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

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

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

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

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

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

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

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 $\quad Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$

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

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

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

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

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

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

↓

single-valueness of the wave function

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

- This is closely related to the quantization of angular momentum
- m is known as magnetic quantum number.

θ - equation

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

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

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

associated Legendre equation.

Physical requirement:

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

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

m must be from $-l$ to l, i.e.,

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

Θ is labelled by l, m

$\Theta(x) \propto P_l^m(x) \rightarrow$ 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.

Central Force Problem. time independent

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

1. Three Dimensional Problem in Spherical Coordinate.

Key Step

∇^2 in spherical coordinate.

See Appendix 1 → See (B.22)

Time - independent Schrodinger equation in spherical coordinate equation

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

$2m \to \mu$

$V(r)$ is a function of r only

⇒ Central force problem.

Key step

Seperation of variable method should be used.

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

$\uparrow$ Ansatz

B

Angular Momentum in Spherical Coordinates

In this appendix, we will show how to derive the expressions of the gradient $\vec{\nabla}$, the Laplacian ∇^2, and the components of the orbital angular momentum in spherical coordinates.

B.1 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

$$dr = \sin\theta \cos\varphi \, dx + \sin\theta \sin\varphi \, dy + \cos\theta \, dz \tag{B.8}$$
$$d\theta = \frac{1}{r} \cos\theta \cos\varphi \, dx + \frac{1}{r} \cos\theta \sin\varphi \, dy - \frac{1}{r} \sin\theta \, dz, \tag{B.9}$$
$$d\varphi = -\frac{\sin\varphi}{r \sin\theta} \, dx + \frac{\cos\varphi}{r \sin\theta} \, dy. \tag{B.10}$$

3

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

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

B.3 Angular Momentum in Spherical Coordinates

The orbital angular momentum operator $\vec{L}$ can be expressed in spherical coordinates as:

$$\hat{\vec{L}} = \hat{\vec{R}} \times \hat{\vec{P}} = (-i\hbar r)\hat{r} \times \vec{\nabla} = (-i\hbar r)\hat{r} \times \left[\hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial \theta} + \frac{\hat{\varphi}}{r\sin\theta}\frac{\partial}{\partial\varphi}\right], \tag{B.23}$$

or as

$$\hat{\vec{L}} = -i\hbar\left(\hat{\varphi}\frac{\partial}{\partial\theta} - \frac{\hat{\theta}}{\sin\theta}\frac{\partial}{\partial\varphi}\right). \tag{B.24}$$

Using (B.24) along with (B.2) to (B.4), we express the components $\hat{L}_x, \hat{L}_y, \hat{L}_z$ within the context of the spherical coordinates. For instance, the expression for $\hat{L}_x$ can be written as follows

$$\begin{aligned} \hat{L}_x &= \hat{x}.\vec{L} = -i\hbar\left(\hat{r}\sin\theta\cos\varphi + \hat{\theta}\cos\theta\cos\varphi - \hat{\varphi}\sin\varphi\right)\cdot\left(\hat{\varphi}\frac{\partial}{\partial\theta} - \frac{\hat{\theta}}{\sin\theta}\frac{\partial}{\partial\varphi}\right) \\ &= i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right). \end{aligned} \tag{B.25}$$

Similarly, we can easily obtain

$$\hat{L}_y = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right) \tag{B.26}$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}. \tag{B.27}$$

From the expressions (B.25) and (B.26) for $\hat{L}_x$ and $\hat{L}_y$, we infer that

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y = \hbar e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right), \tag{B.28}$$

$$\hat{L}_- = \hat{L}_x - i\hat{L}_y = \hbar e^{-i\varphi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\varphi}\right). \tag{B.29}$$

The expression for $\vec{L}^2$ is

$$\vec{L}^2 = -\hbar^2 r^2(\hat{r}\times\vec{\nabla})\cdot(\hat{r}\times\vec{\nabla}) = -\hbar^2 r^2\left[\nabla^2 - \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right]; \tag{B.30}$$

it can be easily written in terms of the spherical coordinates as

$$\vec{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]; \tag{B.31}$$

this expression was derived by substituting (B.22) into (B.30).

Note that, using the expression (B.30) for $\vec{L}^{\,2}$, we can rewrite ∇^2 as

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\vec{L}^{\,2} = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{1}{\hbar^2 r^2}\vec{L}^{\,2}. \tag{B.32}$$

Substitute back into the Schrodinger equation

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

$$\left. + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}RY\right\} + V(r)RY = ERY$$

$$-\frac{\hbar^2}{2m}\left\{Y\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{dR}{dr}\right\} + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}Y$$

$$+ \frac{R}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y\} + V(r)RY = ERY$$

Divide through by RY and rearrange

Multiply by r^2

$$-\frac{1}{R}\frac{d}{dr}r^2\frac{dR}{dr} + \frac{2mr^2}{\hbar^2}(V(r)-E)$$

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

LHS is a function of r only

RHS is a function of θ, ϕ

Choose the seperation constant to be $\ell(\ell+1)$

$$-\frac{1}{R}\frac{d}{dr}r^2\frac{dR}{dr} + \frac{2mr^2}{\hbar^2}(V(r)-E) = \ell(\ell+1)$$

$$-\hbar^2\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + 2\frac{mr^2}{\hbar^2}(V(r)-E)R = \ell(\ell+1)R$$

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

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

$\downarrow$

radial equation for $R(r)$

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

$\downarrow$

angular equation

Choose the seperation constant to be $l(l+1)$

$$\Rightarrow \frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2\overset{\mu}{m}r^2}{\hbar^2}[V(r)-E] = l(l+1)$$

$m \leftrightarrow \mu$ (for hydrogen atom) to avoid confusion

This is known as the radial equation

Remarks.

· It depends on $V(r)$

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

· $Y(\theta,\phi)$ is a function of θ,ϕ

angular part of the wave function

· The equation is known as the angular equation.

· The equation is independent of $V(r)$

It is valid for all central force problem.

· The angular equation is closely related to the angular momentum operator.

· The radial equation is related to the angular equation through the seperation constant $l(l+1)$

Again, use the seperation of variable method

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

The angular equation becomes

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

This equation is known as the θ - equation

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

This is the Φ equation

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

It is related to the ϕ equation through the seperation constant m^2

Physical requirement:

$\underbrace{\Phi(\phi+2\pi) = \Phi(\phi)}_{\text{single valueness of the wave function}} \Rightarrow m$ must be integer

$\Phi = e^{im\phi}$, $m = 0, \pm 1, \pm 2, \cdots$

is the physically allowed solution of the ϕ-equation

Of cource $Ae^{im\phi}$ is also a solution of the ϕ

A can be determined through normalization.

For central force problem, it is usual done together with θ part of the wave equation.

Now we shall study the θ - equation.

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

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

Change variable $x = \cos\theta$

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

↓ associated Legendre equation

Physical requirement

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

$$\Rightarrow \Theta_\ell^m(x) \propto P_\ell^m(x)$$

↓ associate Legendre polynomial.

ℓ must be positive (or zero) integers, i.e., $\ell = 0, 1, 2, \cdots$

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

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

$P_\ell(x)$ is the Legendre polynomial of degree ℓ

$P_\ell(x)$ is a solution of

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

↓ Legendre equation

$$P(x) = \sum_{k=0}^{\infty} c_k x^k \quad \text{with}$$

$$c_k = \frac{(k-2)(k-1) - \ell(\ell+1)}{k(k-1)} c_{k-2}$$

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

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

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

$$= -3c_0$$

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

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

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

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

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

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

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

Normalization

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

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

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

$$|A|^2 2\pi \frac{2}{15} = 1$$

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

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

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

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Orthonormal Relation of Spherical Harmonics

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

(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 $\ell = r$

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

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

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

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.

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

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

Need $\int_{-1}^{1} [P_\ell^0(x)]^2 dx = \frac{2}{2\ell+1}$ $\quad P_\ell^0(x) = P_\ell(x)$

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

Rodriguez formula

we shall show this formula in the Appendix

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

Repeatly use integration by part

$$= \frac{(-1)^\ell}{2^{2\ell}(\ell!)^2} \int_{-1}^{1} (x^2-1)^\ell \frac{d^{2\ell}}{dx^{2\ell}} (x^2-1)^\ell dx$$

In the $\frac{d^{2\ell}}{dx^{2\ell}}$ only the leading term will contribute

$$= \frac{(-1)^\ell}{2^{2\ell}(\ell!)^2} \int (x^2-1)^\ell 2\ell(2\ell-1)(2\ell-2)\cdots(2\ell-(2\ell-1)) dx$$

$$= \frac{(-1)^\ell (2\ell)!}{2^{2\ell}(\ell!)^2} \int_{-1}^{1} (x^2-1)^\ell dx$$

Change of variable $x = 2u-1$ $\quad [x^2-1 = (x+1)(x-1)]$

$$= \frac{(-1)^\ell 2(2\ell)!}{(\ell!)^2} \int_0^1 u^\ell (1-u)^\ell du$$

given by calculus

$$= \frac{\Gamma(\ell+1)\Gamma(\ell+1)}{\Gamma(2\ell+2)}$$

$\Gamma(\ell+1) = \ell!$

$\Gamma(2\ell) = (2\ell-1)!$

$\Gamma(2\ell+2) = (2\ell+1)!$

$$= \frac{2}{2\ell+1}$$

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

$$x = \cos\theta \qquad dx \longrightarrow -\sin\theta\, d\theta$$
$$(-1, 1) \longleftrightarrow (\pi, 0)$$

Define

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

Properties of spherical harmonics

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

  $P_\ell^{-m}(x)$ and $P_\ell^m(x)$ are proportional, since the differential equation depend on m^2 and m is an integer

  The proportional constant is fixed through the normalization formula.

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

  $\downarrow$

  orthonormal condition.

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

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

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

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

$\mu = \cancel{n}(n+1)$, where n 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 $-\frac{M}{2}\left[\ln(1+x)+\ln(1-x)\right]=\mathfrak{Z}_1(x)$

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 $\frac{M}{2}\left[\ln(1+x)-\ln(1-x)\right]=\mathfrak{Z}_2(x)$

Note: $\mathfrak{Z}_1(x)$, $\mathfrak{Z}_2(x)$ 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

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

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

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

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

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

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

↓

Legendre polynomial

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

2. Rodrigues Formula

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

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

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

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

$$= P_n(x)$$

$$\Rightarrow \quad P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2-1)^n$$

↓

Rodrigues formula.

3. Generating Function

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

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

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

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

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

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

$$n^2-3n+2-n^2-n = -4n+2$$

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

(-1) has been absorbed

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

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

obviously, the equation is satisfied

Claim

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

satisfies the normalization

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

$\downarrow$

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)

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

$\Rightarrow$ We need to prove

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

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

$$\frac{\overbrace{(2n-2r)}^{2\cancel{(n-r)}}(2n-2r-1)\cancel{(2n-2r-2)!}}{(n-r-1)!\cancel{(n-r)}\cdot(n-2r-2)!(n-2r-1)(n-2r)} \stackrel{?}{=} \frac{(4n-4r-2)}{(n-2r)(n-2r-1)} \frac{\cancel{(2n-2r-2)!}}{(n-r-1)!(n-2r-2)!}$$

$$2(2n-2r-1) = 4n-4r-2$$

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

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

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

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

$2^{m-(n-m)} \to 2^{2m-n}$, $x^{m-(n-m)} \to x^{2m-n}$

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

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

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

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

$\Rightarrow$ $(1-x^2)^{1/2} \frac{dP_n(x)}{dx}$ 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.

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

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 $= \sum_{n=0}^{\infty} n(n+1)\zeta^n P_n(x)$

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

$\{z^n\}$ 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

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

$$\frac{d^m}{dx^m}(1-x^2)\frac{d^2P_\ell(x)}{dx^2} = (1-x^2)\underbrace{\frac{d^{m+2}}{dx^{m+2}}}_{\text{(m) on the second}} P_\ell(x) - \underbrace{2mx}_{\binom{m}{1}} \underbrace{\frac{d^{m+1}}{dx^{m+1}}}_{\substack{m-1 \text{ on the second} \\ 1 \text{ on the first}}} P_\ell(x)$$

$$- \underbrace{m(m-1)}_{\binom{m}{2} \to \frac{m(m-1)}{2}} \frac{d^m P_\ell(x)}{dx^m} \quad m-2 \text{ on the second, twice on } (1-x^2) \to -2x$$

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

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

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

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

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

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

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

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

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

$\Downarrow$

$P_\ell^m(x)$ 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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.

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

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

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

$$x = \cos\theta$$

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

$\downarrow$ use associated

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

(Orbital) Angular Momentum

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

In Cartesian coordinate

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

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

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

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

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

$$[AB, C] = ABC - ACB + ACB - CAB$$

$$ABC - ACB = A[B, C] \qquad ACB - CAB = [A, C]B$$

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

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

$$[A, BC] = ABC - BAC + BAC - BCA$$

$$ABC - BAC = [A, B]C \qquad BAC - BCA = B[A, C]$$

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

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

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

$$(\mathrm{I}) = [yP_z, zP_x]$$

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

$$y[P_z, zP_x] = y\big([P_z, z]P_x + z\underbrace{[P_z, P_x]}_{=0}\big)$$

$$[y, zP_x]P_z = \underbrace{[y, z]}_{=0}P_x P_z - z\underbrace{[y, P_x]}_{=0}P_z$$

$$\downarrow$$

$$y[P_z, z]P_x$$

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

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

分類:	
編號:	18
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(II), (III) are obviously zero

$$(\mathrm{IV}) = [zP_y, xP_z]$$

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

$$[L_x, L_y] = i\hbar(xP_y - yP_x) = i\hbar L_z$$

Use similar method, we can show

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

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

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

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

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

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

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

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

Angular Momentum in Spherical Coordinate

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

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

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

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

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

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

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

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

Put it together

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

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

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

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

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

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

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

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

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

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

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

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

分類:	
編號:	21
總號:	

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

分類：	
編號：	22
總號：	

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

A

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

Coefficient of $\frac{\partial^2}{\partial\theta\partial\phi}$: $\cot\theta\cos\phi\sin\phi - \cot\theta\sin\phi\cos\phi = 0$

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

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$\langle L_x \rangle$, $\langle L_y \rangle$ 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

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

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

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

L_x, L_y, L_z in spherical coordinates.

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

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

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

From L_x, L_y, L_z and $L^2 = L_x^2 + L_y^2 + L_z^2$

One can show

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

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 $\ell(\ell+1)\hbar^2$

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

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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

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

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

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

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

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

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

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

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

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

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

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

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

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 probilility 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.

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Radial equation

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2\mu r^2}{\hbar^2}\left(-\frac{e^2}{4\pi\epsilon_0 r} - E\right)R = \ell(\ell+1) R$$

$$R = R(r)$$

Change of variable

$$u(r) = rR(r)$$

$$R(r) = \frac{u(r)}{r}$$

$$\frac{dR(r)}{dr} = \frac{1}{r^2}\left(r\frac{du}{dr} - u\right)$$

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) = \frac{d}{dr}\left(r\frac{du}{dr} - u\right) = r\frac{d^2u}{dr^2} + \frac{du}{dr} - \frac{du}{dr}$$

$$= r\frac{d^2u}{dr^2}$$

$$\Rightarrow -\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} + \Big[\underbrace{V + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}}_{V_{eff}}\Big]u = Eu$$

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

$$\Rightarrow -\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}\right]u = Eu$$

Change of variable $\rho = \kappa r$

$$\kappa = \frac{\sqrt{-2mE}}{\hbar} \qquad (E<0,\ \kappa \text{ is real.})$$

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

$$v(\rho) = \sum_{j=0}^{\infty} a_j \rho^j$$

with $$a_{j+1} = \frac{2(j+\ell+1) - \rho_0}{(j+1)(j+2\ell+2)} a_j$$

$$\rho_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$$

In order to have physically acceptable solutions the series must be terminated, i.e., there exists a j_{max} such that

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

Define $n = j_{max}+l+1$

$= $ principal quantum

$$2n = \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$$

$$\Rightarrow \quad \kappa = \frac{me^2}{4\pi\epsilon_0\hbar^2 n}$$

$$\frac{\sqrt{-2mE}}{\hbar} = \frac{me^2}{4\pi\epsilon_0\hbar^2 n}$$

$$-\frac{2mE}{\hbar^2} = \frac{m^2e^4}{(4\pi\epsilon_0\hbar)^2\hbar^2n^2}$$

$$\Rightarrow \quad \underset{E_n}{\underset{\parallel}{E}} = -\frac{me^4}{2(4\pi\epsilon_0\hbar)^2n^2}$$

$$= -\frac{13.6\ eV}{n^2}$$

$$\rho = \kappa r = \frac{me^2}{4\pi\epsilon_0\hbar}\frac{1}{n}r$$

$$= \frac{r}{na}.$$

Example: $n=3$, $l=2$

$$3 = j_{max}+2+1 \Rightarrow j_{max}$$

$$u(\rho) = \rho^3 e^{-\rho}\cdot \underset{\text{constant}}{\underset{\downarrow}{c}}$$

$$R_{n\ell} = \frac{u(r)}{r}$$

$$\rho = \frac{r}{na}$$

$$u_{n\ell}(\rho) \longrightarrow u_{32}(\rho) = c\, e^{-\rho} \rho^3$$
$$= c\, e^{-r/3a} \left(\frac{r}{3a}\right)^3$$

$$R_{n\ell}(r) = A r^2 e^{-r/3a}$$

Now we want to determine the normalization constant A

$$\int_0^\infty |R_{n\ell}(r)|^2 r^2 dr = 1$$

$$\Rightarrow |A|^2 \int_0^\infty r^6 e^{-2r/3a} dr = 1$$

From calculus, we have

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

if n is a positive integer or zero, and $a > 0$

$$\Rightarrow |A|^2 \frac{6!}{\left(\frac{2}{3a}\right)^7} = 1$$

$$|A|^2 \frac{6!}{\frac{2\cdot 2\cdot 2\cdot 2\cdot 2\cdot 2\cdot 2}{3\cdot 3\cdot 3\cdot 3\cdot 3\cdot 3\cdot 3}} a^7 = 1$$

$$\Rightarrow |A|^2 \frac{3^7\, \cancel{6}^{3}\cdot 5\cdot \cancel{4}^{2}\cdot 3\cdot \cancel{2}\cdot 1}{2\cdot 2\cdot 2\cdot 2\cdot \cancel{2}\cdot \cancel{2}\cdot \cancel{2}} a^7 = 1$$

$$\Rightarrow |A|^2 \frac{3^8\ 30}{4^2} a^7 = 1$$

$$|A| = \frac{4}{3^4\sqrt{30}} a^{-7/2} = \frac{4}{81\sqrt{3}} (a)^{-3/2} (a)^{-2}$$

Put it altogether

$$R_{32} = \frac{4}{81\sqrt{30}} a^{-3/2} \left(\frac{r}{a}\right)^2 e^{-r/3a}$$

given in the table
and the
figure.

Example $n=3$, $\ell=1$

$$3 = j_{max}+1+1 \Rightarrow j_{max}=1$$

$j=0$, a_0

$j=1$ $a_1 = \frac{2(0+1+1)-6}{(0+1)(0+2+2)} a_0 = -\frac{1}{2}$

$$v(\rho) = a_0 - \frac{1}{2}a_0\rho = a_0(1-\frac{1}{6}\frac{r}{a})$$

(Note $\rho = \frac{r}{an} = \frac{r}{3a}$)

$$\underset{u(r)}{\overset{\shortparallel}{u(\rho)}} = \rho^2 e^{-\rho} v(\rho)$$

$$= (\frac{r}{3a})^2 e^{-\frac{r}{3a}} a_0 (1-\frac{1}{6}\frac{r}{a})$$

$$R_{31}(r) = A r e^{-r/3a}(1-\frac{1}{6}\frac{r}{a})$$

$\uparrow$ A is a constant to be determined

$$\int_0^\infty |R_{31}|^2 r^2 dr = 1$$

$$|A^2| \int_0^\infty (1-\frac{1}{6}\frac{r}{a})^2 r^4 dr\, e^{-2r/3a}$$

$$= |A|^2 \left[\int_0^\infty r^4 e^{-2r/3a} dr - \frac{1}{3a}\int_0^\infty r^5 e^{-2r/3a} dr + \frac{1}{36a^2}\int_0^\infty r^6 e^{-2r/3a} dr\right] = 1$$

$$\int_0^\infty r^4 e^{-2r/3a} dr = \frac{4!}{(\frac{2}{3a})^5}$$

$$= \frac{4!\, 3^5}{2^5} = \frac{4\cdot3\cdot2\cdot1\cdot 3^4\cdot 3^1}{2^5} a^5$$

$$= \frac{3^6}{4} a^5$$

$$-\frac{1}{3a}\int_0^\infty r^5 e^{-2r/3a} dr$$

$$= -\frac{1}{3a} \frac{5!}{(\frac{2}{3a})^6} = -\frac{1}{3}\frac{5\cdot4\cdot3\cdot2\cdot1}{2^6}\cdot 3^6 a^5$$

$$= -\frac{5}{8} \cdot 3^6 \, a^5$$

$$\frac{1}{36a^2}\int_0^\infty r^6 e^{-2r/3a}\, dr$$

$$= \frac{1}{36a^2} \frac{6!}{\frac{2^7}{3^7} \cdot \frac{1}{a^7}}$$

$$= \frac{1}{\cancel{36}} \cdot \frac{\cancel{6}\cdot 5 \cdot \cancel{4} \cdot \cancel{3} \cdot \cancel{2}}{\cancel{2}^7 \, 2^5} 3^7 \, a^5$$

$$= \frac{15 \cdot 3^6}{32} a^5$$

$$|A|^2 \left(\frac{1}{4} - \frac{1}{8} + \frac{15}{32} \right) 3^6 a^5 = 1$$

$$\overset{\shortparallel}{\frac{8 - 20 + 15}{32}} = \frac{3}{32} = \frac{6}{64}$$

$$\Rightarrow \quad |A|^2 \cdot \frac{6}{64} \cdot 3^6 \, a^5 = 1$$

$$|A| = \frac{8}{27\sqrt{6}} a^{-5/2}$$

$$\Rightarrow \quad R_{31}(r) = \frac{8}{27\sqrt{6}} a^{-3/2} \left(\frac{r}{a}\right) e^{-r/3a}$$

the desired result.

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Summary

$\phi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi)$ is

the simultaneous eigenfunction of H, L^2, L_z

with eigenvalue $E_n = -\frac{13.6\,eV}{n^2}$, $\ell(\ell+1)\hbar^2$, $m\hbar$

respectively.

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

m, ℓ, n are integers

$H \phi_{n\ell m} = E_n \phi_{n\ell m}$ (The energy depends on n

only, this is valid for hydrogen atom.

For other central force problem, $E_n \to E_{n,\ell}$

i.e., energy may also depend on ℓ]

$\phi_{n\ell m}(r, \theta, \phi)$ with the same n, but different ℓ, m

will have the same energy $\Rightarrow$ they are degenerate

Number of independent state that have the same

energy = degree of denergency

With n fixed

$\ell = 0, 1, 2, \cdots n-1$

$m = -\ell, \cdots \ell$ $\Rightarrow$ there are $2\ell+1$ different m states

Number of states with the same energy (fixed n)

$$= \sum_{\ell=0}^{n-1} (2\ell+1) = 2\sum_{\ell=0}^{n-1} \ell + \sum_{\ell=0}^{n-1} = n(n-1) + n$$

$$= n^2$$

Example $n=3$

$$l = 0, \quad 1, \quad 2$$
$$\downarrow \quad \downarrow \quad \downarrow$$
$$1 \quad 3 \quad 5$$

$$1+3+5 = 9 = 3^2$$

$\phi_{nlm}(r,\theta,\phi)$ is a solution of the time independent Schrodinger equation

$$H\,\phi_{nlm}(r,\theta,\phi) = E_n\,\phi_{nlm}(r,\theta,\phi)$$

$\Rightarrow$ $\phi_{nlm}(r,\theta,\phi)\,e^{-iE_nt/\hbar}$ is a solution of the (time-dependent) Schrodinger equation

Example : A hydrogen atom is in state

$$\phi(r,\theta,\phi;0) = \frac{1}{\sqrt{2}}\phi_{200}(\vec{r}) + \frac{1}{\sqrt{3}}\phi_{311}(\vec{r}) + \frac{1}{\sqrt{6}}\phi_{322}(\vec{r})$$

at time t

$$\Rightarrow \phi(r,\theta,\phi;t) = \frac{1}{\sqrt{2}}\phi_{200}\,e^{-iE_2t/\hbar} + \frac{1}{\sqrt{3}}\phi_{311}(\vec{r})\,e^{-iE_3t/\hbar} + \frac{1}{\sqrt{6}}\phi_{322}(\vec{r})\,e^{-iE_3t/\hbar}$$

is time-dependent wave function since it satisfies the time-dependent Schrodinger equation. and the initial condition

$$H\,\phi_{nlm} = E_n\,\phi_{nlm}$$

$$L^2\phi_{nlm} = l(l+1)\hbar^2\,\phi_{nlm}$$

$$L_z\,\phi_{nlm} = m\hbar\,\phi_{nlm}$$

Example: An electron in the Coulomb field of a proton is in a state described by the wave function

$$\psi(\vec{r}) = \frac{1}{6}\left[4\phi_{100}(\vec{r}) + 3\phi_{211}(\vec{r}) - \phi_{210}(\vec{r}) + \sqrt{10}\,\phi_{21,-1}\right]$$

$$\langle H\rangle = \iiint \psi^*(\vec{r})\, H\, \psi(\vec{r})\, d^3r$$

$$= \frac{1}{36}\iiint\left[4\phi_{100}(\vec{r}) + 3\phi_{211}(\vec{r}) - \phi_{210}(\vec{r}) + \sqrt{10}\,\phi_{21-1}\right]^*$$

$$H\left[4\phi_{100}(\vec{r}) + 3\phi_{211}(\vec{r}) - \phi_{210}(\vec{r}) + \sqrt{10}\,\phi_{21-1}\right] d^3r$$

Since $\phi_{n\ell m}$ are eigenstate of H, the calculation is simple

$$= \frac{1}{36}\iiint\left[4\phi_{100}(\vec{r}) + 3\phi_{211}(r) - \phi_{210}(\vec{r}) + \sqrt{10}\,\phi_{21-1}\right]^*$$

$$\left(4E_1\phi_{100}(\vec{r}) + 3E_2\phi_{211}(\vec{r}) - E_2\phi_{210}(\vec{r}) + \sqrt{10}\,E_2\phi_{2,1,1}\right]$$

$$r^2 \sin\theta\, d\theta\, d\phi$$

(ℓ, m) are different

Use the orthonormal condition of $Y_{\ell m}$

$\Rightarrow$ only term contribute

$$= \frac{16}{36}E_1 + \frac{9}{36}E_2 + \frac{1}{36}E_2 + \frac{10}{36}E_2$$

$$= \frac{16}{36}E_1 + \frac{20}{36}\underset{\frac{1}{4}E_1}{\underset{\|}{E_2}}$$

$$= \frac{21}{36}E_1 = \frac{7}{12}(-13.6\text{ eV})$$

$$\langle L^2\rangle = \frac{16}{36}0(0+1)\hbar^2 + \frac{20}{36}1(1+1)\hbar^2$$

$$= \frac{20}{36}\cdot 2\hbar^2 = \frac{10}{9}\hbar$$

$$\langle L_z\rangle = \frac{16}{36}\cdot 0\hbar + \frac{9}{36}\hbar + \frac{1}{36}(0\hbar) - \frac{10}{36}\hbar$$

$$= -\frac{\hbar}{36}$$

Expectation value for r^k

$$\phi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r) Y_{\ell m}(\theta,\phi)$$

$$\langle r^k \rangle = \iiint \phi^*_{n\ell m}(r,\theta,\phi)\, r^k\, \phi_{n\ell m}(r,\theta,\phi)\, r^2 dr \sin\theta\, d\theta\, d\phi$$

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

$$= \int |R_{n\ell}(r)|^2 r^{k+2} dr$$

$n = 2,\ \ell = 1;\ k = 1$

$$R_{21}(r) = \frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} e^{-r/2a} \qquad a = \text{Bohr radius}$$

$$|R_{21}(r)|^2 = \frac{1}{24} a^{-5} r^2 e^{-r/a}$$

$$\langle r \rangle = \frac{1}{24} a^{-5} \int_0^\infty r^5 e^{-r/a} dr$$

Key definite integral

$$\int_0^\infty x^n e^{-bx} dx = \frac{n!}{b^{n+1}}$$

$$\langle r \rangle = \frac{1}{24} a^{-5} \frac{5!}{(\frac{1}{a})^6}$$

$$= 5a.$$

$k = -1;\quad n = 2,\ \ell = 1$

$$\langle \frac{1}{r} \rangle = \frac{1}{24} a^{-5} \int_0^\infty r^3 e^{-r/a} dr$$

$$= \frac{1}{24} a^{-5} \frac{3!}{(\frac{1}{a})^4}$$

$$= \frac{1}{4a}.$$

For $\Phi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\phi)$

Expectation value of $x = r\sin\theta\cos\phi$

$$\langle x \rangle = \iiint R_{n\ell}^*(r)\, Y_{\ell m}^*(\theta,\phi)\, [r\sin\theta\cos\phi]\, R_{n\ell}(r) Y_{\ell m}(\theta,\phi)\; r^2\, dr \sin\theta\, d\theta\, d\phi$$

$$= \int_0^\infty |R_{n\ell}(r)|^2 r^3\, dr \iint \sin\theta\, d\theta\; Y_{\ell m}^*(\theta,\phi)\, Y_\ell^m(\theta,\phi)\; \sin\theta\cos\phi \;\; d\phi$$

Look at the ϕ integration involves

$$\int_0^{2\pi} e^{+im\phi} \cos\phi\, e^{-im\phi}\, d\phi$$

$$= \int_0^{2\pi} \cos\phi \;\; d\phi = 0$$

$\Rightarrow \langle x \rangle = 0$

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

$$\langle L_x \rangle = \iiint R_{n\ell}^*(r)\, Y_{\ell m}^*(\theta,\phi) \left[i\hbar\left(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]\right.$$

$$\cancel{Y_{\ell m}(\theta,\phi) R_{n\ell}(r)\;\; r^2\, dr\, \sin\theta\, d\phi}$$

$$= \underbrace{\int_0^\infty |R_{n\ell}|^2 r^2\, dr}_{1}\;\; Y_{\ell m}^*(\theta,\phi)\left[i\hbar \sin\phi \frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right] Y_{\ell m}(\theta,\phi)\; d\phi$$

ϕ - dependent integration

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

$Y_{\ell m}(\theta,\phi \sim e^{-im\phi}$

(I) $\quad \int_0^{2\pi} e^{im\phi} \sin\phi\, e^{-im\phi}\, d\phi = \int_0^{2\pi} \sin\phi\, d\phi = 0$

(II) $\sim \int_0^{2\pi} e^{im\phi} \cos\phi\, e^{-im\phi} = \int_0^{2\pi} \cos\phi\, d\phi$

$\Rightarrow \langle L_x \rangle = 0$

When we deals with transition from n', ℓ', m' $\rightarrow n, \ell, m$; we encounter transition elements such as

$$\iiint \phi^{*}_{n',\ell',m'}(r,\theta,\phi) \underset{\underset{r\sin\theta\cos\phi}{\parallel}}{x} \phi_{n\ell m}(r,\theta,\phi)\, r^2 dr \sin\theta\, d\phi$$

The calculation follows the same procedure.

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Hydrogen Atom
Appendix F

. The Radial Wave Function

Our first task is to tidy up the notation. Let

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}. \tag{4.54}$$

(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

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

so that

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

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

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

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

$$u(\rho) \sim Ae^{-\rho} \tag{4.58}$$

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

$$u(\rho) \sim C\rho^{l+1} \tag{4.59}$$

[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.

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Defining

$$n \equiv j_{\max} + l + 1 \tag{4.67}$$

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

$$\rho_0 = 2n. \tag{4.68}$$

But ρ_0 determines E (Equations 4.54 and 4.55):

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

so the allowed energies are

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

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

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

where

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

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

$$\rho = \frac{r}{an}. \tag{4.73}$$

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

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

where (referring back to Equations 4.36 and 4.60)

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

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

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

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

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

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

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

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

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

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

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

If $n = 2$ the energy is

$$E_2 = \frac{-13.6 \text{ eV}}{4} = -3.4 \text{ eV}; \qquad [4.81]$$

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

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

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

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

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

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

(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

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

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

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

The Isotropic Harmonic Oscillator

The radial Schrödinger equation for a particle of mass M in an isotropic harmonic oscillator potential

$$V(r) = \frac{1}{2}M\omega^2 r^2 \tag{6.77}$$

is obtained from (6.56):

$$-\frac{\hbar^2}{2M}\frac{d^2U_{nl}(r)}{dr^2} + \left[\frac{1}{2}M\omega^2 r^2 + \frac{l(l+1)\hbar^2}{2Mr^2}\right]U_{nl}(r) = EU_{nl(r)}. \tag{6.78}$$

We are going to solve this equation by invoking the behavior of the solutions at very small and very large values of r. As $r \to 0$ this equation reduces to

$$-\frac{\hbar^2}{2M}\frac{d^2U(r)}{dr^2} + \frac{l(l+1)\hbar^2}{2Mr^2}U(r) = 0; \tag{6.79}$$

its solution is of the form $U(r) \sim r^{l+1}$. The asymptotic form of (6.78) for $r \to \infty$ is

$$-\frac{\hbar^2}{2M}\frac{d^2U}{dr^2} + \frac{1}{2}M\omega^2 r^2 U(r) = 0, \tag{6.80}$$

which admits solutions of type $U(r) \sim e^{-M\omega r^2/2\hbar}$. Combining (6.79) and (6.80), we can write the solutions of (6.78) as

$$U(r) = f(r)r^{l+1}e^{-M\omega r^2/2\hbar}, \tag{6.81}$$

where $f(r)$ is a function of r. Substituting this expression into (6.78), we obtain an equation for $f(r)$:

$$\frac{d^2f(r)}{dr^2} + 2\left(\frac{l+1}{r} - \frac{M\omega}{\hbar}r\right)\frac{df(r)}{dr} + \left[\frac{2ME}{\hbar^2} - (2l+3)\frac{M\omega}{\hbar}\right]f(r) = 0. \tag{6.82}$$

Let us try a power series solution

$$f(r) = \sum_{n=0}^{\infty} a_n r^n = a_0 + a_1 r + a_2 r^2 + \cdots + a_n r^n + \cdots. \tag{6.83}$$

Substituting this function into (6.82), we obtain

$$\sum_{n=0}^{\infty}\left\{n(n-1)a_n r^{n-2} + 2\left(\frac{l+1}{r} - \frac{M\omega}{\hbar}r\right)na_n r^{n-1} + \left[\frac{2ME}{\hbar^2} - (2l+3)\frac{M\omega}{\hbar}\right]a_n r^n\right\} = 0, \tag{6.84}$$

which in turn reduces to

$$\sum_{n=0}^{\infty}\left\{n(n+2l+1)a_n r^{n-2} + \left[-\frac{2M\omega}{\hbar}n + \frac{2ME}{\hbar^2} - (2l+3)\frac{M\omega}{\hbar}\right]a_n r^n\right\} = 0. \tag{6.85}$$

For this equation to hold, the coefficients of the various powers of r must vanish separately. For instance, when $n = 0$ the coefficient of r^{-2} is indeed zero:

$$0 \cdot (2l+1)a_0 = 0. \tag{6.86}$$

Note that a_0 need not be zero for this equation to hold. The coefficient of r^{-1} corresponds to $n = 1$ in (6.85); for this coefficient to vanish, we must have

$$1 \cdot (2l+2)a_1 = 0. \tag{6.87}$$

Since $(2l+2)$ cannot be zero, because the quantum number l is a positive integer, a_1 must vanish.

The coefficient of r^n results from the relation

$$\sum_{n=0} \left\{ (n+2)(n+2l+3)a_{n+2} + \left[\frac{2ME}{\hbar^2} - \frac{M\omega}{\hbar}(2n+2l+3) \right] a_n \right\} r^n = 0, \tag{6.88}$$

which leads to the recurrence formula

$$(n+2)(n+2l+3)a_{n+2} = \left[\frac{-2ME}{\hbar^2} + \frac{M\omega}{\hbar}(2n+2l+3) \right] a_n. \tag{6.89}$$

This recurrence formula shows that all coefficients a_n corresponding to odd values of n are zero, since $a_1 = 0$ (see (6.87)). The function $f(r)$ must therefore contain only even powers of r:

$$f(r) = \sum_{n=0}^{\infty} a_{2n} r^{2n} = \sum_{n'=0,2,4,\cdots}^{\infty} a_{n'} r^{n'}, \tag{6.90}$$

where all coefficients a_{2n}, with $n \geq 1$, are proportional to a_0.

Now note that when $n \to +\infty$ the function $f(r)$ diverges, for it behaves asymptotically like e^{r^2}. To obtain a finite solution, we must require the series (6.90) to stop at a maximum power $r^{n'+2}$, hence it must be *polynomial*. For this, we require $a_{n'+2}$ to be zero. The recurrence formula (6.89) therefore yields the *quantization condition*

$$2\frac{M}{\hbar^2} E_{n'l} - \frac{M\omega}{\hbar}(2n' + 2l + 3) = 0, \tag{6.91}$$

or

$$E_{n'l} = \left(n' + l + \frac{3}{2} \right) \hbar\omega, \tag{6.92}$$

where n' is even (see (6.90)). Denoting n' by $2N$, where $N = 0, 1, 2, 3, \ldots$, we rewrite this energy expression as

$$\boxed{E_n = \left(n + \frac{3}{2} \right) \hbar\omega \qquad (n = 0, 1, 2, 3, \ldots),} \tag{6.93}$$

where $n = n' + l = 2N + l$.

The ground state, whose energy is $E_0 = \frac{3}{2}\hbar\omega$, is not degenerate; the first excited state, $E_1 = \frac{5}{2}\hbar\omega$, is threefold degenerate; and the second excited state, $E_2 = \frac{7}{2}\hbar\omega$, is sixfold degenerate (Table 6.4). As shown in the following example, the degeneracy relation for the nth level is given by

$$\boxed{g_n = \frac{1}{2}(n+1)(n+2).} \tag{6.94}$$

Finally, we should note that the radial wave function is given by (6.81), where $f(r)$ is a polynomial in r^{2l} of degree $(n-l)/2$, hence the total wave function for the isotropic harmonic oscillator is

$$\psi_{nlm}(r, \theta, \varphi) = r^{l+1} f(r) Y_{lm}(\theta, \varphi) e^{-M\omega r^2/2\hbar} = R_{nl}(r) Y_{lm}(\theta, \varphi), \tag{6.95}$$

Table 6.4 Energy levels E_n and degeneracies g_n for an isotropic harmonic oscillator.

n	E_n	$N l$	m	g_n
0	$\frac{3}{2}\hbar\omega$	0 0	0	1
1	$\frac{5}{2}\hbar\omega$	0 1	$\pm 1, 0$	3
2	$\frac{7}{2}\hbar\,\omega$	1 0	0	6
		0 2	$\pm 2, \pm 1, 0$	
3	$\frac{9}{2}\hbar\omega$	1 1	$\pm 1, 0$	10
		0 3	$\pm 3, \pm 2, \pm 1, 0$	

where l takes only odd or only even values. For instance, the ground state corresponds to $(n, l, m) = (0, 0, 0)$; its wave function is

$$\psi_{000}(r, \theta, \varphi) = R_{00}(r)Y_{00}(\theta, \varphi) = \frac{2}{\sqrt{\sqrt{\pi}}}\left(\frac{M\omega}{\hbar}\right)^{3/4} e^{-M\omega r^2/2\hbar}Y_{00}(\theta, \varphi), \qquad (6.96)$$

As for the configurations of the first, second and third excited states, they correspond to: $(n, l, m) = (1, 1, m)$, $(2, 0, 0)$, and $(3, 1, m)$, respectively; their wave functions are given by

$$\psi_{11m}(r, \theta, \varphi) = R_{11}(r)Y_{1m}(\theta, \varphi) = \sqrt{\frac{8}{3\sqrt{\pi}}}\left(\frac{M\omega}{\hbar}\right)^{5/4} re^{-M\omega r^2/2\hbar}Y_{1m}(\theta, \varphi), \qquad (6.97)$$

$$\psi_{200}(r, \theta, \varphi) = R_{20}(r)Y_{00}(\theta, \varphi) = \sqrt{\frac{8}{3\sqrt{\pi}}}\left(\frac{M\omega}{\hbar}\right)^{3/4}\left(\frac{3}{2} - \frac{M\omega}{\hbar}r^2\right)e^{-M\omega r^2/2\hbar}Y_{00}(\theta, \varphi), \qquad (6.98)$$

$$\psi_{31m}(r, \theta, \varphi) = R_{31}(r)Y_{1m}(\theta, \varphi) = \frac{4}{\sqrt{15\sqrt{\pi}}}\left(\frac{M\omega}{\hbar}\right)^{7/4} r^2e^{-M\omega r^2/2\hbar}Y_{1m}(\theta, \varphi). \qquad (6.99)$$

Example 6.2 (Degeneracy relation for an isotropic oscillator)
Prove the degeneracy relation (6.94) for an isotropic harmonic oscillator.

Solution
Since $n = 2N + l$ the quantum numbers n and l must have the same parity. Also, since the isotropic harmonic oscillator is spherically symmetric, its states have definite parity[2]. In addition, since the parity of the states corresponding to a central potential is given by $(-1)^l$, the quantum number l (hence n) can take only even or only odd values. Let us consider separately the cases when n is even or odd.

[2]Recall from Chapter 4 that if the potential of a system is symmetric, $V(x) = V(-x)$, the states of the system must be either odd or even.

First, when n is even the degeneracy g_n of the nth excited state is given by

$$g_n = \sum_{l=0,2,4,\ldots}^{n}(2l+1) = \sum_{l=0,2,4,\ldots}^{n} 1 \; + \; 2\sum_{l=0,2,4,\ldots}^{n} l = \frac{1}{2}(n+2) + \frac{n(n+2)}{2} = \frac{1}{2}(n+1)(n+2). \quad (6.100)$$

A more explicit way of obtaining this series consists of writing it in the following two equivalent forms:

$$g_n = 1+5+9+13+\cdots+(2n-7)+(2n-3)+(2n+1), \quad (6.101)$$
$$g_n = (2n+1)+(2n-3)+(2n-7)+(2n-11)+\cdots+13+9+5+1. \quad (6.102)$$

We then add them, term by term, to get

$$2g_n = (2n+2)+(2n+2)+(2n+2)+(2n+2)+\cdots+(2n+2) = (2n+2)\left(\frac{n}{2}+1\right). \quad (6.103)$$

This relation yields $g_n = \frac{1}{2}(n+1)(n+2)$, which proves (6.94) when n is even.

Second, when n is odd, a similar treatment leads to

$$g_n = \sum_{l=1,3,5,7,\ldots}^{n}(2l+1) = \sum_{l=1,3,5,7,\ldots}^{n} 1 \; + \; 2\sum_{l=1,3,5,7,\ldots}^{n} l = \frac{1}{2}(n+1)+\frac{1}{2}(n+1)^2 = \frac{1}{2}(n+1)(n+2), \quad (6.104)$$

which proves (6.94) when n is odd. Note that this degeneracy relation is, as expected, identical with the degeneracy expression (6.36) obtained for a harmonic oscillator in Cartesian coordinates.