+1)\sin^2\theta\right]$$
$$= -\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}$$

LHS is function of θ only
RHS is function of ϕ only

$$\Rightarrow \underbrace{\frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right] + \ell(\ell+1)\sin^2\theta = m^2}_{\theta \text{ equation}}$$

$$\underbrace{\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2}_{\phi \text{ equation}}$$

ϕ equation

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2$$

$$\Phi(\phi) = e^{\pm im\phi}$$

Physical Requirement

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

$\downarrow$

single-valueness

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

θ equation

$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi$$

$\Rightarrow \quad \Phi(\phi) = e^{im\phi}$ Normalization $\frac{1}{\sqrt{2\pi}}$

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

$\downarrow$ single-valueness of the wave function

$\Rightarrow \quad e^{2\pi i m} = 1 \Rightarrow$ m must be integer.

· This is closely related to the quantization of angular momentum.

· m is known as magnetic quantum number.

Θ - equation

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + [\ell(\ell+1)\sin^2\theta - m^2]\Theta = 0$$

Note: $m = 0, \pm 1, \pm 2, \cdots$

Change variable $x = \cos\theta$

[using the chain rule

$$\frac{d}{d\theta} = \frac{dx}{d\theta}\frac{d}{dx} = -\sin\theta\frac{d}{dx} = -\sqrt{1-x^2}\frac{d}{dx}$$

$\sin^2\theta = 1 - x^2$]

The above equation becomes

$$(1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx} + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right]\Theta = 0$$

$\downarrow$ associated Legendre equation.

Physical requirement:

$\Theta(x)$ must be well-behaved at $x = \pm 1$

$\Rightarrow$ ℓ must be integers, i.e. $\ell = 0, 1, 2, \cdots$

m must be from $-\ell$ to ℓ, i.e.,

$m = -\ell, -\ell+1, -\ell+2, \cdots -1, 0, +1, \cdots \ell-2, \ell-1, \ell$

Θ is labelled by ℓ, m

$\Theta(x) \propto P_\ell^m(x) \rightarrow$ associated Legendre polynomial

A more general discussion of Legendre equation, Legendre polynomial is given in Appendix. B.

Radial equation depends on the $V(r)$ given, and will be discussed later.

Appendix B

Legendre Equation

1. Legendre Equation and Legendre Polynomial

$$\frac{d}{dx}(1-x^2)\frac{dy}{dx} + \mu y = 0$$

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \mu y = 0$$

Legendre equation

Physical requirement: when $x = \cos\theta$, $y(x)$ is a physical quantity, we would require $y(x)$ to be finite in $-1 \le x \le 1$

We want to show this requirement can only be met for

$$\mu = n(n+1) \quad , \text{ where } n \text{ is integer}$$

$\ell(\ell+1)$

Use a series expansion

$$y(x) = \sum_{k=0}^{\infty} c_k x^k$$

Substitute back into the Legendre equation

$$(1-x^2)\sum_{k=0}^{\infty} c_k k(k-1)x^{k-2} - 2x\sum_{k=0}^{\infty} c_k k x^{k-1} + \mu\sum_{k=0}^{\infty} c_k x^k = 0$$

Compare coefficient of x^k

$$c_{k+2}(k+2)(k+1) - c_k k(k-1) - 2c_k k + \mu c_k = 0$$

$$\Rightarrow \quad c_{k+2} = \frac{k(k+1)-\mu}{(k+1)(k+2)} c_k$$

recursive formula

$$y(x) = y_1(x) + y_2(x)$$

$$= \underbrace{\sum_{k=0}^{\infty} c_{2k} x^{2k}}_{\text{even terms}} + \underbrace{\sum_{k=0}^{\infty} c_{2k+1} x^{2k+1}}_{\text{odd terms}}$$

$$c_k = \frac{(k-2)(k-1)-\mu}{k(k-1)}\, c_{k-2}$$

$$= \frac{1}{k}\left[1-\frac{\mu}{(k-1)(k-2)}\right](k-2)\, c_{k-2}$$

$$= \frac{1}{k}\left[1-\frac{\mu}{(k-1)(k-2)}\right]\left[1-\frac{\mu}{(k-3)(k-4)}\right] c_{k-4}$$

$$= \frac{1}{k}\left[1-\frac{\mu}{(k-1)(k-2)}\right]\left[1-\frac{\mu}{(k-3)(k-4)}\right]\cdots\left[1-\frac{\mu}{(N+1)N}\right] N c_N$$

As N sufficient large, with μ fixed

$$c_k \longrightarrow \frac{1}{k}\underbrace{M}_{\text{constant, i.e., } N c_N}$$

Even term $y_1(x)$ asymptotically has the form

$$\sum_{2m>N} \frac{M}{2m} x^{2m}$$

$\downarrow$ has the same form as $-\frac{M}{2}\left[\ln(1+x)+\ln(1-x)\right] = z_1(x)$

Odd term $y_2(x)$ asymptotically has the form

$$\sum_{2m+1>N} \frac{M}{2m+1} x^{2m+1}$$

$\downarrow$ has the same form as $\frac{M}{2}\left[\ln(1+x)-\ln(1-x)\right] = z_2(x)$

Note: $z_1(x)$, $z_2(x)$ both are divergent at $x=\pm 1$

To insure $y(x)$ to be finite for $-1 \le x \le 1$, there are two possible solutions

(i) Choose $c_0 = 0 \Rightarrow y_1(x) = 0$, and truncate $y_2(x)$

$\Rightarrow \mu = \overset{\ell(\ell+1)}{n(n+1)}$ where n is an odd integers

(ii) Choose $c_1 = 0 \Rightarrow y_2(x) = 0$, and truncate $y_1(x)$

$\Rightarrow \mu = \overset{\ell(\ell+1)}{n(n+1)}$ where n is an even integer

$\Rightarrow$ Legendre polynomial

Since Legendre equation is linear, we can choose the normalization constant

With $\mu = n(n+1)$, we shall choose

$$C_n = \frac{(2n)!}{2^n (n!)^2} \Rightarrow P_n(1) = 1$$

Use the recursive formula and by induction, it can be shown that

$$C_{n-2r} = (-1)^r \frac{(2n-2r)!}{2^n r!(n-r)!(n-2r)!}, \quad r = 0, 1, 2, \cdots, [\tfrac{n}{2}]$$

$$[\tfrac{n}{2}] = \frac{n}{2} \quad \text{if } n \text{ is even}$$

$$= \frac{n-1}{2} \quad \text{if } (n-1) \text{ is odd}$$

$$\Rightarrow \underbrace{P_n(x) = \sum_{r=0}^{[\frac{n}{2}]} (-1)^r \frac{(2n-2r)!}{2^n r!(n-r)!(n-2r)!} x^{n-2r}}_{\text{Legendre polynomial}}$$

Note, the method is similar to the one use for Hermite polynomial.

2. Rodrigues Formula

$$(x^2-1)^n = \sum_{r=0}^{n} \frac{(-1)^r n!}{r!(n-r)!} x^{2n-2r}$$

$$\frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2-1)^n = \frac{1}{2^n n!} \sum_{r=0}^{n} \frac{(-1)^r n!}{r!(n-r)!} \frac{d^n}{dx^n} x^{2n-2r}$$

$$= \frac{1}{2^n n!} \sum_{r=0}^{[\frac{n}{2}]} \frac{(-1)^r n!}{r!(n-r)!} (2n-2r)(2n-2r-1)\cdots(n-2r+1) x^{n-2r}$$

$$= \frac{1}{2^n} \sum_{r=0}^{[\frac{n}{2}]} (-1)^r \frac{(2n-2r)!}{r!(n-r)!(n-2r)!} x^{n-2r}$$

$$= P_n(x)$$

$$\Rightarrow \underbrace{P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2-1)^n}_{\text{Rodrigues formula}}$$

3. Generating Function

$$F(x, z) = \frac{1}{\sqrt{1-2xz+z^2}} = \sum_{n=0}^{\infty} z^n P_n(x)$$

$r=0 \qquad C_n = (-1)^0 \frac{(2n)!}{2^n 0!\, n!\, n!}$

$= \frac{2n!}{2^n (n!)^2}$

$r=1$

$C_{n-2} = (-1) \frac{(2n-2)!}{2^n 1!\,(n-1)!\,(n-2)!}$

$k+2=n$, the recursive relation reads

$C_n \overset{?}{=} \frac{(n-2)(n-1)-n(n+1)}{(n-1)\,n} C_{n-2}$ $\qquad n^2-3n+2-n^2-n = -4n+2$

$C_n = \frac{-4n+2}{n(n+1)} C_{n-2}$

$\parallel \qquad$ (-1) has been absorbed

$\frac{2n!}{2^n (n!)^2} \overset{?}{=} \frac{4n-2}{n(n-1)} \frac{(2n-2)!}{2^n (n-1)!\,(n-2)!}$

$\frac{2\cancel{n}\cdot(2n-1)\cdot\cancel{(2n-2)!}}{\cancel{(n-1)!}\, \cancel{n}\, \cancel{(n)(n-1)(n-2)!}} = \frac{4n-2}{n(n-1)} \frac{\cancel{(2n-2)!}}{\cancel{(n-1)!\,(n-2)!}}$

$\downarrow$

obviously, the equation is satisfied

Claim

$$C_{n-2r} = (-1)^r \frac{(2n-2r)!}{2^n r!(n-r)!(n-2r)!}$$

satisfies the normalization

$$C_n = \frac{(2n)!}{2^n (n!)^2}$$

this we can choose
since the equation
is linear

and the recursive relation

$$C_{k+2} = \frac{k(k+1) - n(n+1)}{(k+1)(k+2)} C_k$$

We need to prove

$$C_{n-2r} = \underbrace{\frac{(n-2r-2)(n-2r-1) - n(n+1)}{(n-2r-1)(n-2r)}}_{(I)} C_{n-2r-2}$$

$$n-2r = k+2 \quad \Rightarrow \quad k = n-2r+2$$

Now the upstair of (I)

$$\begin{aligned}
&= (n-2r)^2 - 3(n-2r) + 2 - n^2 - n \\
&= \cancel{n^2} - 4rn + 4r^2 - 3n + 6r + 2 - \cancel{n^2} - n \\
&= 4r^2 - 4rn - 4n + 6r + 2 \\
&= 4r^2 + 6r + 2 - 4n(r+1) \\
&= (r+1)\,[4r + 2 - 4n]
\end{aligned}$$

$\Rightarrow$ We need to prove

$$C_{n-2r} \overset{?}{=} \frac{(r+1)(4r+2-4n)}{(n-2r-1)(n-2r)} C_{n-2r-2}$$

$$\cancel{(-1)^r} \frac{(2n-2r)!}{\cancel{2^n} r!(n-r)!(n-2r)!} \overset{?}{=} \frac{\cancel{(r+1)}(4r+2-4n)}{(n-2r-1)(n-2r)} \frac{(2n-2r-2)!\ (-1)^{r+1}}{2^n \cancel{(r+1)!}(n-r-1)!(n-2r-2)!}$$

$$\frac{(2n-2r)(2n-2r-1)\,(2n-2r-2)!}{(n-r-1)!\,\underbrace{(n-r)}_{}\cdot(n-2r-2)!(n-2r-1)(n-2r)} \overset{?}{=} \frac{(4n-4r-2)}{(n-2r)(n-2r-1)} \frac{(2n-2r-2)!}{(n-r-1)!(n-2r-2)!}$$

$$\| \\ 4n-4r-2$$

∴ Obviously, the recursive equation is satisfied. ⇒ Equation (A)

$$(1-2xz+z^2)^{-\frac{1}{2}} = [1-z(2x-z)]^{-\frac{1}{2}}$$

$$= \sum_{m=0}^{\infty} (-1)^m \binom{-\frac{1}{2}}{m} z^m \underbrace{(2x-z)^m}_{\sum_{r=0}^{m} (-1)^r \binom{m}{r} z^r 2^{m-r} x^{m-2}}$$

$$= \sum_{n=0}^{\infty} z^n \sum_{m=0}^{n} (-1)^m \binom{-\frac{1}{2}}{m} (-1)^{n-m} \binom{m}{n-m} \underset{\downarrow\, 2^{2m-n}}{2^{m-(n-m)}} \underset{\downarrow\, x^{2m-n}}{x^{m-(n-m)}}$$

$\downarrow$ rearrange terms $\quad m+r=n \quad \binom{-\frac{1}{2}}{m} = (-1)^m \frac{1\cdot 3\cdot 5\cdots 2m-1}{2\cdot 4\cdot 6\cdots 2m}$

If we define $(1-2xz+z^2) = \sum_{n=0}^{\infty} z^n P_n(x)$, then $P_n(x)$ is a polynomial of degree n.

Now we shall show $P_n(x)$ defined here satisfies the Legendre equation

$$\frac{1}{(1-2xz+z^2)^{\frac{1}{2}}} = \sum z^n P_n(x)$$

Differentiate with respect to x

$$\frac{-\frac{1}{2}(-2z)}{(1-2xz+z^2)^{3/2}} = \sum_{n=0}^{\infty} z^n \frac{dP_n(x)}{dx}$$

$$\Rightarrow \frac{z}{(1-2xz+z^2)^{3/2}} = \sum_{n=0}^{\infty} z^n \frac{dP_n(x)}{dx}$$

Differentiate with respect to x again

$$\frac{z(-\frac{3}{2})(-2z)}{(1-2xz+z^2)^{5/2}} = \sum_{n=0}^{\infty} z^n \frac{d^2P_n(x)}{dx^2}$$

$$\Rightarrow \sum_{n=0}^{\infty} z^n \left[(1-x^2)\frac{d^2P_n(x)}{dx^2} - 2x\frac{dP_n(x)}{dx}\right]$$

$$= \frac{(1-x^2)3z^2}{(1-2xz+z^2)^{5/2}} - \frac{2xz}{(1-2xz+z^2)^{3/2}}$$

$$= \frac{3z^2-3z^2x^2-2xz+4x^2z^2-2xz^3}{(1-2xz+z^2)^{5/2}}$$

$$= \frac{3z^2-2xz+x^2z^2-2xz^3}{(1-2xz+z^2)^{5/2}}$$

Differentiate with respect to z

$$\frac{(-\frac{1}{2})(-2x+2z)}{(1-2xz+z^2)^{3/2}} = \sum_{n=0}^{\infty} n z^{n-1} P_n(x)$$

$$\frac{(x-z)}{(1-2xz+z^2)^{3/2}} z^2 = \sum_{n=0}^{\infty} n z^{n+1} P_n(x)$$

Differentiate with respect to z

$$(x-z)z^2 \cdot \frac{3(x-z)}{(1-2xz+z^2)^{5/2}} + \frac{2zx-3z^2}{(1-2xz+z^2)^{3/2}} = \sum_{n=0}^{\infty} n(n+1) z^n P_n(x)$$

$$\frac{3z^2(x^2-2xz+z^2)+(2zx-3z^2)(1-2zx+z^2)}{(1-2xz+z^2)^{5/2}} = \sum_{n=0}^{\infty} n(n+1)z^n P_n(x)$$

$$\frac{2xz-x^2z^2+2z^3x-3z^2}{(1-2xz+z^2)^{5/2}} = \sum_{n=0}^{\infty} (n+1)n z^n P_n(x) \checkmark$$

$$\Rightarrow \sum_{n=0}^{\infty} z^n \left[(1-x^2)\frac{d^2P_n(x)}{dx^2} - 2x\frac{dP_n(x)}{dx} + n(n+1)P_n(x)\right] = 0$$

$\Rightarrow$ $P_n(x)$ satisfies the Legendre equation.

Then we compare the expression of $P_0(x)$ and $P_1(x)$ obtained here with those obtained from the Rodrigues formula

$\Rightarrow$ $P_n(x)$ defined by the generating function

$$F(x,z) = \frac{1}{\sqrt{1-2xz+z^2}} = \sum_{n=0}^{\infty} z^n P_n(x)$$

is indeed the Legendre polynomial

4. Associated Legendre Polynomial.

$$\frac{d}{dx}(1-x^2)\frac{dy}{dx} + \left[\mu - \frac{m^2}{1-x^2}\right]y = 0 \rightarrow \text{Associated Legendre equation}$$

Ansatz $\quad y(x) = (1-x^2)^{m/2} v(x)$

Substitute back into the associated Legendre equation

$$\Rightarrow (1-x^2)\frac{d^2v}{dx^2} + 2(m+1)x\frac{dv}{dx} + [\mu - m(m+1)]v = 0 \qquad (A)$$

Differentiate (A) with respect to x

$$(1-x^2)\frac{d^2}{dx^2}\left(\frac{dv}{dx}\right) - 2(m+2)x\frac{d}{dx}\left(\frac{dv}{dx}\right) + [\mu-(m+1)(m+2)]\frac{dv}{dx} = 0$$

For $\mu = n(n+1)$, $m=0$, $P_n(x)$ is a solution of the associated Legendre equation

$\Rightarrow$ $(1-x^2)^{1/2} \dfrac{dP_n(x)}{dx}$ is a solution of the associated Legendre equation with $\mu = n(n+1)$ and $m=1$

Continuity this process, it can be seen that

$$P_n^m(x) = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_n(x)$$

is a solution of the associated Legendre equation.

$$(1-2x\zeta-\zeta^2)^{-\frac{1}{2}} \equiv \sum_n \zeta^n P_n(x)$$

direct prove (3A-4)

$$\frac{1}{(1-2x\zeta+\zeta^2)^{1/2}} = \sum_n \zeta^n P_n(x) \qquad (A)$$

Want to prove $P_n(x)$ satisfies the Legendre

$\frac{\partial}{\partial x}$ above equation

$$\frac{(-\frac{1}{2})(-2\zeta)}{(1-2x\zeta+\zeta^2)^{3/2}} = \sum_{n=0}^{\infty} \zeta^n \frac{dP_n(x)}{dx}$$

$$\Rightarrow \frac{\zeta}{(1-2x\zeta+\zeta^2)^{3/2}} = \sum_{n=0}^{\infty} \zeta^n \frac{dP_n(x)}{dx}$$

$\frac{\partial}{\partial x}$ above equation

$$\frac{\zeta(-\frac{3}{2})(-2\zeta)}{(1-2x\zeta+\zeta^2)^{5/2}} = \sum_{n=0}^{\infty} \zeta^n \frac{d^2P_n(x)}{dx^2}$$

$$\frac{3\zeta^2}{(1-2x\zeta+\zeta^2)^{5/2}} = \sum_{n=0}^{\infty} \zeta^n \frac{d^2P_n(x)}{dx^2}$$

$$\sum_{n=0}^{\infty} \zeta^n \left[(1-x^2)\frac{d^2P_n}{dx^2} - 2x\frac{dP_n(x)}{dx}\right]$$

$$= \frac{(1-x^2)3\zeta^2}{(1-2x\zeta+\zeta^2)^{5/2}} - \frac{2x\zeta}{(1-2x\zeta+\zeta^2)^{3/2}}$$

$$= \frac{3\zeta^2 - 2x\zeta + x^2\zeta^2 - 2x\zeta^3}{(1-2x\zeta+\zeta^2)^{5/2}} = (B)$$

Differentiate A with respect to ζ

$$\frac{-\frac{1}{2}(-2x+2\zeta)}{(1-2x\zeta+\zeta^2)^{3/2}} = \sum_{n=0}^{\infty} n\zeta^{n-1} P_n(x)$$

Multiple by ζ^2

$$\frac{(x-\zeta)\zeta^2}{(1-2x\zeta+\zeta^2)^{3/2}} = \sum_{n=0}^{\infty} n\zeta^{n+1} P_n(x)$$

$\frac{\partial}{\partial \zeta}$ above equation

LHS = RHS of (B) $\qquad$ $RHS = \sum_{n=0}^{\infty} n(n+1)\zeta^n P_n(x)$

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$$\Rightarrow \sum_{n=0}^{\infty} z^n \left[(1-x^2)\frac{d^2P_n(x)}{dx^2} - 2x\frac{dP_n(x)}{dx} + n(n+1)P_n(x) \right] = 0$$

$\because \{z^n\}$ are linearly independent

$\Rightarrow$ $P_n(x)$ satisfies the Legendre equation.

Associated Legendre Function

$$P_\ell^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x)$$

Want to show it satisfies the associated Legendre equation

Start with Legendre equation

$$(1-x^2)\frac{d^2P_\ell(x)}{dx^2} - 2x\frac{dP_\ell(x)}{dx} + \ell(\ell+1)P_\ell(x) = 0$$

Differentiate above equation m times with respect to x

Use Leibnz's rule

$$\frac{d^n}{dx^n}(uv) = (\underset{\substack{\downarrow \\ \text{act only} \\ \text{on } u}}{D_u} + \underset{\substack{\downarrow \\ \text{act only} \\ \text{on } v}}{D_v})^n (uv)$$

$$\frac{d^m}{dx^m}(1-x^2)\frac{d^2P_\ell(x)}{dx^2} = (1-x^2)\frac{d^{m+2}}{dx^{m+2}}P_\ell(x) - \underset{\substack{\downarrow \\ \binom{m}{1}}}{2m} x \frac{d^{m+1}}{dx^{m+1}}P_\ell(x)$$

$\binom{m}{m}$ on the second; $m-1$ on the second, 1 on the first

$$- m(m-1)\frac{d^m P_\ell(x)}{dx^m}$$

$\binom{m}{2} \rightarrow \frac{m(m-1)}{2}$ $m-2$ on the second, twice on $(1-x^2) \to -2x$

$$\frac{d^m}{dx^m}\left(-2x\frac{dP_\ell(x)}{dx}\right) = -2x\frac{d^{m+1}}{dx^{m+1}}P_\ell(x) - 2m\frac{d^m}{dx^m}P_\ell(x)$$

$$\frac{d^m}{dx^m}\ell(\ell+1)P_\ell(x) = \ell(\ell+1)\frac{d^m}{dx^m}P_\ell(x)$$

$$\Rightarrow (1-x^2)\frac{d^{m+2}}{dx^{m+2}}P_\ell(x) - 2(m+1)x\frac{d^{m+1}}{dx^{m+1}}P_\ell(x) + (\ell-m)(\ell+m+1)\frac{d^m}{dx^m}P_\ell(x) = 0$$

$$\frac{d^m}{dx^m}P_\ell(x) = (-1)^{-m}(1-x^2)^{-m/2}P_\ell^m(x)$$

$$\Rightarrow (1-x^2)\frac{d^2}{dx^2}\left[(1-x^2)^{-\frac{m}{2}}P_\ell^m(x)\right] - 2(m+1)x\frac{d}{dx}\left[(1-x^2)^{-\frac{1}{2}m}P_\ell^m(x)\right]$$

$$+(\ell-m)(\ell+m+1)(1-x^2)^{-\frac{1}{2}m}P_\ell^m(x) = 0$$

$$(1-x^2)\left\{P_\ell^m(x)\frac{d^2}{dx^2}(1-x^2)^{-\frac{m}{2}} + 2\frac{d}{dx}(1-x^2)^{-\frac{m}{2}}\frac{d}{dx}P_\ell^m(x) + (1-x^2)^{-\frac{1}{2}m}\frac{d^2}{dx^2}P_\ell^m(x)\right\} - 2(m+1)x\left\{\left[\frac{d}{dx}(1-x^2)^{-\frac{1}{2}m}\right]P_\ell^m(x)\right.$$

$$+ (1-x^2)^{-\frac{1}{2}m} \frac{d}{dx} P_\ell^m(x) + (\ell-m)(\ell+m+1)(1-x^2)^{-\frac{1}{2}m} P_\ell^m(x) = 0$$

$$\Rightarrow (1-x^2)\frac{d^2}{dx^2} P_\ell^m(x) - 2x\frac{d}{dx} P_\ell^m(x) + [\ell(\ell+1) - \frac{m^2}{1-x^2}] P_\ell^m(x) = 0$$

$$\Rightarrow \frac{d}{dx}[(1-x^2)\frac{dP_\ell^m(x)}{dx}] + \{\ell(\ell+1) - \frac{m^2}{1-x^2}\} P_\ell^m(x) = 0$$

$\Downarrow$

$P_\ell^m(x)$ satisfies the Associated Legendre Equation

Orthogonality and Normalization

$$\int_{-1}^{1} P_\ell^m(x) P_r^m(x)\, dx = 0 \quad \text{if } \ell = r$$

$$\frac{d}{dx}(1-x^2)\frac{dP_r^m}{dx} + [r(r+1) - \frac{m^2}{1-x^2}] P_r^m(x) = 0$$

$\int P_\ell^m(x)\, dx$, integrate by part

$$-\int_{-1}^{1}(1-x^2)\frac{dP_\ell^m}{dx}\frac{dP_r^m}{dx}\, dx + \int_{-1}^{1}(r(r+1) - \frac{m^2}{1-x^2}) P_\ell^m(x) P_r^m(x)\, dx = 0$$

Interchange $\ell \leftrightarrow r$ and substrate

$$\underbrace{[\ell(\ell+1) - r(r+1)]}_{(\ell-r)(\ell+r+1)} \int_{-1}^{1} P_\ell^m(x) P_r^m(x)\, dx = 0$$

$$\Rightarrow \text{If } \ell \neq r, \quad \int_{-1}^{1} P_\ell^m(x) P_r^m(x)\, dx = 0$$

$$\int_{-1}^{1} [P_\ell^m(x)]^2\, dx = \frac{(\ell+m)!}{(\ell-m)!}\frac{2}{2n+1}$$

$$\int_{-1}^{1}[P_\ell^m(x)]^2 dx = \int_{-1}^{1} \underbrace{(1-x^2)^m \frac{d^m}{dx^m} P_\ell(x)\frac{d^m}{dx^m}}_{(1-x^2)^m} P_\ell(x)\, dx$$

$$= -\int_{-1}^{1}[\frac{d^{m-1}}{dx^{m-1}} P_\ell(x)][\frac{d}{dx}(1-x^2)^m \frac{d^m}{dx^m} P_\ell(x)]\, dx$$

partial integration

Lemma $\frac{d}{dx}(1-x^2)\frac{d^m}{dx^m} P_\ell(x) = -(\ell+m)(\ell-m+1)(1-x^2)^{m-1}\frac{d^{m-1}}{dx^{m-1}} P_\ell(x)$

Start with Legendre equation

Differentiate with respect to x ; $m-1$ time

Multiply by $(1-x^2)^{m-1}$

$$+ (1-x^2)^{-\frac{1}{2}m}\frac{d}{dx}P_\ell^m(x) + (\ell-m)(\ell+m+1)(1-x^2)^{-\frac{1}{2}m}P_\ell^m(x) = 0$$

$$\Rightarrow (1-x^2)\frac{d^2}{dx^2}P_\ell^m(x) - 2x\frac{d}{dx}P_\ell^m(x) + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right]P_\ell^m(x) = 0$$

$$\Rightarrow \frac{d}{dx}\left[(1-x^2)\frac{dP_\ell^m(x)}{dx}\right] + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right]P_\ell^m(x) = 0$$

$\Downarrow$

$P_\ell^m(x)$ satisfies the Associated Legendre Equation

Orthogonality and Normalization

$$\int_{-1}^{1} P_\ell^m(x)P_r^m(x)\,dx = 0 \quad \text{if } \ell = r$$

$$\frac{d}{dx}(1-x^2)\frac{dP_r^m}{dx} + \left[r(r+1) - \frac{m^2}{1-x^2}\right]P_r^m(x) = 0$$

$\int P_\ell^m(x)\,dx$, integrate by part

$$-\int_{-1}^{1}(1-x^2)\frac{dP_\ell^m}{dx}\frac{dP_r^m}{dx}\,dx + \int_{-1}^{1}\left(r(r+1) - \frac{m^2}{1-x^2}\right)P_\ell^m(x)P_r^m(x)\,dx = 0$$

Interchange $\ell \leftrightarrow r$ and substrate

$$\underbrace{[\ell(\ell+1) - r(r+1)]}_{(\ell-r)(\ell+r+1)}\int_{-1}^{1}P_\ell^m(x)P_r^m(x)\,dx = 0$$

$$\Rightarrow \text{If } \ell \neq r, \quad \int_{-1}^{1}P_\ell^m(x)P_r^m(x)\,dx = 0$$

$$\int_{-1}^{1}[P_\ell^m(x)]^2\,dx = \frac{(\ell+m)!}{(\ell-m)!}\frac{2}{2n+1}$$

$$\int_{-1}^{1}[P_\ell^m(x)]^2\,dx = \int_{-1}^{1}(1-x^2)^m\frac{d^m}{dx^m}P_\ell(x)\frac{d^m}{dx^m}P_\ell(x)\,dx$$

$$= -\int_{-1}^{1}\left[\frac{d^{m-1}}{dx^{m-1}}P_\ell(x)\right]\left[\frac{d}{dx}(1-x^2)^m\frac{d^m}{dx^m}P_\ell(x)\right]dx$$

partial integration

Lemma $\frac{d}{dx}(1-x^2)\frac{d^m}{dx^m}P_\ell(x) = -(\ell+m)(\ell-m+1)(1-x^2)^{m-1}\frac{d^{m-1}}{dx^{m-1}}P_\ell(x)$

Start with Legendre equation

Differentiate with respect to x ; $m-1$ time

Multiply by $(1-x^2)^{m-1}$

Legendre equation

$$(1-x^2)\frac{d^2}{dx^2}P_\ell(x) - 2x\frac{d}{dx}P_\ell(x) + \ell(\ell+1)P_\ell(x) = 0$$

Differentiate with respect to x $(m-1)$ times

$$(1-x^2)\frac{d^{m+1}}{dx^{m+1}}P_\ell(x) - 2(m-1)x\frac{d^m}{dx^m}P_\ell(x) - (m-1)(m-2)\frac{d^{m-1}}{dx^{m-1}}P_\ell(x)$$

$$-2x\frac{d^m}{dx^m}P_\ell(x) - 2(m-1)\frac{d^{m-1}}{dx^{m-1}}P_\ell(x) + \ell(\ell+1)\frac{d^{m-1}}{dx^{m-1}}P_\ell(x) = 0$$

$$\Rightarrow (1-x^2)\frac{d^{m+1}}{dx^{m+1}}P_\ell(x) - 2mx\frac{d^m}{dx^m}P_\ell(x) = -(\ell+m)(\ell-m+1)\frac{d^{m-1}}{dx^{m-1}}P_\ell(x)$$

Multiply by $(1-x^2)^{m-1}$

$$(1-x^2)^m\frac{d^{m+1}}{dx^{m+1}}P_\ell(x) - 2mx(1-x^2)^{m-1}\frac{d^m}{dx^m}P_\ell(x)$$

$$= -(\ell+m)(\ell-m+1)(1-x^2)^{m-1}\frac{d^{m-1}}{dx^{m-1}}P_\ell(x)$$

$$\frac{d}{dx}\left[(1-x^2)^m\frac{d^m}{dx^m}P_\ell(x)\right] = -(\ell+m)(\ell-m+1)(1-x^2)^{m-1}\frac{d^{m-1}}{dx^{m-1}}P_\ell(x)$$

$$\int_{-1}^{1}[P_\ell^m(x)]^2dx = -\int_{-1}^{1}\left(\frac{d^{m-1}}{dx^{m-1}}P_\ell(x)\right]\left[\frac{d}{dx}(1-x^2)^m\frac{d^m}{dx^m}P_\ell(x)\right]dx$$

$$= +(\ell+m)(\ell-m+1)\int_{-1}^{1}\left[\frac{d^{m-1}}{dx^{m-1}}P_\ell(x)\right]\underbrace{(1-x^2)^{m-1}}_{(1-x^2)^{\frac{m-1}{2}}(1-x^2)^{\frac{m-1}{2}}}\left[\frac{d^{m-1}}{dx^{m-1}}P_\ell(x)\right]$$

$$= (\ell+m)(\ell-m+1)\int_{-1}^{1}[P_\ell^{m-1}(x)]^2dx$$

$$\int_{-1}^{1}[P_\ell^m(x)]^2dx = (\ell+m)(\ell-m+1)\int_{-1}^{1}[P_\ell^{m-1}(x)]^2dx$$

$$= (\ell-m+1)(\ell-m+2)\cdots\ell\,(\ell+m)(\ell+m-1)\cdots(\ell+1)\underbrace{\int_{-1}^{1}[P_0(x)]^2dx}_{=\frac{2}{2\ell+1}}$$

$$= \frac{\ell!}{(\ell-m)!}\frac{(\ell+m)!}{\ell!}\frac{2}{2\ell+1}$$

$$= \frac{(\ell+m)!}{(\ell-m)!}\frac{2}{2\ell+1}$$

This equation gives the normalization

$\left\{\sqrt{\frac{(2\ell+1)(\ell-m)!}{2(\ell+m)!}}\,P_\ell^m(x)\right\}$ forms an orthonormal set of function in the interval $(-1, 1)$

Spherical harmonics

$$Y_{\ell m}(\theta,\phi) = \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}\,P_\ell^m(\cos\theta)\,e^{im\phi}$$

Properties:

(i) $Y_{\ell,-m}(\theta,\phi) = (-1)^m Y_{\ell m}^*(\theta,\phi)$

$$P_\ell^{-m}(x) = (-1)^m\frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(x)$$

$P_\ell^{-m}(x)$ and $P_\ell^m(x)$ are proportional, since differential equation depend on m^2 and m are integer.
The proportionality constant are fixed through the normalization formula

(ii) $\int_0^{2\pi}d\phi\int_0^{\pi}\sin\theta\,d\theta\;Y_{\ell' m'}^*(\theta,\phi)\,Y_{\ell,m}(\theta,\phi) = \delta_{\ell'\ell}\,\delta_{m'm}$

(iii) $f(\theta,\phi) = \sum_\ell\sum_m a_{\ell m}Y_{\ell m}(\theta,\phi)$

$$a_{\ell m} = \int_{-1}^{1}d(\cos\theta)\int_0^{2\pi}d\phi\;Y_{\ell m}^*(\theta,\phi)f(\theta,\phi)$$

$$\Rightarrow f(\theta,\phi) = \int_{-1}^{1}d(\cos\theta')\int_0^{2\pi}\left\{\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}Y_{\ell m}^*(\theta',\phi')Y_{\ell m}(\theta,\phi)\right\}f(\theta',\phi')$$

$$\Rightarrow \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}Y_{\ell m}^*(\theta',\phi')\,Y_{\ell m}(\theta,\phi) = \delta(\cos\theta-\cos\theta')\,\delta(\phi-\phi')$$

this is the completness relation.

(iv) $Y_{\ell 0}(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}}\,P_\ell(\cos\theta)$

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Theorem a.

$$Y_{\ell m}(\theta,\phi) \sim P_\ell^m(\cos\theta)\, e^{im\phi}$$

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial}{\partial\phi}\right]\underbrace{P_\ell^m(\cos\theta)\, e^{im\phi}}_{Y_{\ell m}(\theta,\phi)}$$

$$= \left[\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d}{d\theta}P_\ell^m(\cos\theta) + \frac{1}{\sin^2\theta}(-m^2)P_\ell^m(\cos\theta)\right]e^{im\phi}$$

$x = \cos\theta$

$$= \left[\frac{d}{dx}(1-x^2)\frac{d}{dx}P_\ell^m(x) - \frac{m^2}{1-x^2}P_\ell^m(x)\right]e^{im\phi}$$

↓ use associated

$$= -\ell(\ell+1)\underbrace{P_\ell^m(\theta,\phi)\, e^{im\phi}}_{Y_{\ell m}(\theta,\phi)}$$

Example $\ell = 2, \quad m = 1$

$$P_\ell(x) = \sum_{k=0}^{\infty} c_k x^k \underset{\ell=2}{=} c_0 + c_2 x^2$$

$$c_2 = \frac{0\cdot 1 - 2(2+1)}{2(2-1)} c_0$$

$$= -3c_0$$

$$P_2(x) = c_0(1-3x^2)$$

$$\cancel{P_2^1(x) = (-1)^1(1-x^2)^{1/2}\frac{d}{dx}c_0(1-3x^2)}$$

$$= (-1)(1-x)^{1/2} c_0(-6x)$$

$$= +6c_0(1-x^2)^{1/2} x$$

$$\Theta_2^1(\cos\theta) \propto (1-x^2)^{\frac{1}{2}} x = \sin\theta\cos\theta$$

$$Y_2^1(\theta,\phi) \propto (\sin\theta\cos\theta)e^{i\phi}$$

$$Y_2^1(\theta,\phi) = A(\sin\theta\cos\theta)e^{i\phi}$$

Normalization

$$\iint Y_{21}^*(\theta,\phi)\, Y_{21}(\theta,\phi)\sin\theta\, d\theta\, d\phi = 1$$

$$\Rightarrow |A|^2\int_0^{\pi}\int_0^{2\pi} d\theta\, d\phi\, \sin^3\theta\cos^2\theta = 1$$

$$\Rightarrow |A|^2\, 2\pi\int_{-1}^{1}(1-x^2)\,x^2\,dx = 1$$

$$|A|^2\, 2\pi\,\frac{4}{15} = 1 \qquad 2\left(\frac{1}{3}-\frac{1}{5}\right) = 2\cdot\frac{2}{15}$$

$$A = \sqrt{\frac{15}{8\pi}}$$

$$Y_{2,1}(\theta,\phi) = \sqrt{\frac{15}{8\pi}}\, e^{i\phi}\sin\theta\cos\theta.$$

$$Y_{\ell,-m}(\theta,\phi) = (-1)^m\, Y_{\ell,m}(\theta,\phi) \qquad m \geq 0$$

Orthonormal Relation of Spherical Harmonics

$Y_{\ell m} \propto P_\ell^m(\theta)\, e^{im\phi}$

(i) $\int_0^{2\pi} e^{-im'\phi}\, e^{im\phi}\, d\phi = \delta_{m'm} \cdot 2\pi$

first $m \neq m'$ the integral vanishs

when $m = m'$ the integral $= 2\pi$.

(ii) $\int_{-1}^{1} P_\ell^m(x) P_r^m(x)\, dx = 0$ if $\ell = r$

$$\frac{d}{dx}(1-x^2)\frac{dP_r^m}{dx} + \left[(r+1)r - \frac{m^2}{1-x^2}\right] P^m(x) = 0$$

Multiply $\int_{-1}^{1} P_\ell^m(x)$

$$\int_{-1}^{1} P_\ell^m(x)\frac{d}{dx}(1-x^2)\frac{dP_r^m}{dx}\, dx + \int_{-1}^{1} P_\ell^m(x)\left[r(r+1) - \frac{m^2}{1-x^2}\right] P_r^m(x)\, dx$$

$= 0$

integral by part

$$\Rightarrow -\int_{-1}^{1}(1-x^2)\frac{dP_\ell^m(x)}{dx}\frac{dP_r^m(x)}{dx}\, dx + \int_{-1}^{1}\left(r(r+1) - \frac{m^2}{1-x^2}\right) P_\ell^m(x) P_r^m(x)\, dx$$

$= 0$

Interchange $\ell \leftrightarrow r$ and subtract

$$[\underbrace{\ell(\ell+1) - r(r+1)}_{(\ell-r)(\ell+r+1)}]\int_{-1}^{1} P_\ell^m(x) P_r^m(x)\, dx = 0$$

If $\ell \neq r$, then $\int_{-1}^{1} P_\ell^m(x) P_r^m(x)\, dx$

(iii) $\int_{-1}^{1} [P_\ell^m(x)]^2\, dx = \frac{(\ell+m)!}{(\ell-m)!}\frac{2}{2\ell+1}$

Similar method gives $Y_{\ell,m}(\theta,\phi)$

When ℓ, m is small; the spherical harmonics can be written down explicitly.

For ℓ, m are large, it is better to look up in a table.

But, at least, how it is obtain.

$Y_{\ell,m}(\theta,\phi)$ is the solution of the angular equation specified by ℓ, m.

The physical meaning of $Y_{\ell m}(\theta,\phi)$ is related to the orbital angular momentum.

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(Orbital) Angular Momentum

$$\vec{L} = \vec{r} \times \vec{p} \rightarrow -i\hbar\, \vec{r} \times \nabla$$

In Cartesian coordinate

$$\vec{L} = \begin{vmatrix} i & j & k \\ x & y & z \\ P_x & P_y & P_z \end{vmatrix}$$

$$L_x = yP_z - zP_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$L_y = zP_x - xP_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$L_z = xP_y - yP_y = -i\hbar\left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right)$$

Commutators between the angular momentum components

$$L_x L_y - L_y L_x = i\hbar L_z$$

$$L_y L_z - L_z L_y = i\hbar L_x$$

$$L_z L_x - L_x L_z = i\hbar L_y$$

Write in compact form

$$[L_i, L_j] = i\hbar\, \epsilon_{ijk} L_k$$

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } i, j, k \text{ is even permutation of } 1, 2, 3 \\ -1 & \text{if } i, j, k \text{ is odd permutation of } 1, 2, 3 \\ 0 & \text{if two or more indices are equal} \end{cases}$$

Fundamental commutator

$$[x, P_x] = [y, P_y] = [z, P_z] = i\hbar$$

$$[x, P_y] = [x, P_z] = [y, P_x] = [y, P_z] = [z, P_x] = [z, P_y] = 0$$

Theorem $[A+B, C+D]$

$$= (A+B)(C+D) - (C+D)(A+B)$$

$$= AC + BC + AD + BD - CA - DA - CB - DB$$

$$= [A,C] + [B,C] + [A,D] + [B,D]$$

Theorem $[AB, C] = A[B,C] + [A,C]B$

$$\| $$

$$ABC - ACB + ACB - CAB$$

$$\| \qquad\qquad \|$$

$$A[B,C] \quad + \quad [A,C]B$$

Theorem $[A, BC] = [A,B]C + B[A,C]$

$$\|$$

$$ABC - BAC + BAC - BCA$$

$$\|$$

$$[A,B]C + B[A,C]$$

$$[L_x, L_y] = [yP_z - zP_y, zP_x - xP_z]$$

$$= \underbrace{[yP_z, zP_x]}_{(I)} - \underbrace{[zP_y, zP_x]}_{(II)} - \underbrace{[zP_y, zP_x]}_{(III)} + \underbrace{[zP_y, xP_z]}_{(IV)}$$

$$(I) = [yP_z, zP_x]$$

$$y[P_z, zP_x] + [y, zP_x]P_z$$

$$y\left([P_z, z]P_x + z\underbrace{[P_z, P_x]}_{0}\right) \qquad \underbrace{[y,z]}_{0}P_xP_z - z\underbrace{[y,P_x]}_{0}P_z$$

$$\downarrow$$

$$y[P_z, z]P_x$$

$$\|$$

$$y(-i\hbar P_x)$$

$$= -i\hbar\, yP_x$$

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(II), (III) are obviously zero

$$(\text{IV}) = [z P_y, x P_z]$$

$$= z \underbrace{[P_y, x P_z]}_{=0} + \underbrace{[z, x P_z]}_{=\underbrace{[z, x]}_{=0} P_z P_y + x \underbrace{[z, P_z]}_{=i\hbar} P_y} P_y$$

$$[L_x, L_y] = i\hbar (x P_y - y P_x) = i\hbar L_z$$

Use similar method, we can show

$$[L_y, L_z] = i\hbar L_x$$

$$[L_z, L_x] = i\hbar L_y$$

$$\vec{L}^2 = L_x^2 + L_y^2 + L_z^2$$

$$[\vec{L}^2, L_z] = [L_x^2 + L_y^2 + L_z^2, L_z]$$

$$= [L_x^2, L_z] + [L_y^2, L_z] + \underbrace{[L_z^2, L_z]}_{=0}$$

$$[L_x^2, L_z] = \underbrace{L_x [L_x, L_z]}_{L_x(-i\hbar L_y)} + \underbrace{[L_x, L_z] L_x}_{-i\hbar L_y L_x}$$

$$[L_y^2, L_z] = \underbrace{L_y [L_y, L_z]}_{=i\hbar L_y L_x} + \underbrace{[L_y, L_z] L_y}_{=i\hbar L_x L_y}$$

$$\Rightarrow [L^2, L_z] = 0$$

Angular Momentum in Spherical Coordinate

$$L_x = yP_z - zP_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi}$$

$$= \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial \theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial \phi}$$

$$\underset{r\cos\theta}{\underset{\|}{z}}\frac{\partial}{\partial y} = r\cos\theta\sin\theta\sin\phi\frac{\partial}{\partial r} + \cos^2\theta\sin\phi\frac{\partial}{\partial \theta} + \frac{\cos\theta\cos\phi}{\sin\theta}\frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial z}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial z}\frac{\partial}{\partial \phi}$$

$$= \cos\theta\frac{\partial}{\partial r} + \left(-\frac{\sin\theta}{r}\right)\frac{\partial}{\partial \theta} + 0$$

$$y\frac{\partial}{\partial z} = r\sin\theta\sin\phi\left[\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\right]$$

$$= r\cos\theta\sin\theta\sin\phi\frac{\partial}{\partial r} - \sin^2\theta\sin\phi\frac{\partial}{\partial \theta}$$

Put it together

$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial \theta} + \cot\theta\cos\phi\frac{\partial}{\partial \phi}\right)$$

$$L_y = zP_x - xP_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi}$$

$$= \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial \theta} + \left(-\frac{\sin\phi}{r\sin\theta}\right)\frac{\partial}{\partial \phi}$$

$$z\frac{\partial}{\partial x} = r\cos\theta\left(\sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial \theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial \phi}\right)$$

$$= r\cos\theta\sin\theta\cos\phi\frac{\partial}{\partial r} + \cos^2\theta\cos\phi\frac{\partial}{\partial \theta} - \frac{\cos\theta\sin\phi}{\sin\theta}\frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial z}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial z}\frac{\partial}{\partial \phi}$$

$$= \cos\theta\frac{\partial}{\partial r} + \left(-\frac{\sin\theta}{r}\right)\frac{\partial}{\partial \theta} + 0$$

$$x\frac{\partial}{\partial z} = r\sin\theta\cos\phi\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\right)$$

$$= r\cos\theta\sin\theta\cos\phi\frac{\partial}{\partial r} - \sin^2\theta\cos\phi\frac{\partial}{\partial\theta}$$

Put it together

$$L_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$L_z = xP_y - yP_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial y}\frac{\partial}{\partial\phi}$$

$$= \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$x\frac{\partial}{\partial y} = r\sin\theta\cos\phi\left(\sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}\right)$$

$$= r\sin^2\theta\cos\phi\sin\phi\frac{\partial}{\partial r} + \sin\theta\cos\phi\cos\theta\sin\phi\frac{\partial}{\partial\theta} + \cos^2\phi\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial x}\frac{\partial}{\partial\phi}$$

$$y\frac{\partial}{\partial x} = r\sin^2\theta\cos\phi\sin\phi\frac{\partial}{\partial r} + \sin\theta\cos\theta\cos\phi\sin\phi\frac{\partial}{\partial\theta} - \sin^2\phi\frac{\partial}{\partial\phi}$$

Put it together

$$L_z = -i\hbar\frac{\partial}{\partial\phi} = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

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$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$L_x^2 = -\hbar^2\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$\sin\phi\frac{\partial}{\partial\theta}\sin\phi\frac{\partial}{\partial\theta} = \sin^2\phi\frac{\partial^2}{\partial\theta^2}.$$

$$\cot\theta\cos\phi\frac{\partial}{\partial\phi}\left(\sin\phi\frac{\partial}{\partial\theta}\right) = \cot\theta\cos\phi\sin\phi\frac{\partial^2}{\partial\theta\partial\phi}$$

$$+\cot\theta\cos\phi\cos\phi\frac{\partial}{\partial\theta}$$

$$\sin\phi\frac{\partial}{\partial\theta}\cot\theta\cos\phi\frac{\partial}{\partial\phi}$$

$$= \sin\phi\cos\phi\cot\theta\frac{\partial^2}{\partial\theta\partial\phi} + \sin\phi\cos\phi(-\csc^2\theta)\frac{\partial}{\partial\phi}$$

$$\cot\theta\cos\phi\frac{\partial}{\partial\phi}\cot\theta\cos\phi\frac{\partial}{\partial\phi}$$

$$= \cot^2\theta\cos\phi(-\sin\phi)\frac{\partial}{\partial\phi} + \cot^2\theta\cos^2\phi\frac{\partial^2}{\partial\phi^2}$$

$$L_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$L_y^2 = -\hbar^2\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$-\cos\phi\frac{\partial}{\partial\theta}\left(-\cos\phi\frac{\partial}{\partial\theta}\right) = \cos^2\phi\frac{\partial^2}{\partial\theta^2}.$$

$$\cot\theta\sin\phi\frac{\partial}{\partial\phi}\left(-\cos\phi\frac{\partial}{\partial\theta}\right) = -\cot\theta\sin\phi\cos\phi\frac{\partial^2}{\partial\theta\partial\phi}$$

$$+\cot\theta\sin^2\phi\frac{\partial}{\partial\theta}$$

$$-\cos\phi\frac{\partial}{\partial\theta}\left(\cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) = -\cos\phi\sin\phi\cot\theta\frac{\partial^2}{\partial\theta\partial\phi}$$

$$-\cos\phi(\sin\phi)(-\csc^2\theta)\frac{\partial}{\partial\phi}$$

$$\cot\theta\sin\phi\frac{\partial}{\partial\phi}\left(\cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) = \cot^2\theta\sin\phi\cos\phi\frac{\partial}{\partial\phi}$$

$$+\cot^2\theta\sin^2\phi\frac{\partial^2}{\partial\phi^2}$$

分類:

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$L_x^2 + L_y^2 \qquad -\hbar^2 \, [\ A\ ]$

A

Coefficient of $\frac{\partial^2}{\partial\theta^2}$: $\quad \sin^2\phi + \cos^2\phi = 1$

Coefficient of $\frac{\partial^2}{\partial\theta\partial\phi}$: $\quad \cot\theta\cos\phi\sin\phi - \cot\theta\sin\phi\cos\phi$

$= 0$

Coefficient of $\frac{\partial}{\partial\theta}$ $\quad \cot\theta\cos^2\phi + \cot\theta\sin^2\phi$

$= \cot\theta$

Coefficient of $\frac{\partial}{\partial\phi}$ $\quad -\csc^2\theta\sin\phi\cos\phi - \cot^2\theta\cos\phi\sin\phi$

$+ \csc^2\theta\sin\phi\cos\phi + \cot^2\theta\sin\phi\cos\phi$

$= 0$

Coefficient of $\frac{\partial^2}{\partial\phi^2}$ $\quad \cot^2\theta\cos^2\phi + \cot^2\theta\sin^2\phi$

$= \cot^2\theta$

$$\Rightarrow \quad L_x^2 + L_y^2 = \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2}$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$\Rightarrow \quad L_z^2 = -\hbar^2\frac{\partial^2}{\partial\phi^2}$$

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$= -\hbar^2\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\phi^2}\right]$$

$$= -\hbar^2\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \csc^2\theta\frac{\partial^2}{\partial\phi^2}\right]$$

$$* \quad \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} = \frac{1}{\sin\theta}\sin\theta\frac{\partial^2}{\partial\theta^2} + \frac{1}{\sin\theta}\cos\theta\frac{\partial}{\partial\theta}$$

$$= \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta}$$

$$** \quad \csc^2\theta\frac{\partial^2}{\partial\phi} = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$\Rightarrow \quad L^2 = L_x^2 + L_y^2 + L_z^2$$

$$= -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

Going back to the θ - equation

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + [\ell(\ell+1)\sin^2\theta - m^2]\Theta = 0$$

$$\Rightarrow \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{m^2}{\sin^2\theta}\Theta = -\ell(\ell+1)\Theta$$

ϕ - equation

$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi$$

$$Y_{\ell m} \propto \Theta_{\ell m}(\theta)\,\Phi_m(\phi) \Rightarrow Y_{\ell m} = A\Theta\Phi$$

Claim $L^2 Y_{\ell m}(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_{\ell m}(\theta,\phi)$

Proof:

$$L^2 Y_{\ell m}(\theta,\phi) = -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\} A\Theta_{\ell m}(\theta)\Phi_m(\phi)$$

$$= A\Phi_m(\phi)\left\{-\frac{\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta_{\ell m}\right\} - \left\{\frac{\hbar^2}{\sin^2\theta}\Theta_{\ell m}\frac{\partial^2}{\partial\phi^2}\Phi\right\}$$

$$= -\hbar^2 A\Phi_m(\phi)\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta_{\ell m}\right\}$$

$$-\frac{\hbar^2(-m^2)\Theta_{\ell m}A\Phi_m(\phi)}{\sin^2\theta}$$

$$= -\hbar^2 A\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\Theta_{\ell m} - \frac{m^2}{\sin^2\theta}\Theta_{\ell m}\right\}\Phi_m(\phi)$$

$$= -\hbar^2 A(-\ell(\ell+1))\Theta_{\ell m}\Phi_m$$

$$= \ell(\ell+1)\hbar^2 Y_{\ell m}(\theta,\phi)$$

$Y_{\ell m}(\theta,\phi)$ is eigenfunction of L^2 with eigenvalue $\ell(\ell+1)\hbar^2$

$$L_z Y_{\ell m} = -i\hbar\frac{\partial}{\partial\phi}A\Theta\Phi \qquad \Phi = e^{im\phi}$$

$$= -i\hbar A\Theta\Phi(im) = m\hbar Y_{\ell m}$$

$Y_{\ell,m}(\theta,\phi)$ is eigenfunction of L_z with eigenvalue $m\hbar$

Thus $Y_{\ell m}(\theta,\phi)$ is simultaneous eigenfunction of $\vec{L}^2$, L_z with eigenvalues $\ell(\ell+1)\hbar^2$, $m\hbar$ respectively.

This is possible because of $[L^2, L_z] = 0$

Let us go back to the central force problem.

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

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

$$= -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right) + \frac{L^2}{2mr^2}$$

Now it is obvious that $[H, L^2]$

L^2 operates on θ, ϕ; not on r

$[L^2, L^2] = 0$

Furthermore, $[H, L_z] = 0$

L_z operators on ϕ only, not on r

$[L^2, L_z] = 0$

Therefore, L^2, L_z are conserved

$$\frac{d\langle L^2\rangle}{dt} = \frac{d\langle L_z\rangle}{dt} = 0$$

$\Rightarrow$ $\langle L^2\rangle$, $\langle L_z\rangle$ are independent of time

$\Rightarrow$ $\langle L^2\rangle$, $\langle L_z\rangle$ are independent of time

$\Rightarrow$ they are conserved.

We can use the same method to show

$\langle L_x \rangle$, $\langle L_y \rangle$ are also conserved.

$\downarrow$

conservation of angular momentum.

However, we cannot find simultaneous eigenfunctions of L_x, L_y (or L_y, L_z, etc) because they do not commute.

Orbital Angular Momentum

$[L_i, L_j] = i\hbar\epsilon_{ijk} L_k$

$L^2 = L_x^2 + L_y^2 + L_z^2$

$[\vec{L}^2, L_z] = 0$

L_x, L_y, L_z in spherical coordinates.

$L_x = i\hbar(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}$

$L_y = i\hbar(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi})$

$L_z = -i\hbar\frac{\partial}{\partial\phi}$

From L_x, L_y, L_z and $\vec{L}^2 = L_x^2 + L_y^2 + L_z^2$

One can show

$L^2 = -\hbar^2\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$

Since $Y_{\ell,m} \propto \Theta_{\ell m}(\theta)\Phi_m(\phi)$; $\Theta_{\ell m}$, $\Phi_m(\phi)$ are solution of the θ- and ϕ- equation

$\Rightarrow \quad L^2 Y_{\ell m}(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_{\ell m}(\theta,\phi)$

$L_z Y_{\ell m}(\theta,\phi) = m\hbar Y_{\ell m}(\theta,\phi)$

If a state has angular wave function $Y_{\ell m}(\theta,\phi)$ and we measure L^2, it will have definite value $\ell(\ell+1)\hbar^2$

$\Rightarrow$ $Y_{\ell m}(\theta,\phi)$ is an eigenfunction of L^2 with eigenvalue $\ell(\ell+1)\hbar^2$

$Y_{\ell m}(\theta,\phi)$ is also an eigenfunction of L_z with eigenvalue $m\hbar$

ℓ, m are quantum numbers that specifies $\vec{L}^2$, L_z

$Y_{\ell m}(\theta,\phi)$ are simultaneous eigenfunctions of $\vec{L}^2$, L_z

Summary of $Y_{\ell,m}(\theta,\phi)$

$$\iint Y^*_{\ell',m'}(\theta,\phi)\, Y_{m}(\theta,\phi)\sin\theta\, d\theta\, d\phi = \delta_{\ell'\ell}\,\delta_{mm'}$$

For ℓ, m small, we can find $Y_{\ell,m}$ through the method outlined above

See the example and table.

$$L^2\, Y_{\ell m}(\theta,\phi) = \ell(\ell+1)\hbar^2\, Y_{\ell m}(\theta,\phi)$$

$$L_z\, Y_{\ell m}(\theta,\phi) = m\hbar.$$

Expansion

$$\text{Any function } \overset{\psi(\theta,\phi)}{f(\theta,\phi)} = \sum_{l}\sum_{m} a_{lm} Y_{lm}(\theta,\phi)$$

$$\Rightarrow \quad a_{lm} = \int_{-1}^{1} d(\cos\theta') \int_{0}^{2\pi} d\phi\, Y^{*}_{lm}(\theta,\phi) f(\theta,\phi)$$

In usual application, we shall just use the orthonormal condition and the tabulated $Y_{lm}(\theta,\phi)$

Example $\quad \underset{}{\overset{\psi(\theta,\phi)}{\overset{\parallel}{f(\theta,\phi)}}} = A\cos^2\theta$

Normalization $\quad \iint |f(\theta,\phi)|^2 \sin\theta\, d\theta\, d\phi = 1$

$$|A|^2 \int \cos^4\theta \sin\theta\, d\phi = 1$$

$$|A|^2\, 2\pi\, \frac{2}{5} = 1$$

$$|A| = \sqrt{\frac{5}{4\pi}}$$

$$f(\theta,\phi) = \sqrt{\frac{5}{4\pi}} \cos^2\theta$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}}$$

$$\parallel$$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta - 1)$$

$$= \sqrt{\frac{5}{4\pi}} \cdot \frac{1}{2}\, 3\cos^2\theta - \sqrt{\frac{5}{4\pi}} \cdot \frac{1}{2}$$

$$= \frac{3}{2} f(\theta,\phi) - \sqrt{5}\, Y_{00}\, \frac{1}{2}$$

$$\frac{3}{2} f(\theta,\phi) = Y_{2,0} + \frac{\sqrt{5}}{2} Y_{0,0}$$

$$f(\theta,\phi) = \frac{2}{3} Y_{2,0} + \frac{\sqrt{5}}{3} Y_{0,0}$$

If the angular part of the wave function is given by $f(\theta,\phi)$

Measure L^2, the expectation value is

$$\langle L^2 \rangle = \iint f^*(\theta,\phi)\, L^2 f(\theta,\phi) \sin\theta\, d\theta\, d\phi$$

$$= \iint \left(\frac{2}{3} Y_{2,0} + \frac{\sqrt{5}}{3} Y_{00}\right) L^2 \left(\frac{2}{3} Y_{2,0} + \frac{\sqrt{5}}{3} Y_{0,0}\right) \sin\theta\, d\theta\, d\phi$$

Due to the orthonormal relation, only the direct term will contribute

$$= \frac{4}{9} \iint Y_{2,0}\, 2(2+1)\hbar^2\, Y_{2,0} \sin\theta\, d\theta\, d\phi$$

$$+ \frac{5}{9} \iint Y_{0,0}\, 0(0+1)\hbar\, Y_{00} \sin\theta\, d\phi$$

$$= \frac{4}{9} \cdot 6\hbar^2 = \frac{8}{3}\hbar^2$$

By inspection

The state has probability $\frac{4}{9} = \left(\frac{2}{3}\right)^2$ in $Y_{2,0}$

In $Y_{2,0}$, the L^2 measurement gives $2(2+1)\hbar^2$

The state has probability $\frac{5}{9} = \left(\frac{\sqrt{5}}{3}\right)^2$ in $Y_{0,0}$

In $Y_{0,0}$, the L^2 measurement gives $0(0+1)\hbar^2$

$$\langle L_z \rangle = \iint \left(\frac{2}{3} Y_{2,0} + \frac{\sqrt{5}}{3} Y_{0,0}\right) L_z \left(\frac{2}{3} Y_{2,0} + \frac{\sqrt{5}}{3} Y_{0,0}\right) \sin\theta\, d\theta\, d\phi$$

$$= 0$$

Example: $\psi(\theta,\phi) = \frac{1}{\sqrt{5}} Y_{1,-1}(\theta,\phi) + \sqrt{\frac{3}{5}}\, Y_{10}(\theta,\phi) + \frac{1}{\sqrt{5}} Y_{1,1}(\theta,\psi)$

If L_z is measured, the probability of finding

the value to be $-\hbar$ is $\left(\frac{1}{\sqrt{5}}\right)^2 = \frac{1}{5}$

the value to be 0 is $\left(\sqrt{\frac{3}{5}}\right)^2 = \frac{3}{5}$

the value to be $+\hbar$ is $\left(\frac{1}{\sqrt{5}}\right)^2 = \frac{1}{5}$

If $\vec{L}^2$ is measured, the probility of finding the value to be $2(2+1)\hbar^2$ is 1.

If after measuring, we find $L_z = -\hbar$, then

$$\psi(\theta,\phi) \longrightarrow Y_{1,-1}(\theta,\phi)$$

$$\langle L_x \rangle = \iint Y^*_{1,-1}(\theta,\phi)\, L_x\, Y_{1,-1}(\theta,\phi) \sin\theta\, d\theta\, d\phi$$

$$= \int_0^{\pi}\!\!\int_0^{2\pi} \left(\frac{21}{64\pi}\right)^{\frac{1}{2}} \sin\theta(5\cos^2\theta - 1)e^{+i\phi} \left[-i\hbar \sin\phi \frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]\left(\frac{21}{64\pi}\right)^{\frac{1}{2}} \sin\theta(5\cos^2\theta - 1)e^{i\phi}) \sin\theta\, d\theta\, d\phi$$

$\downarrow$

this integral can be carried out $\Rightarrow \langle L_x \rangle = 0$

$\downarrow$

we will later use operator method to show this in a quicker way.

5

Angular Momentum

5.1 Introduction

Angular momentum plays an important role in classical mechanics. The study of the dynamics of those systems that possess certain symmetries, such as rotational invariance in space, is made simple by the use of the angular momentum concept; for instance, the angular momentum of an isolated system is conserved.

Angular momentum is just as important in quantum mechanics as it is in classical mechanics. It is very useful for studying the dynamics of systems that move under the influence of *spherically symmetric*, or *central*, potentials, $V(\vec{r}) = V(r)$, for, as in classical mechanics, the orbital angular momenta of these systems are *conserved*. Angular momentum plays a critical role in the description of, for instance, molecular rotations, the motion of electrons in atoms and the motion of nucleons in nuclei. The quantum theory of angular momentum is thus a prerequisite for studying molecular, atomic and nuclear systems.

In this chapter we are going to consider the general formalism of angular momentum. We will examine the various properties of the angular momentum operator, and then focus on determining its eigenvalues and eigenstates. Finally, we will apply this formalism to the determination of the eigenvalues and eigenvectors of the orbital and spin angular momenta.

5.2 Orbital Angular Momentum

In classical physics the angular momentum of a particle with momentum $\vec{p}$ and position $\vec{r}$ is defined by

$$\vec{L} = \vec{r} \times \vec{p} = (yp_z - zp_y)\vec{i} + (zp_x - xp_z)\vec{j} + (xp_y - yp_x)\vec{k}. \tag{5.1}$$

The orbital angular momentum operator $\hat{\vec{L}}$ can be obtained at once by replacing $\vec{r}$ and $\vec{p}$ by the corresponding operators in the position representation, $\hat{\vec{R}}$ and $\hat{\vec{P}} = -i\hbar\vec{\nabla}$:

$$\boxed{\hat{\vec{L}} = \hat{\vec{R}} \times \hat{\vec{P}} = -i\hbar\hat{\vec{R}} \times \vec{\nabla}\,.} \tag{5.2}$$

The Cartesian components of $\hat{\vec{L}}$ are

$$\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y = -i\hbar\left(\hat{Y}\frac{\partial}{\partial z} - \hat{Z}\frac{\partial}{\partial y}\right), \tag{5.3}$$

$$\hat{L}_y = \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z = -i\hbar\left(\hat{Z}\frac{\partial}{\partial x} - \hat{X}\frac{\partial}{\partial z}\right), \tag{5.4}$$

$$\hat{L}_z = \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x = -i\hbar\left(\hat{X}\frac{\partial}{\partial y} - \hat{Y}\frac{\partial}{\partial x}\right). \tag{5.5}$$

Note that angular momentum does not exist in a one-dimensional space.

Commutation relations

Since $\hat{X}$, $\hat{Y}$ and $\hat{Z}$ mutually commute and so do $\hat{P}_x$, $\hat{P}_y$ and $\hat{P}_z$, and since $[\hat{X}, \hat{P}_x] = i\hbar$, $[\hat{Y}, \hat{P}_y] = i\hbar$, $[\hat{Z}, \hat{P}_z] = i\hbar$, we have

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= [\hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y,\ \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] \\
&= [\hat{Y}\hat{P}_z, \hat{Z}\hat{P}_x] - [\hat{Y}\hat{P}_z, \hat{X}\hat{P}_z] - [\hat{Z}\hat{P}_y, \hat{Z}\hat{P}_x] + [\hat{Z}\hat{P}_y, \hat{X}\hat{P}_z] \\
&= \hat{Y}[\hat{P}_z, \hat{Z}]\hat{P}_x + \hat{X}[\hat{Z}, \hat{P}_z]\hat{P}_y = i\hbar(\hat{X}\hat{P}_y - \hat{Y}\hat{P}_x) \\
&= i\hbar\hat{L}_z.
\end{aligned} \tag{5.6}$$

A similar calculation yields the other two commutation relations; but it is much simpler to infer them from (5.6) by means of a *cyclic permutation* of the xyz components, $x \to y \to z \to x$:

$$\boxed{[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, \qquad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, \qquad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y.} \tag{5.7}$$

As mentioned in Chapter 3, since $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_x$ do not commute, we cannot measure them simultaneously to arbitrary accuracy.

Note that the commutation relations (5.7) were derived by expressing the orbital angular momentum in the *position representation*. But since these are operator relations, they must be valid in any representation. In the following section we are going to consider the general formalism of angular momentum; a formalism that is restricted to no particular representation.

Example 5.1

(a) Calculate the commutators $[\hat{X},\ \hat{L}_x]$, $[\hat{X},\ \hat{L}_y]$ and $[\hat{X},\ \hat{L}_z]$.

(b) Calculate the commutators: $[\hat{P}_x,\ \hat{L}_x]$, $[\hat{P}_x,\ \hat{L}_y]$ and $[\hat{P}_x,\ \hat{L}_z]$.

(c) Use the results of (a) and (b) to calculate $[\hat{X},\ \hat{\vec{L}}^2]$ and $[\hat{P}_x,\ \hat{\vec{L}}^2]$.

Solution

(a) The only nonzero commutator which involves $\hat{X}$ and the various components of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ is $[\hat{X},\ \hat{P}_x] = i\hbar$. Having stated this result, we can easily evaluate the needed commutators. First, since $\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y$ involves no P_x, the operator $\hat{X}$ commutes separately with $\hat{Y}$, $\hat{P}_z$, $\hat{Z}$ and $\hat{P}_y$, hence

$$[\hat{X},\ \hat{L}_x] = [\hat{X},\ \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y] = 0. \tag{5.8}$$

The evaluation of the other two commutators is straightforward:

$$[\hat{X},\ \hat{L}_y] = [\hat{X},\ \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] = [\hat{X},\ \hat{Z}\hat{P}_x] = \hat{Z}[\hat{X},\ \hat{P}_x] = i\hbar\hat{Z}, \tag{5.9}$$
$$[\hat{X},\ \hat{L}_z] = [\hat{X},\ \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x] = -[\hat{X},\ \hat{Y}\hat{P}_x] = -\hat{Y}[\hat{X},\ \hat{P}_x] = -i\hbar\hat{Y}. \tag{5.10}$$

(b) The only commutator between $\hat{P}_x$ and the components of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ that survive is again $[\hat{P}_x,\ \hat{X}] = -i\hbar$. We may thus infer

$$[\hat{P}_x,\ \hat{L}_x] = [\hat{P}_x,\ \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y] = 0, \tag{5.11}$$
$$[\hat{P}_x,\ \hat{L}_y] = [\hat{P}_x,\ \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] = -[\hat{P}_x,\ \hat{X}\hat{P}_z] = -[\hat{P}_x,\ \hat{X}]\hat{P}_z = i\hbar\hat{P}_z, \tag{5.12}$$
$$[\hat{P}_x,\ \hat{L}_z] = [\hat{P}_x,\ \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x] = [\hat{P}_x,\ \hat{X}\hat{P}_y] = [\hat{P}_x,\ \hat{X}]\hat{P}_y = -i\hbar\hat{P}_y. \tag{5.13}$$

(c) Using the commutators derived in (a) and (b), we infer

$$\begin{aligned}[\hat{X},\ \hat{\vec{L}}^2] &= [\hat{X},\ \hat{L}_x^2] + [\hat{X},\ \hat{L}_y^2] + [\hat{X},\ \hat{L}_z^2] \\ &= 0 + \hat{L}_y[\hat{X},\ \hat{L}_y] + [\hat{X},\ \hat{L}_y]\hat{L}_y + \hat{L}_z[\hat{X},\ \hat{L}_z] + [\hat{X},\ \hat{L}_z]\hat{L}_z \\ &= i\hbar(\hat{L}_y\hat{Z} + \hat{Z}\hat{L}_y - \hat{L}_z\hat{Y} - \hat{Y}\hat{L}_y),\end{aligned} \tag{5.14}$$
$$\begin{aligned}[\hat{P}_x,\ \hat{\vec{L}}^2] &= [\hat{P}_x,\ \hat{L}_x^2] + [\hat{P}_x,\ \hat{L}_y^2] + [\hat{P}_x,\ \hat{L}_z^2] \\ &= 0 + \hat{L}_y[\hat{P}_x,\ \hat{L}_y] + [\hat{P}_x,\ \hat{L}_y]\hat{L}_y + \hat{L}_z[\hat{P}_x,\ \hat{L}_z] + [\hat{P}_x,\ \hat{L}_z]\hat{L}_z \\ &= i\hbar(\hat{L}_y\hat{P}_z + \hat{P}_z\hat{L}_y - \hat{L}_z\hat{P}_y - \hat{P}_y\hat{L}_y),\end{aligned} \tag{5.15}$$

5.3 General Formalism of Angular Momentum

An angular momentum operator $\hat{\vec{J}}$ is defined by its three components $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$, which satisfy the commutation relations:

$$\boxed{[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z, \qquad [\hat{J}_y, \hat{J}_z] = i\hbar\hat{J}_x, \qquad [\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y,} \tag{5.16}$$

or equivalently by

$$\hat{\vec{J}} \times \hat{\vec{J}} = i\hbar\hat{\vec{J}}. \tag{5.17}$$

Since $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$ do not mutually commute, they cannot be simultaneously diagonalized; that is, they do not possess common eigenstates. The square of the angular momentum

$$\hat{\vec{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2, \tag{5.18}$$

is a scalar, hence it commutes with $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$:

$$[\hat{\vec{J}}^2, \hat{J}_k] = 0, \tag{5.19}$$

where k stands for x, y, and z. For instance, in the the case $k = x$ we have

$$\begin{aligned} [\hat{\vec{J}}^2, \hat{J}_x] &= [\hat{J}_x^2, \hat{J}_x] + \hat{J}_y[\hat{J}_y, \hat{J}_x] + [\hat{J}_y, \hat{J}_x]\hat{J}_y + \hat{J}_z[\hat{J}_z, \hat{J}_x] + [\hat{J}_z, \hat{J}_x]\hat{J}_z \\ &= \hat{J}_y(-i\hbar\hat{J}_z) + (-i\hbar\hat{J}_z)\hat{J}_y + \hat{J}_z(i\hbar\hat{J}_y) + (i\hbar\hat{J}_y)\hat{J}_z \\ &= 0, \end{aligned} \tag{5.20}$$

because $[\hat{J}_x^2, \hat{J}_x] = 0$, $[\hat{J}_y, \hat{J}_x] = -i\hbar\hat{J}_z$ and $[\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y$.

Eigenstates and eigenvalues of the angular momentum operator

Since $\hat{\vec{J}}^2$ commutes with $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$, each component of $\vec{J}$ can be separately diagonalized (hence it has simultaneous eigenfunctions) with $\hat{\vec{J}}^2$. But since the components $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$ do not mutually commute, we can choose only one of them to be simultaneously diagonalized with $\hat{\vec{J}}^2$. By convention we choose $\hat{J}_z$. There is nothing special about the z-direction, we can just as well take $\hat{\vec{J}}^2$ and $\hat{J}_x$ or $\hat{\vec{J}}^2$ and $\hat{J}_y$.

Let us now look for the joint eigenstates of $\hat{\vec{J}}^2$ and $\hat{J}_z$ and their corresponding eigenvalues. Denoting the joint eigenstates by $\mid \alpha,\ \beta\rangle$ and the eigenvalues of $\hat{\vec{J}}^2$ and $\hat{J}_z$ by $\hbar^2\alpha$ and $\hbar\beta$, respectively, we have

$$\hat{\vec{J}}^2 \mid \alpha,\ \beta\rangle = \hbar^2\alpha \mid \alpha,\ \beta\rangle, \tag{5.21}$$

$$\hat{J}_z \mid \alpha,\ \beta\rangle = \hbar\beta \mid \alpha,\ \beta\rangle. \tag{5.22}$$

The factor $\hbar$ is introduced so that α and β are dimensionless, since the angular momentum has the dimensions of $\hbar$: energy$\times$time. For simplicity, we will assume that these eigenstates are orthonormal

$$\langle\alpha',\ \beta' \mid \alpha,\ \beta\rangle = \delta_{\alpha'\alpha}\delta_{\beta'\beta}. \tag{5.23}$$

Now we need to introduce *raising* and *lowering* operators $\hat{J}_+$ and $\hat{J}_-$, just as we did when we studied the harmonic oscillator in Chapter 4:

$$\boxed{\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y.} \tag{5.24}$$

This leads to

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-), \qquad \hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-), \tag{5.25}$$

hence

$$\hat{J}_x^2 = \frac{1}{4}(\hat{J}_+^2 + \hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ + \hat{J}_-^2), \qquad \hat{J}_y^2 = -\frac{1}{4}(\hat{J}_+^2 - \hat{J}_+\hat{J}_- - \hat{J}_-\hat{J}_+ + \hat{J}_-^2). \tag{5.26}$$

Using (5.16) we can easily obtain the following commutation relations:

$$[\hat{\vec{J}}^2,\ \hat{J}_\pm] = 0, \qquad [\hat{J}_+,\ \hat{J}_-] = 2\hbar\hat{J}_z, \qquad [\hat{J}_z,\ \hat{J}_\pm] = \pm\hbar\hat{J}_\pm. \tag{5.27}$$

In addition, $\hat{J}_+$ and $\hat{J}_-$ satisfy

$$\hat{J}_+\hat{J}_- = \hat{J}_x^2 + \hat{J}_y^2 + \hbar\hat{J}_z = \hat{\vec{J}}^2 - \hat{J}_z^2 + \hbar\hat{J}_z, \tag{5.28}$$

$$\hat{J}_-\hat{J}_+ = \hat{J}_x^2 + \hat{J}_y^2 - \hbar\hat{J}_z = \hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z. \tag{5.29}$$

These relations lead to

$$\boxed{\hat{\vec{J}}^2 = \hat{J}_\pm\hat{J}_\mp + \hat{J}_z^2 \mp \hbar\hat{J}_z,} \tag{5.30}$$

which in turn yield

$$\boxed{\hat{\vec{J}}^2 = \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) + \hat{J}_z^2.} \tag{5.31}$$

Let us see how $\hat{J}_\pm$ operate on $\mid \alpha,\ \beta\rangle$. First, since $\hat{J}_\pm$ do not commute with $\hat{J}_z$, the kets $\mid \alpha,\ \beta\rangle$ are not eigenstates of $\hat{J}_\pm$. Using the relations (5.27) we have

$$\hat{J}_z(\hat{J}_\pm \mid \alpha,\ \beta\rangle) = (\hat{J}_\pm\hat{J}_z\ \pm\ \hbar\hat{J}_\pm) \mid \alpha,\ \beta\rangle = \hbar(\beta \pm 1)(\hat{J}_\pm \mid \alpha,\ \beta\rangle), \tag{5.32}$$

hence the ket $(\hat{J}_\pm \mid \alpha,\ \beta\rangle)$ is an eigenstate of $\hat{J}_z$ with eigenvalues $\hbar(\beta \pm 1)$. Now since $\hat{J}_z$ and $\hat{\vec{J}}^2$ commute, $(\hat{J}_\pm \mid \alpha,\ \beta\rangle)$ must also be an eigenstate of $\hat{\vec{J}}^2$. The eigenvalue of $\hat{\vec{J}}^2$ when acting on $\hat{J}_\pm \mid \alpha,\ \beta\rangle$ can be determined by making use of the commutator $[\hat{\vec{J}}^2, \hat{J}_\pm] = 0$. The state $(\hat{J}_\pm \mid \alpha,\ \beta\rangle)$ is also an eigenstate of $\hat{\vec{J}}^2$ with eigenvalue $\hbar^2\alpha$:

$$\hat{\vec{J}}^2(\hat{J}_\pm \mid \alpha,\ \beta\rangle) = \hat{J}_\pm\hat{\vec{J}}^2 \mid \alpha,\ \beta\rangle = \hbar^2\alpha(\hat{J}_\pm \mid \alpha,\ \beta\rangle). \tag{5.33}$$

From (5.32) and (5.33) we infer that when $\hat{J}_\pm$ acts on $\mid \alpha,\ \beta\rangle$, it does not affect the first quantum number α, but it raises or lowers the second quantum number β by one unit. That is, $J_\pm \mid \alpha,\ \beta\rangle$ is proportional to $\mid \alpha,\ \beta \pm 1\rangle$

$$\hat{J}_\pm \mid \alpha,\ \beta\rangle = C_{\alpha\beta}^\pm \mid \alpha,\ \beta \pm 1\rangle, \tag{5.34}$$

we will determine later on the constant $C_{\alpha\beta}^\pm$.

Note that, for a given eigenvalue α of $\hat{\vec{J}}^2$, there exists an *upper limit* for the quantum number β. This is due to the fact that the operator $\hat{\vec{J}}^2 - \hat{J}_z^2$ is positive, since $\hat{\vec{J}}^2 - \hat{J}_z^2 = \hat{J}_x^2 + \hat{J}_y^2 \geq 0$; we can therefore write

$$\langle \alpha,\ \beta \mid \hat{\vec{J}}^2 - \hat{J}_z^2 \mid \alpha,\ \beta\rangle = \hbar^2(\alpha - \beta^2) \geq 0, \quad \Longrightarrow \quad \alpha \geq \beta^2. \tag{5.35}$$

Since β has an upper limit β_{max}, there must exist a state $\mid \alpha,\ \beta_{max}\rangle$ which cannot be raised further:

$$\hat{J}_+ \mid \alpha,\ \beta_{max}\rangle = 0. \tag{5.36}$$

Using this relation along with $\hat{J}_-\hat{J}_+ = \hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z$, we see that $\hat{J}_-\hat{J}_+ \mid \alpha,\ \beta_{max}\rangle = 0$ or

$$(\hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z) \mid \alpha,\ \beta_{max}\rangle = \hbar^2(\alpha - \beta_{max}^2 - \beta_{max}) \mid \alpha,\ \beta_{max}\rangle, \tag{5.37}$$

hence

$$\alpha = \beta_{max}(\beta_{max} + 1). \tag{5.38}$$

After n successive applications of $\hat{J}_-$ on $\mid \alpha,\ \beta_{max}\rangle$, we must be able to reach a state $\mid \alpha,\ \beta_{min}\rangle$ which cannot be lowered further:

$$\hat{J}_- \mid \alpha,\ \beta_{min}\rangle = 0. \tag{5.39}$$

Using $\hat{J}_+\hat{J}_- = \hat{\vec{J}}^2 - \hat{J}_z^2 + \hbar\hat{J}_z$, and by analogy with (5.37) and (5.38), we infer that

$$\alpha = \beta_{min}(\beta_{min} - 1). \tag{5.40}$$

Comparing (5.38) and (5.40) we obtain

$$\beta_{max} = -\beta_{min}. \tag{5.41}$$

Since β_{min} was reached by n applications of $\hat{J}_-$ on $\mid \alpha,\ \beta_{max}\rangle$, it follows that

$$\beta_{max} = \beta_{min} + n; \tag{5.42}$$

and since $\beta_{min} = -\beta_{max}$ we conclude that

$$\beta_{max} = \frac{n}{2}. \tag{5.43}$$

Hence β_{max} can be integer or half-odd-integer, depending on n being even or odd.

It is now appropriate to introduce the notation j and m to denote β_{max} and β, respectively:

$$j = \beta_{max} = \frac{n}{2}, \qquad m = \beta, \tag{5.44}$$

hence the eigenvalue of $\hat{\vec{J}}^2$ is given by

$$\alpha = j(j+1). \tag{5.45}$$

Now since $\beta_{min} = -\beta_{max}$, and with n positive, we infer that the allowed values of m lie between $-j$ and $+j$:

$$\boxed{-j \le m \le j.} \tag{5.46}$$

The results obtained thus far can be summarized as follows: the eigenvalues of $\hat{\vec{J}}^2$ and J_z corresponding to the joint eigenvectors $\mid j,\ m\rangle$ are given, respectively, by $\hbar^2 j(j+1)$ and $\hbar m$

$$\boxed{\hat{\vec{J}}^2 \mid j,\ m\rangle = \hbar^2 j(j+1) \mid j,\ m\rangle \quad \text{and} \quad \hat{J}_z \mid j,\ m\rangle = \hbar m \mid j,\ m\rangle,} \tag{5.47}$$

where $j = 0, 1/2, 1, 3/2, \ldots$ and $m = -j, -(j-1), \ldots, j-1, j$. So for each j there are $2j+1$ values of m. For example, if $j = 1$ then m takes the three values $-1, 0, 1$; if $j = 5/2$ then m takes the six values $-5/2, -3/2, -1/2, 0, 1/2, 3/2, 5/2$. The values of j are either integer of half-integer. We see that the spectra of the angular momentum operators $\hat{\vec{J}}^2$ and $\hat{J}_z$ are discrete. Since the eigenstates corresponding to different angular momenta are orthogonal, and since the angular momentum spectra are discrete, the orthonormality condition is

$$\boxed{\langle j',\ m' \mid j,\ m\rangle = \delta_{j'\,j}\delta_{m'\,m}.} \tag{5.48}$$

Let us now look for the eigenvalues of $\hat{J}_\pm$ within the $\{\mid j,\ m\rangle\}$ basis; $\mid j,\ m\rangle$ is not an eigenstate of $\hat{J}_\pm$. We can rewrite the eigenvalue equation (5.34) as

$$\hat{J}_\pm \mid j,\ m\rangle = C^{\pm}_{jm} \mid j,\ m \pm 1\rangle. \tag{5.49}$$

We are going to derive C^+_{jm} and then infer C^-_{jm}. Since $\mid j,\, m\rangle$ is normalized, we can use (5.49) to obtain the following two expressions

$$\left(\hat{J}_+ \mid j,\, m\rangle\right)^\dagger \left(\hat{J}_+ \mid j,\, m\rangle\right) = |C^+_{jm}|^2\langle j,\, m+1 \mid j,\, m+1\rangle = |C^+_{jm}|^2, \tag{5.50}$$

$$\left|C^+_{jm}\right|^2 = \langle j,\, m|\hat{J}_-\hat{J}_+ \mid j,\, m\rangle. \tag{5.51}$$

But since $\hat{J}_-\hat{J}_+$ is equal to $(\hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z)$, and assuming the arbitrary phase of C^+_{jm} to be zero, we conclude that

$$C^+_{jm} = \sqrt{\langle j,\, m|\hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z \mid j,\, m\rangle} = \hbar\sqrt{j(j+1) - m(m+1)}. \tag{5.52}$$

By analogy with C^+_{jm} we can easily infer the expression for C^-_{jm}:

$$C^-_{jm} = \hbar\sqrt{j(j+1) - m(m-1)}. \tag{5.53}$$

Thus, the eigenvalue equations for $\hat{J}_+$ and $\hat{J}_-$ are given by

$$\boxed{\hat{J}_\pm \mid j,\, m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\ \mid j,\, m\pm 1\rangle,} \tag{5.54}$$

or

$$\boxed{\hat{J}_\pm \mid j,\, m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\ \mid j,\, m\pm 1\rangle,} \tag{5.55}$$

which in turn leads to the two relations:

$$\begin{aligned}\hat{J}_x \mid j,\, m\rangle &= \frac{1}{2}(\hat{J}_+ + \hat{J}_-) \mid j,\, m\rangle \\ &= \frac{\hbar}{2}\left[\sqrt{(j-m)(j+m+1)}\ \mid j,\, m+1\rangle + \sqrt{(j+m)(j-m+1)}\ \mid j,\, m-1\rangle\right],\end{aligned} \tag{5.56}$$

$$\begin{aligned}\hat{J}_y \mid j,\, m\rangle &= \frac{1}{2i}(\hat{J}_+ - \hat{J}_-) \mid j,\, m\rangle \\ &= \frac{\hbar}{2i}\left[\sqrt{(j-m)(j+m+1)}\ \mid j,\, m+1\rangle - \sqrt{(j+m)(j-m+1)}\ \mid j,\, m-1\rangle\right].\end{aligned} \tag{5.57}$$

The expectation values of $\hat{J}_x$ and $\hat{J}_y$ are therefore zero:

$$\langle j,\, m \mid \hat{J}_x \mid j,\, m\rangle = \langle j,\, m \mid \hat{J}_y \mid j,\, m\rangle = 0 \tag{5.58}$$

We will show later in (5.204) that the expectation values $\langle j,\, m \mid \hat{J}_x^2 \mid j,\, m\rangle$ and $\langle j,\, m \mid \hat{J}_y^2 \mid j,\, m\rangle$ are equal and given by

$$\boxed{\langle \hat{J}_x^2\rangle = \langle \hat{J}_y^2\rangle = \frac{1}{2}\left[\langle j,\, m \mid \hat{\vec{J}}^2 \mid j,\, m\rangle - \langle j,\, m \mid \hat{J}_z^2 \mid j,\, m\rangle\right] = \frac{\hbar^2}{2}\left[j(j+1) - m^2\right].} \tag{5.59}$$

5.7.2 Eigenfunctions of $\hat{\vec{L}}^2$

Let us now focus on determining the eigenfunctions $\Theta_{lm}(\theta)$ of $\hat{\vec{L}}^2$. We are going to follow two methods. The first method involves differential equations and gives $\Theta_{lm}(\theta)$ in terms of the well-known associated Legendre functions. The second method is algebraic; it deals with the operators $\hat{L}_{\pm}$ and enables an explicit construction of $Y_{lm}(\theta, \varphi)$, the spherical harmonics.

5.7.2.1 First Method for Determining the Eigenfunctions of $\hat{\vec{L}}^2$

We begin by applying $\hat{\vec{L}}^2$ of (5.130) to the eigenfunctions

$$Y_{lm}(\theta, \varphi) = \frac{1}{\sqrt{2\pi}}\Theta_{lm}(\theta)e^{im\varphi}. \tag{5.144}$$

This gives

$$\begin{aligned} \hat{\vec{L}}^2 Y_{lm}(\theta, \varphi) &= \frac{-\hbar^2}{\sqrt{2\pi}}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\Theta_{lm}(\theta)e^{im\varphi} \\ &= \frac{\hbar^2 l(l+1)}{\sqrt{2\pi}}\Theta_{lm}(\theta)e^{im\varphi}, \end{aligned} \tag{5.145}$$

which, after eliminating the φ-dependence, reduces to

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d(\Theta_{lm}(\theta))}{d\theta}\right) + \left[l(l+1) - \frac{m^2}{\sin^2\theta}\right]\Theta_{lm}(\theta) = 0. \tag{5.146}$$

This equation is known as the *Legendre differential equation*. Its solutions can be expressed in terms of the *associated Legendre functions* $P_l^m(\cos\theta)$:

$$\Theta_{lm}(\theta) = C_{lm}P_l^m(\cos\theta), \tag{5.147}$$

which are defined by

$$P_l^m(x) = (1 - x^2)^{|m|/2}\frac{d^{|m|}}{dx^{|m|}}P_l(x). \tag{5.148}$$

This shows that

$$P_l^{-m}(x) = P_l^m(x), \tag{5.149}$$

where $P_l(x)$ is the lth *Legendre polynomial* which is defined by the *Rodrigues formula*

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2 - 1)^l. \tag{5.150}$$

We can obtain at once the first few Legendre polynomials:

$$P_0(x) = 1, \qquad P_1(x) = \frac{1}{2}\frac{d(x^2 - 1)}{dx} = x \tag{5.151}$$

$$P_2(x) = \frac{1}{8}\frac{d^2(x^2 - 1)^2}{dx^2} = \frac{1}{2}(3x^2 - 1), \qquad P_3(x) = \frac{1}{48}\frac{d^3(x^2 - 1)^3}{dx^3} = \frac{1}{2}(5x^3 - 3x), \tag{5.152}$$

Table 5.1 First few Legendre polynomials and associated Legendre functions.

Legendre Polynomials	Associated Legendre Functions
$P_0(\cos\theta) = 1$	$P_1^1(\cos\theta) = \sin\theta$
$P_1(\cos\theta) = \cos\theta$	$P_2^1(\cos\theta) = 3\cos\theta\sin\theta$
$P_2(\cos\theta) = (3\cos^2\theta - 1)/2$	$P_2^2(\cos\theta) = 3\sin^2\theta$
$P_3(\cos\theta) = (5\cos^3\theta - 3\cos\theta)/2$	$P_3^1(\cos\theta) = 3\sin\theta(5\cos^3\theta - 1)/2$
$P_4(\cos\theta) = (35\cos^4\theta - 30\cos^2\theta + 3)/8$	$P_3^2(\cos\theta) = 15\sin^2\theta\cos\theta$
$P_5(\cos\theta) = (63\cos^5\theta - 70\cos^3\theta + 15\cos\theta)/8$	$P_3^3(\cos\theta) = 15\sin^3\theta$

$$P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3), \qquad P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x). \tag{5.153}$$

The Legendre polynomials satisfy the following closure or completeness relation:

$$\frac{1}{2}\sum_{l=0}^{\infty}(2l+1)P_l(x')P_l(x) = \delta(x - x') \tag{5.154}$$

and

$$P_l(-x) = (-1)^l P_l(x). \tag{5.155}$$

A similar calculation leads to the first few associated Legendre functions:

$$P_1^1(x) = \sqrt{1 - x^2}, \tag{5.156}$$

$$P_2^1(x) = 3x\sqrt{1 - x^2}, \qquad P_2^2(x) = 3(1 - x^2), \tag{5.157}$$

$$P_3^1(x) = \frac{3}{2}(5x^2 - 1)\sqrt{1 - x^2}, \quad P_3^2(x) = 15x(1 - x^2), \quad P_3^3(x) = 15(1 - x^2)^{3/2}, \tag{5.158}$$

where $P_l^0(x) = P_l(x)$, with $l = 0, 1, 2, 3, \ldots$. The first few expressions for the associated Legendre functions and the Legendre polynomials are listed in Table 5.1.

The constant C_{lm} of (5.147) can be determined from the orthonormalization condition

$$\langle l', m' \mid l, m\rangle = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\ \sin\theta \langle l'm'|\theta\,\varphi\rangle\langle\theta\varphi \mid l, m\rangle = \delta_{l'l}\delta_{m'm}, \tag{5.159}$$

which can be written as

$$\boxed{\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\ \sin\theta\ Y_{l'm'}^*(\theta,\varphi)Y_{lm}(\theta,\varphi) = \delta_{l'l}\delta_{m'm}.} \tag{5.160}$$

This relation is known as the normalization condition of spherical harmonics. Using the form (5.144) for $Y_{lm}(\theta,\varphi)$, we obtain

$$\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\ \sin\theta\,|Y_{lm}(\theta,\varphi)|^2 = \frac{|C_{lm}|^2}{2\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta |P_l^m(\cos\theta)|^2 = 1. \tag{5.161}$$

From the theory of associated Legendre functions, we have

$$\int_0^\pi d\theta\, \sin\theta P_l^m(\cos\theta) P_{l'}^m(\cos\theta) = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'}, \tag{5.162}$$

which is known as the normalization condition of associated Legendre functions. A combination of the previous two relations leads to an expression for the coefficient C_{lm}:

$$C_{lm} = (-1)^m \sqrt{\left(\frac{2l+1}{2}\right)\frac{(l-m)!}{(l+m)!}} \qquad (m \geq 0). \tag{5.163}$$

Inserting this equation into (5.147), we obtain the eigenfunctions of $\hat{\vec{L}}^2$:

$$\Theta_{lm}(\theta) = (-1)^m \sqrt{\left(\frac{2l+1}{2}\right)\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta). \tag{5.164}$$

Finally, the joint eigenfunctions, $Y_{lm}(\theta, \varphi)$, of $\hat{\vec{L}}^2$ and $\hat{J}_z$ can be obtained by substituting (5.139) and (5.164) into (5.135) are given by

$$\boxed{Y_{lm}(\theta,\varphi) = (-1)^m \sqrt{\left(\frac{2l+1}{4\pi}\right)\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta) e^{im\varphi} \qquad (m \geq 0).} \tag{5.165}$$

These are called the *normalized spherical harmonics*.

5.7.2.2 Second Method for Determining the Eigenfunctions of $\hat{\vec{L}}^2$

The second method deals with a direct construction of $Y_{lm}(\theta, \varphi)$; it starts with the case $m = l$ (this is the maximum value of m). By analogy with the general angular momentum algebra developed in the previous section, the action of $\hat{L}_+$ on Y_{ll} gives zero

$$\langle \theta\ \varphi | \hat{L}_+ \mid l,\ l\rangle = \hat{L}_+ Y_{ll}(\theta, \varphi) = 0, \tag{5.166}$$

since Y_{ll} cannot be raised further as $Y_{ll} = Y_{lm_{max}}$.

Using the expression (5.131) for $\hat{L}_+$ in the spherical coordinates, we can rewrite (5.166) as follows:

$$\frac{\hbar e^{i\varphi}}{\sqrt{2\pi}}\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right]\Theta_{ll}(\theta)e^{i\,l\varphi} = 0, \tag{5.167}$$

which leads to

$$\frac{\partial\Theta_{ll}(\theta)}{\partial\theta} = l\cot\theta. \tag{5.168}$$

The solution to this differential equation is of the form

$$\Theta_{ll}(\theta) = C_l \sin^l\theta, \tag{5.169}$$

where C_l is a constant to be determined from the normalization condition (5.160) of $Y_{ll}(\theta, \varphi)$:

$$Y_{ll}(\theta,\varphi) = \frac{C_l}{\sqrt{2\pi}} e^{il\varphi}\sin^l\theta. \tag{5.170}$$

We can ascertain that C_l is given by

$$C_l = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)!}{2}}. \tag{5.171}$$

The action of L_- on $Y_{ll}(\theta, \varphi)$ is given on the one hand by

$$\hat{L}_- Y_{ll}(\theta, \varphi) = \sqrt{2l}\, Y_{l,l-1}(\theta, \varphi), \tag{5.172}$$

and, on the other hand, by

$$\hat{L}_- Y_{ll}(\theta, \varphi) = \frac{(-1)^l}{2^l\, l!}\sqrt{\frac{(2l+1)!}{4\pi}}\, e^{i(l-1)\varphi}(\sin\theta)^{1-l}\frac{d}{d(\cos\theta)}[(\sin\theta)^{2l}], \tag{5.173}$$

where we have used the spherical coordinate form (5.131).

Similarly, we can show that the action of L_-^{l-m} on $Y_{ll}(\theta, \varphi)$ is given, on the one hand, by

$$L_-^{l-m} Y_{ll}(\theta, \varphi) = \hbar^{l-m}\sqrt{\frac{(2l)!(l+m)!}{(l-m)!}}\, Y_{lm}(\theta, \varphi), \tag{5.174}$$

and, on the other hand, by

$$L_-^{l-m} Y_{ll}(\theta, \varphi) = \hbar^{l-m}\frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l)!(2l+1)!}{4\pi}}\, e^{im\varphi}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\sin\theta)^{2l}, \tag{5.175}$$

where $m \geq 0$. Equating the previous two relations, we obtain the expression of the spherical harmonic $Y_{lm}(\theta, \varphi)$ for $m \geq 0$

$$\boxed{Y_{lm}(\theta, \varphi) = \frac{(-1)^l}{2^l l!}\sqrt{\left(\frac{2l+1}{4\pi}\right)\frac{(l+m)!}{(l-m)!}}\, e^{im\varphi}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\sin\theta)^{2l}.} \tag{5.176}$$

5.7.3 Properties of the Spherical Harmonics

Since the spherical harmonics $Y_{lm}(\theta, \varphi)$ are joint eigenfunctions of $\hat{\vec{L}}^2$ and $\hat{L}_z$ and are orthonormal (5.160), they constitute an orthonormal basis in the Hilbert space of square-integrable functions of θ and φ. The completeness relation is given by

$$\sum_{m=-l}^{l} \mid l,\ m\rangle\langle l,\ m \mid = 1, \tag{5.177}$$

or

$$\begin{aligned}\sum_m \langle\theta\varphi \mid l,\ m\rangle\langle l,\ m \mid \theta'\varphi' > &= \sum_m Y_{lm}^*(\theta', \varphi')Y_{lm}(\theta, \varphi) = \delta(\cos\theta - \cos\theta')\delta(\varphi - \varphi') \\ &= \frac{\delta(\theta - \theta')}{\sin\theta}\delta(\varphi - \varphi'). \end{aligned} \tag{5.178}$$

Let us mention some essential properties of the spherical harmonics. First, the spherical harmonics are complex functions; their complex conjugate is given by

$$\boxed{[Y_{lm}(\theta, \varphi)]^* = (-1)^m Y_{l,-m}(\theta, \varphi).} \tag{5.179}$$

Table 5.2 Spherical harmonics and their expressions in Cartesian coordinates.

$Y_{lm}(\theta, \varphi)$	$Y_{lm}(x, y, z)$
$Y_{00}(\theta, \varphi) = \frac{1}{\sqrt{4\pi}}$	$Y_{00}(x, y, z) = \frac{1}{\sqrt{4\pi}}$
$Y_{10}(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta$	$Y_{10}(x, y, z) = \sqrt{\frac{3}{4\pi}} \frac{z}{r}$
$Y_{1,\pm 1}(\theta, \varphi) = \mp\sqrt{\frac{3}{8\pi}} e^{\pm i\varphi} \sin\theta$	$Y_{1,\pm 1}(x, y, z) = \mp\sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$
$Y_{20}(\theta, \varphi) = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1)$	$Y_{20}(x, y, z) = \sqrt{\frac{5}{16\pi}} \frac{3z^2 - r^2}{r^2}$
$Y_{2,\pm 1}(\theta, \varphi) = \mp\sqrt{\frac{15}{8\pi}} e^{\pm i\varphi} \sin\theta \cos\theta$	$Y_{2,\pm 1}(x, y, z) = \mp\sqrt{\frac{15}{8\pi}} \frac{(x \pm iy)z}{r^2}$
$Y_{2,\pm 2}(\theta, \varphi) = \sqrt{\frac{15}{32\pi}} e^{\pm 2i\varphi} \sin^2\theta$	$Y_{2,\pm 2}(x, y, z) = \mp\sqrt{\frac{15}{32\pi}} \frac{x^2 - y^2 \pm 2ixy}{r^2}$

We can verify that $Y_{lm}(\theta, \varphi)$ is an eigenstate of the parity operator $\hat{\mathcal{P}}$ with an eigenvalue $(-1)^l$:

$$\hat{\mathcal{P}} Y_{lm}(\theta, \varphi) = Y_{lm}(\pi - \theta, \varphi + \pi) = (-1)^l Y_{lm}(\theta, \varphi), \tag{5.180}$$

since a spatial reflection about the origin, $\vec{r}\,' = -\vec{r}$, corresponds to $r' = r$, $\theta' = \pi - \theta$ and $\varphi' = \pi + \varphi$, which leads to $P_l^m(\cos\theta') = P_l^m(-\cos\theta) = (-1)^{l+m} P_l^m(\cos\theta)$ and $e^{im\varphi'} = e^{im\pi} e^{im\varphi} = (-1)^m e^{im\varphi}$.

We can establish a connection between the spherical harmonics and the Legendre polynomials by simply taking $m = 0$. Then equation (5.176) yields

$$Y_{l0}(\theta, \varphi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{2l+1}{4\pi}} \frac{d^l}{d(\cos\theta)^l} ((\sin\theta)^{2l}) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta), \tag{5.181}$$

with

$$P_l(\cos\theta) = \frac{1}{2^l l!} \frac{d^l}{d(\cos\theta)^l} (\cos^2\theta - 1)^l. \tag{5.182}$$

From the expression of Y_{lm}, we can verify that

$$Y_{lm}(0, \varphi) = \sqrt{\frac{2l+1}{4\pi}} \delta_{m0}. \tag{5.183}$$

The expressions for the spherical harmonics corresponding to $l = 0$, $l = 1$, and $l = 2$ are listed in Table 5.2.

Spherical harmonics in Cartesian coordinates

Note that $Y_{lm}(\theta, \varphi)$ can also be expressed in terms of the Cartesian coordinates. For this, we need only to substitute

$$\sin\theta\cos\varphi = \frac{x}{r}, \qquad \sin\theta\sin\varphi = \frac{y}{r}, \qquad \cos\theta = \frac{z}{r} \tag{5.184}$$

in the expression for $Y_{lm}(\theta, \varphi)$.

Radial Equation

Coulomb potential

Boundary condition.

$r \to \infty$

$r \to 0$

$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$

$v(\rho)$ should be slowly varying

Hydrogen Atom
Appendix F

. . The Radial Wave Function

Our first task is to tidy up the notation. Let

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}. \qquad [4.54]$$

(For bound states, $E < 0$, so κ is real.) Dividing Equation 4.53 by E, we have

$$\frac{1}{\kappa^2}\frac{d^2u}{dr^2} = \left[1 - \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}\frac{1}{(\kappa r)} + \frac{l(l+1)}{(\kappa r)^2}\right]u.$$

This suggests that we let

$$\rho \equiv \kappa r, \quad \text{and} \quad \rho_0 \equiv \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}, \qquad [4.55]$$

so that

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u. \qquad [4.56]$$

Next we examine the asymptotic form of the solutions. As $\rho \to \infty$, the constant term in the brackets dominates, so (approximately)

$$\frac{d^2u}{d\rho^2} = u.$$

The general solution is

$$u(\rho) = Ae^{-\rho} + Be^{\rho}, \qquad [4.57]$$

but e^{ρ} blows up (as $\rho \to \infty$), so $B = 0$. Evidently,

$$u(\rho) \sim Ae^{-\rho} \qquad [4.58]$$

for large ρ. On the other hand, as $\rho \to 0$ the centrifugal term dominates[12]; approximately, then,

$$\frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2}u.$$

The general solution (check it!) is

$$u(\rho) = C\rho^{l+1} + D\rho^{-l},$$

but ρ^{-l} blows up (as $\rho \to 0$), so $D = 0$. Thus

$$u(\rho) \sim C\rho^{l+1} \qquad [4.59]$$

[12]This argument does not apply when $l = 0$ (although the conclusion, Equation 4.59, is in fact valid for that case too). But never mind: All I am trying to do is provide some *motivation* for a change of variables (Equation 4.60.)

for small ρ.

The next step is to peel off the asymptotic behavior, introducing the new function $v(\rho)$:

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho), \qquad [4.60]$$

in the hope that $v(\rho)$ will turn out to be simpler than $u(\rho)$. The first indications are not auspicious:

$$\frac{du}{d\rho} = \rho^l e^{-\rho}\left[(l+1-\rho)v + \rho\frac{dv}{d\rho}\right],$$

and

$$\frac{d^2u}{d\rho^2} = \rho^l e^{-\rho}\left\{\left[-2l-2+\rho+\frac{l(l+1)}{\rho}\right]v + 2(l+1-\rho)\frac{dv}{d\rho} + \rho\frac{d^2v}{d\rho^2}\right\}.$$

In terms of $v(\rho)$, then, the radial equation (Equation 4.56) reads

$$\rho\frac{d^2v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0. \qquad [4.61]$$

Finally, we assume the solution, $v(\rho)$, can be expressed as a power series in ρ:

$$v(\rho) = \sum_{j=0}^{\infty} a_j \rho^j. \qquad [4.62]$$

Our problem is to determine the coefficients $(a_0, a_1, a_2, \ldots)$. Differentiating term by term,

$$\frac{dv}{d\rho} = \sum_{j=0}^{\infty} j a_j \rho^{j-1} = \sum_{j=0}^{\infty}(j+1)a_{j+1}\rho^j.$$

[In the second summation I have renamed the "dummy index": $j \to j+1$. If this troubles you, write out the first few terms explicitly, and *check* it. You might say that the sum should now begin at $j=-1$, but the factor $(j+1)$ kills that term anyway, so we might as well start at zero.] Differentiating again,

$$\frac{d^2v}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1)a_{j+1}\rho^{j-1}.$$

Inserting these into Equation 4.61, we have

$$\sum_{j=0}^{\infty} j(j+1)a_{j+1}\rho^j + 2(l+1)\sum_{j=0}^{\infty}(j+1)a_{j+1}\rho^j$$

$$-2\sum_{j=0}^{\infty} j a_j \rho^j + [\rho_0 - 2(l+1)]\sum_{j=0}^{\infty} a_j\rho^j = 0.$$

Equating the coefficients of like powers yields

$$j(j+1)a_{j+1} + 2(l+1)(j+1)a_{j+1} - 2ja_j + [\rho_0 - 2(l+1)]a_j = 0,$$

or

$$a_{j+1} = \left\{ \frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)} \right\} a_j. \qquad [4.63]$$

This recursion formula determines the coefficients, and hence the function $v(\rho)$: We start with $a_0 = A$ (this becomes an overall constant, to be fixed eventually by normalization), and Equation 4.63 gives us a_1; putting this back in, we obtain a_2, and so on.[13]

Now let's see what the coefficients look like for large j (this corresponds to large ρ, where the higher powers dominate). In this regime the recursion formula says

$$a_{j+1} \cong \frac{2j}{j(j+1)} a_j = \frac{2}{j+1} a_j,$$

so

$$a_j \cong \frac{2^j}{j!} A. \qquad [4.64]$$

Suppose for a moment that this were the *exact* result. Then

$$v(\rho) = A \sum_{j=0}^{\infty} \frac{2^j}{j!} \rho^j = Ae^{2\rho},$$

and hence

$$u(\rho) = A\rho^{l+1} e^{\rho}, \qquad [4.65]$$

which blows up at large ρ. The positive exponential is precisely the asymptotic behavior we *didn't* want in Equation 4.57. (It's no accident that it reappears here; after all, it *does* represent the asymptotic form of *some* solutions to the radial equation—they just don't happen to be the ones we're interested in, because they aren't normalizable.) There is only one way out of this dilemma: *The series must terminate.* There must occur some maximal integer, $j_{\max}$, such that

$$a_{j_{\max}+1} = 0 \qquad [4.66]$$

(and beyond which all coefficients vanish automatically). Evidently (Equation 4.63)

$$2(j_{\max} + l + 1) - \rho_0 = 0.$$

[13] You might wonder why I didn't use the series method directly on $u(\rho)$—why factor out the asymptotic behavior before applying this procedure? The reason for peeling off ρ^{l+1} is largely aesthetic: Without this, the sequence would begin with a long string of zeroes (the first nonzero coefficient being a_{l+1}); by factoring out ρ^{l+1} we obtain a series that starts out with ρ^0. The $e^{-\rho}$ factor is more critical—if you *don't* pull that out, you get a three-term recursion formula involving a_{j+2}, a_{j+1}, and a_j (*try* it!), and that is enormously more difficult to work with.

Defining

$$n \equiv j_{\max} + l + 1 \qquad [4.67]$$

(the so-called **principal quantum number**), we have

$$\rho_0 = 2n. \qquad [4.68]$$

But ρ_0 determines E (Equations 4.54 and 4.55):

$$E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{me^4}{8\pi^2\epsilon_0^2\hbar^2\rho_0^2}, \qquad [4.69]$$

so the allowed energies are

$$\boxed{E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2}, \quad n = 1, 2, 3, \ldots.} \qquad [4.70]$$

This is the famous **Bohr formula**—by any measure the most important result in all of quantum mechanics. Bohr obtained it in 1913 by a serendipitous mixture of inapplicable classical physics and premature quantum theory (the Schrödinger equation did not come until 1924).

Combining Equations 4.55 and 4.68, we find that

$$\kappa = \left(\frac{me^2}{4\pi\epsilon_0\hbar^2}\right)\frac{1}{n} = \frac{1}{an}, \qquad [4.71]$$

where

$$\boxed{a \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}\ \text{m}} \qquad [4.72]$$

is the so-called **Bohr radius**. It follows (again, from Equation 4.55) that

$$\rho = \frac{r}{an}. \qquad [4.73]$$

Evidently the spatial wave functions for hydrogen are labeled by three quantum numbers (n, l, and m):

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)\, Y_l^m(\theta, \phi), \qquad [4.74]$$

where (referring back to Equations 4.36 and 4.60)

$$R_{nl}(r) = \frac{1}{r}\rho^{l+1}e^{-\rho}v(\rho), \qquad [4.75]$$

and $v(\rho)$ is a polynomial of degree $j_{\max} = n - l - 1$ in ρ, whose coefficients are determined (up to an overall normalization factor) by the recursion formula

$$a_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)} a_j. \tag{4.76}$$

The **ground state** (that is, the state of lowest energy) is the case $n = 1$; putting in the accepted values for the physical constants, we get

$$E_1 = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right] = -13.6 \text{ eV}. \tag{4.77}$$

Evidently the **binding energy** of hydrogen (the amount of energy you would have to impart to the electron in order to ionize the atom) is 13.6 eV. Equation 4.67 forces $l = 0$, whence also $m = 0$ (see Equation 4.29), so

$$\psi_{100}(r, \theta, \phi) = R_{10}(r) Y_0^0(\theta, \phi). \tag{4.78}$$

The recursion formula truncates after the first term (Equation 4.76 with $j = 0$ yields $a_1 = 0$), so $v(\rho)$ is a constant (a_0) and

$$R_{10}(r) = \frac{a_0}{a} e^{-r/a}. \tag{4.79}$$

Normalizing it, in accordance with Equation 4.31,

$$\int_0^\infty |R_{10}|^2 r^2 \, dr = \frac{|a_0|^2}{a^2} \int_0^\infty e^{-2r/a} r^2 \, dr = |a_0|^2 \frac{a}{4} = 1,$$

so $a_0 = 2/\sqrt{a}$. Meanwhile, $Y_0^0 = 1/\sqrt{4\pi}$, so

$$\boxed{\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}.} \tag{4.80}$$

If $n = 2$ the energy is

$$E_2 = \frac{-13.6 \text{ eV}}{4} = -3.4 \text{ eV}; \tag{4.81}$$

this is the first excited state—or rather, *states*, since we can have either $l = 0$ (in which case $m = 0$) or $l = 1$ (with $m = -1$, 0, or +1), so there are actually four different states that share this energy. If $l = 0$, the recursion relation (Equation 4.76) gives

$$a_1 = -a_0 \text{ (using } j = 0\text{)}, \quad \text{and } a_2 = 0 \text{ (using } j = 1\text{)},$$

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so $v(\rho) = a_0(1-\rho)$, and hence

$$R_{20}(r) = \frac{a_0}{2a}\left(1 - \frac{r}{2a}\right)e^{-r/2a}. \quad [4.82]$$

If $l = 1$ the recursion formula terminates the series after a single term, so $v(\rho)$ is a constant, and we find

$$R_{21}(r) = \frac{a_0}{4a^2} r e^{-r/2a}. \quad [4.83]$$

(In each case the constant a_0 is to be determined by normalization—see Problem 4.11.)

For arbitrary n, the possible values of l (consistent with Equation 4.67) are

$$l = 0, 1, 2, \ldots, n-1. \quad [4.84]$$

For each l, there are $(2l+1)$ possible values of m (Equation 4.29), so the total degeneracy of the energy level E_n is

$$d(n) = \sum_{l=0}^{n-1}(2l+1) = n^2. \quad [4.85]$$

Physical Interpretation

Angular Momentum.

Definition $\vec{L} = \vec{r} \times \vec{p}$, Angular momentum in spherical coordination

Commutator L^2

H in terms of $\vec{L}^2$

$$H \psi_{n\ell m} = E_n \psi_{n\ell m}$$

$$L^2 \psi_{n\ell m} = \ell(\ell+1)\hbar^2 \psi_{n\ell m}. \rightarrow \theta \text{ equation}$$

$$L_z \psi_{n\ell m} = m\hbar \psi_{n\ell m} \rightarrow \phi \text{ equation}$$

$$n \geq \ell+1 \qquad m = -\ell, -\ell+1, \cdots +\ell$$

Normalization

$$\iiint C_{n\ell m} |R_{n\ell}|^2 |Y_{\ell m}|^2 r^2 dr \sin\theta \, d\theta \, d\phi = 1$$

$$\underbrace{\int |R_{n\ell}|^2 r^2 dr}_{=1} \iint |Y_{\ell m}|^2 \sin\theta \, d\theta \, d\phi = 1$$

$\Rightarrow$ $\psi_{n\ell m}(r, \theta, \phi)$ is completed determined.

$[H, \vec{L}^2] = [H, L_z] = 0 \qquad [L^2, L_z] = 0$

simultaneous eigenstate can be found

Example ~~the~~ of the Hydrogen's ~~et~~ wave function

$$\psi(x, 0) = \sum C_{n\ell m} \psi_{n\ell m}$$

$\downarrow$

then $\psi(x, t) = \sum C_{n\ell m} \psi_{n\ell m} e^{-iE_n t/\hbar}$

$|C_{n\ell m}|^2$ = probability of finding

Second Method of solving the $Y_{\ell m}(\theta, \phi)$

$\Rightarrow$ This solved the central force problem with $V(r) = \frac{k}{r}$

$\downarrow$

hydrogen atom with proton at origin $\Rightarrow$ only provide a Colomb potential

Example

$$\psi(r,\theta,\phi) = a\psi_{100} + b\psi_{211}$$

$$|a|^2+|b|^2=1$$

$$\langle E\rangle = |a|^2E_1+|b|^2E_2$$

$$\langle L^2\rangle = |a|^2\cdot 0(0+1)\hbar^2 + |b|^2\cdot 1\cdot(1+1)\hbar^2$$

$$\langle L_z\rangle = |b|^2\hbar$$

$$\langle r^2\rangle = \iiint \psi(r,\theta,\phi)^*\cdot r^2\,\psi(r,\theta,\phi)\,r^2dr\sin\theta\,d\theta\,d\phi$$