ROTATIONAL MOTION (RM)

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BACKGROUND 1

Rules of Operator Constructions

a. Operator for coordinate of position -----> $\hat{x}$ is the multiplier $x\,\cdot$

b. Operator of coordinate of momentum -----> $\hat{p}_x$ is $\frac{\hbar}{i}\frac{d}{dx}$

c. Write the expression for any other physical quantity in terms of coordinates of position (x, y, z) and of momenta (p_x, p_y, p_z) and then replace these coordinates by their operators.

Example 1: Kinetic energy (along x), $T_x = \frac{p_x^2}{2m} = \frac{1}{2m} p_x \cdot px$

$$\text{Or , } T_x = \frac{1}{2m}\frac{\hbar}{i}\frac{d}{dx}\cdot\frac{\hbar}{i}\frac{d}{dx} = -\frac{\hbar^2}{2m}\frac{d}{dx}\left(\frac{d}{dx}\right) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

Kinetic energy operator (along x), $\hat{T}_x = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

BACKGROUND 1

Example 2:

Total energy, E = K.E+ P.E

K.E ----> $T = T_x + T_y + T_z = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

P.E ------> V(x, y, z)

$$E = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z)$$

Operator corresponding to total energy ----> Hamiltonian operator denoted by $\widehat{H}$

$$\widehat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z)$$

BACKGROUND 1

Eigenvalue Problem:

If ψ is wavefunction of a state and $\widehat{H}$ is a corresponding Hamiltonian operator, then the state can be expressed by following mathematical equation,

$$H\psi = E\psi$$

This is eigenvalue problem or eigenvalue equation.

Its solution provides the wavefunction as well as eigenvalue (energy) of the state.

BACKGROUND 1

Free Particle in one-dimension:

- $\hat{H}$?
- Eigenvalue Problem?
- How to solve for eigenfunction (wavefunction) and eigenvalue?

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

- For free particle ----> V(x) is zero

- Eigenvalue problem:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

BACKGROUND 1

Free Particle in one-dimension:

Solution:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \left[k^2 = \frac{2mE}{\hbar^2}\right]$$

It's a 2nd order differential equation with constant coefficient. So its auxiliary solution is

$$\psi = e^{imx}$$

$$\frac{d^2\psi}{dx^2} = -\mathrm{m}^2 e^{imx}$$

BACKGROUND 1

Free Particle in one-dimension:

$$-\mathrm{m}^2 e^{imx} + k^2 e^{imx} = 0$$

$$e^{imx}(k^2 - \mathrm{m}^2) = 0$$

$$k^2 - \mathrm{m}^2 = 0 \qquad \left(\because e^{imx} \neq 0\right)$$

$$\mathrm{m} = \pm k$$

General solution is

$$\psi = Ae^{ikx} + Be^{-ikx} \qquad (1)$$

$$\psi = A\cos kx + iA\sin kx + B\cos kx - iB\sin kx$$

$$\psi = C\cos kx + D\sin kx \qquad (2)$$

$$\psi = C\cos kx \qquad [when\ D = 0] \qquad (3)$$

BACKGROUND 1

Free Particle in one-dimension:

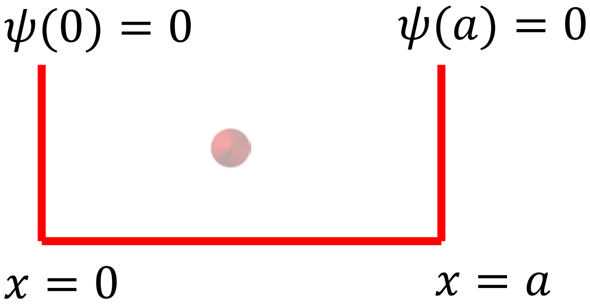
$$\psi = D\sin kx \qquad [when\ C = 0] \tag{4}$$

$$\psi = Ae^{ikx} \qquad [when\ B = 0] \tag{5}$$

$$\psi = Be^{-ikx} \qquad [when\ A = 0] \tag{6}$$

The equations (1)-(6) are the general solutions.

- To get particular solution for a particular problem, the arbitrary constants must be solved by initial boundary conditions.
- For a free particle moving in a box of length a.



Condition 1: $0 = A\cos k\cdot 0 + B\sin k\cdot 0$

$$0 = A\times 1 + B\times 0$$

$$A = 0$$

$$\psi = B\sin kx$$

BACKGROUND 1

Free Particle in one-dimension:

Condition 2:

$$0 = \psi(a) = B \sin ka$$

$$\sin ka = 0$$

$$\sin ka = \sin n\pi \qquad [n = 1, 2, 3, \cdots]$$

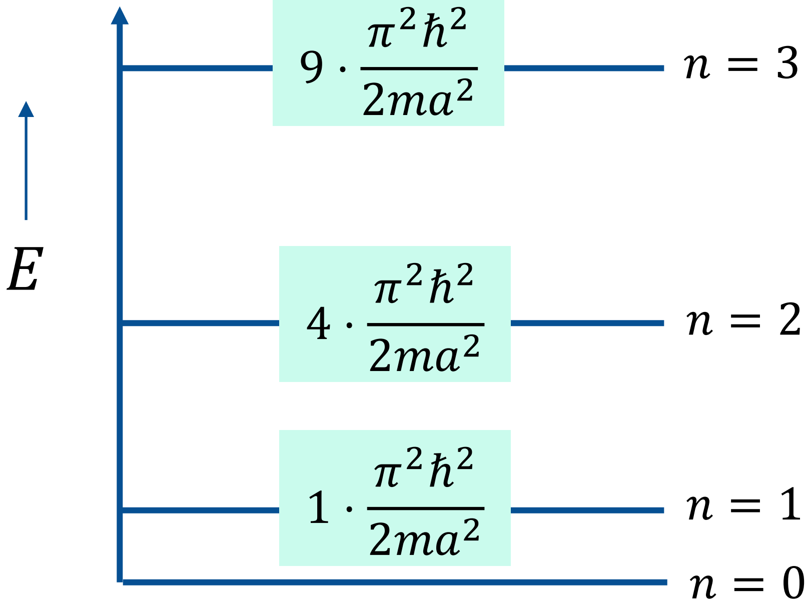
$n \neq 0$ as ψ vanish
$n \neq$ negative integers for generating redundant ψ as positive integers.

$$k = \frac{n\pi}{a}$$

$$k^2 = \frac{n^2\pi^2}{a^2}$$

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

$$E = n^2 \frac{\pi^2\hbar^2}{2ma^2}$$



BACKGROUND 1

Free Particle in one-dimension:

Condition 3:

$$\psi = B\sin\frac{n\pi}{a}x$$

- Normalization condition will give the value of B

$$\int_0^a \psi\psi^* dx = 1 \qquad \Longrightarrow B^2\int_0^a \sin^2\frac{n\pi}{a}x\,dx = 1$$

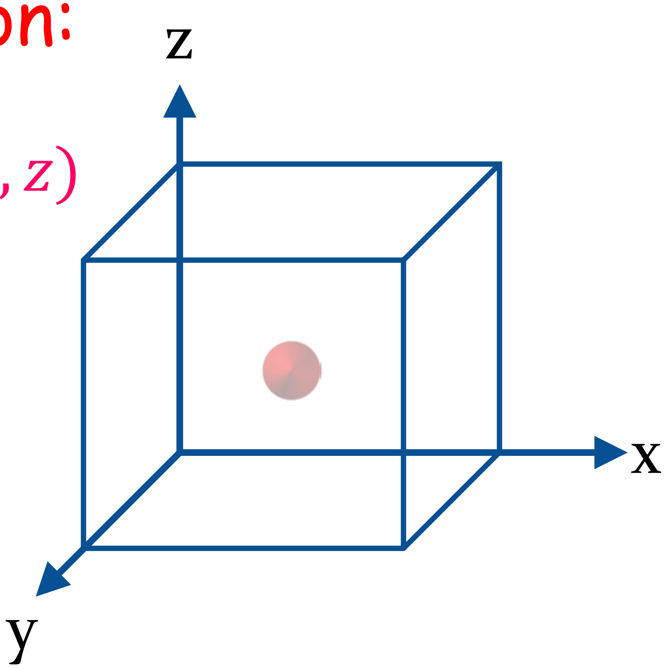
$$B^2\frac{a}{2} = 1 \qquad \Longrightarrow B = \sqrt{\frac{2}{a}}$$

- Normalize (specific) solution:

$$\psi = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x$$

BACKGROUND 1

Free Particle in three-dimension:



$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x,y,z)$$

For free particle,

$V = 0$

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

If ψ is a wavefunction and E is eigenvalue, then SE is

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

This equation cannot be solved directly without converting in ordinary form (to be done by variable separation).

BACKGROUND 1

Free Particle in three-dimension:

Variable Separation:

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi=-\frac{2mE}{\hbar^2}\psi$$

If the x, y and z don't interact each other, then wavefunction, ψ can be expressed as,

$$\psi(x,y,z)=X(x)\cdot Y(y)\cdot Z(z)\quad \text{or, simply }\ \psi=XYZ$$

$$\frac{\partial^2\psi}{\partial x^2}=YZ\frac{d^2X}{dx^2},\qquad \frac{\partial^2\psi}{\partial y^2}=XZ\frac{d^2Y}{dy^2},\qquad \frac{\partial^2\psi}{\partial z^2}=XY\frac{d^2Z}{dz^2}$$

$$YZ\frac{d^2X}{dx^2}+XZ\frac{d^2Y}{dy^2}+XY\frac{d^2Z}{dz^2}=-\frac{2mE}{\hbar^2}XYZ$$

BACKGROUND 1

Free Particle in three-dimension:

Variable Separation:

Dividing both sides by XYZ

$$\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{Z}\frac{d^2Z}{dz^2}=-\frac{2mE}{\hbar^2}$$

Each terms in LHS depends only on single variable and RHS is constant for a particular state. This equation is valid only when each term in LHS becomes constant, i.e.,

$$\frac{1}{X}\frac{d^2X}{dx^2}=-\frac{2mE_x}{\hbar^2}, \qquad \frac{1}{Y}\frac{d^2Y}{dy^2}=-\frac{2mE_y}{\hbar^2}, \qquad \frac{1}{Z}\frac{d^2Z}{dz^2}=-\frac{2mE_z}{\hbar^2}$$

With $E=E_x+E_y+E_z$

BACKGROUND 1

Free Particle in three-dimension:

Variable Separation:

On rearranging gives,

$$\frac{d^2X}{dx^2} = -\frac{2mE_x}{\hbar^2}X \qquad (1)$$

$$\frac{d^2Y}{dy^2} = -\frac{2mE_y}{\hbar^2}Y \qquad (2)$$

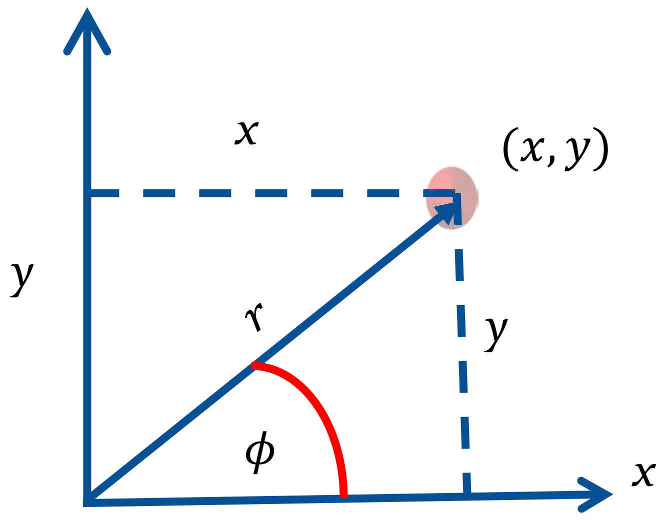
$$\frac{d^2Z}{dz^2} = -\frac{2mE_z}{\hbar^2}Z \qquad (3)$$

The equations (1), (2), (3) now become one-dimensional problems and ordinary differential equation. These can be solved easily as detailed out previous.

BACKGROUND 2

Relation among different coordinate systems:

Cartesian and Polar

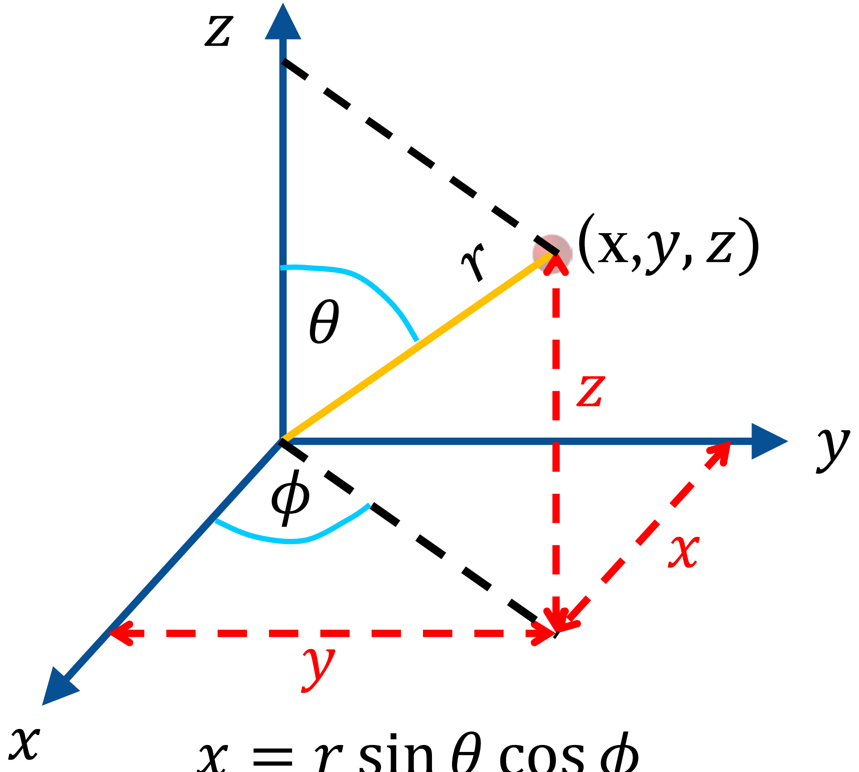


$$x = r\cos\phi$$

$$y = r\sin\phi$$

$$x^2 + y^2 = r^2$$

Cartesian and Spherical

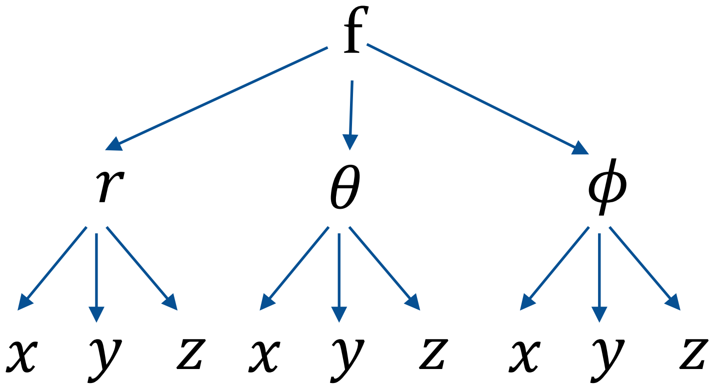


$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$
$$x^2 + y^2 + z^2 = r^2$$

BACKGROUND 1

Conversion of Laplacian in spherical coordinates

Function Tree



Chain Rule

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

$$f_x = f_r r_x + f_\theta \theta_x + f_\phi \phi_x$$

$$f_{xx} = (f_r)_x r_x + f_r r_{xx} + (f_\theta)_x \theta_x + f_\theta \theta_{xx} + \left(f_\phi\right)_x \phi_x + f_\phi \phi_{xx}$$

$$f_{xx} = \left(f_{rr} r_x + f_{r\theta}\theta_x + f_{r\phi}\phi_x\right) r_x + f_r r_{xx} + \left(f_{\theta r} r_x + f_{\theta\theta}\theta_x + f_{\theta\phi}\phi_x\right)\theta_x$$
$$+ f_\theta \theta_{xx} + \left(f_{\phi r} r_x + f_{\phi\theta}\theta_x + f_{\phi\phi}\phi_x\right)\phi_x + f_\phi \phi_{xx}$$

$$f_{xx} = f_r r_{xx} + f_\theta \theta_{xx} + f_\phi \phi_{xx} + f_{rr} r_x^2 + f_{\theta\theta}\theta_x^2 + f_{\phi\phi}\phi_x^2 + 2f_{r\theta} r_x \theta_x +$$
$$2f_{\theta\phi}\theta_x\phi_x + 2f_{\phi r}\phi_x r_x$$

ROTATIONAL MOTION

Free Particle moving on circle (Plane):

The particle of mass *m* travels on a circle of radius *r* in the xy-plane. If particle rotates freely then V(x,y) = 0.

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

Since the motion is circular, it is convenient to express $\hat{H}$ in polar coordinates (r, ϕ).

$$x = r\cos\phi$$
$$y = r\sin\phi$$
$$x^2 + y^2 = r^2$$

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}$$

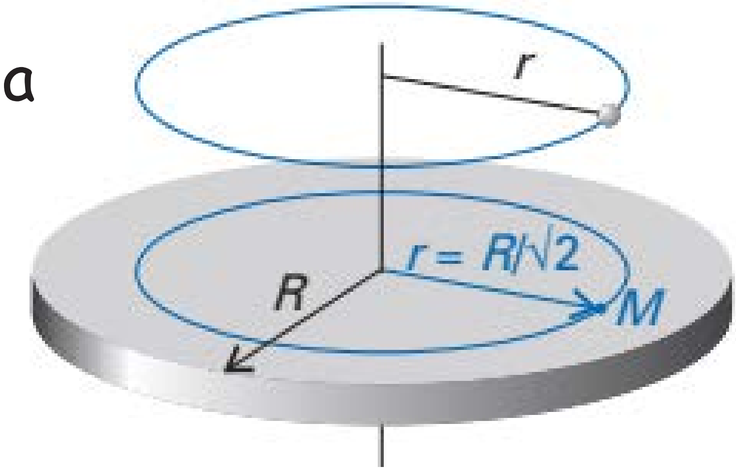


Fig. The rotational characteristics of a uniform disk are represented by the motion of a single mass point at its radius of gyration.

ROTATIONAL MOTION

Free Particle moving on circle (Plane):

Since r is constant, the derivatives with respect to r can be discarded.

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial^2}{\partial\phi^2} = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2}$$

$$I = mr^2$$

I is the moment of intertia

The wavefunction will depend on ϕ only. Denoting wavefunction by $\Phi(\phi)$, simply Φ, the S. E. is

$$-\frac{\hbar^2}{2I}\frac{\partial^2\Phi}{\partial\phi^2} = E\Phi \qquad \Longrightarrow \frac{\partial^2\Phi}{\partial\phi^2} = -\frac{2IE}{\hbar^2}\Phi$$

The general solutions are

$$\Phi = Ae^{im_l\phi} + Be^{-im_l\phi} \qquad \text{where } m_l^2 = \frac{2IE}{\hbar^2}$$

ROTATIONAL MOTION

Free Particle moving on circle (Plane):

Since the particle remains always on the ring, there is no condition for vanishing Φ. However, because wavefunction must be single-valued, it must follow the cyclic boundary condition i.e., $\Phi(\phi + 2\pi) = \Phi(\phi)$.

$$Ae^{im_l(\phi+2\pi)} + Be^{-im_l(\phi+2\pi)} = Ae^{im_l\phi} + Be^{-im_l\phi}$$

This relation is satisfied only if m_l is an integer, for then, using Euler's relation, $e^{2\pi i m_l} = 1$. The boundary conditions therefore imply that

$$m_l = 0, \pm 1, \pm 2, \pm 3, \cdots$$

It follows that the allowed energies are

$$E_{m_l} = \frac{m_l^2 \hbar^2}{2I}, \qquad m_l = 0, \pm 1, \pm 2, \pm 3, \cdots$$

ROTATIONAL MOTION

Free Particle moving on circle (Plane):

Normalization of wavefunctions: For the function with $B = 0$, we write

$$\int_0^{2\pi} \Phi\Phi^* d\phi = A^2 \int_0^{2\pi} e^{im_l\phi} e^{-im_l\phi} d\phi = 1$$

$$A^2 [\phi]_0^{2\pi} = 1 \qquad \Longrightarrow A = \frac{1}{\sqrt{2\pi}}$$

The normalized wavefunction is,

$$\Phi = \frac{1}{\sqrt{2\pi}} e^{im_l\phi}, \qquad m_l = 0, \pm 1, \pm 2, \pm 3, \cdots$$

ROTATIONAL MOTION

Free Particle moving on circle (Plane):

m_l	Φ	E_{m_l}
0	0	0
1	$\frac{1}{\sqrt{2\pi}}e^{i\phi}$	$\frac{\hbar^2}{2I}$
-1	$\frac{1}{\sqrt{2\pi}}e^{-i\phi}$	$\frac{\hbar^2}{2I}$
2	$\frac{1}{\sqrt{2\pi}}e^{2i\phi}$	$\frac{4\hbar^2}{2I}$
-2	$\frac{1}{\sqrt{2\pi}}e^{-2i\phi}$	$\frac{4\hbar^2}{2I}$

Except ground state ($m_l = 0$), the wavefunctions are doubly degenerate.

BACKGROUND 2

Legendre equation & Legendre polynomial

Let us consider a function

$$y = c(x^2-1)^l \tag{A01}$$

Then, differentiating the equation (A01) with respect x gives

$$\frac{dy}{dx} = 2clx(x^2-1)^{l-1} = \frac{2lx}{x^2-1}c(x^2-1)^l = \frac{2lx}{x^2-1}y,$$

$$\Longrightarrow (x^2-1)\frac{dy}{dx} - 2lxy = 0, \ \Longrightarrow (1-x^2)y_1 + 2lxy = 0 \tag{A02}$$

According to Leibnitz's theorem,

$$D^n(uv) = {}^n c_0 u_n v + {}^n c_1 u_{n-1} v_1 + {}^n c_2 u_{n-2} v_2 + \cdots,$$

Differentiating eq(A02) $(l+1)$ times, we obtain,

$$y_{l+2}(1-x^2) + (l+1)y_{l+1}(-2x) + \frac{(l+1)l}{2}y_l(-2) + 2ly_{l+1}x$$
$$+ 2l(l+1)y_l \cdot 1 = 0$$

BACKGROUND 2

Legendre equation & Legendre polynomial

After simplification,

$$(1-x^2)y_{l+2}-2xy_{l+1}+l(l+1)y_l=0$$

Let,

$$y_l=\frac{d^l y}{dx^l}=c\,\frac{d^l\left(x^2-1\right)^l}{dx^l}=\mathrm{z}$$

Substituting y_l by z gives

$$(1-x^2)z_2-2xz_1+l(l+1)z=0$$

$$\Longrightarrow (1-x^2)\frac{d^2z}{dx^2}-2x\frac{dz}{dx}+l(l+1)z=0 \qquad \text{(A03)}$$

This equation (A03) is the Legendre differential equation and it's solution, z written as $P_l(x)$ is a polynomial in x of degree l, i.e.,

$$P_l(x)=c\,\frac{d^l(x^2-1)^l}{dx^l}$$

BACKGROUND 2

Associated Legendre equation & Associated Legendre polynomial

Again differentiating k times the Legendre differential equation, gives

$$z_{k+2}(1-x^2)+kz_{k+1}(-2x)+\frac{k(k-1)}{2}z_k(-2)+$$

$$2z_{k+1}x+2kz_k\cdot 1+l(l+1)z_k=0$$

$$\Longrightarrow (1-x^2)z_{k+2}-2x(k+1)z_{k+1}+(l+k+1)(l-k)z_k=0 \qquad \text{(A04)}$$

Let

$$Q=z_k=\frac{d^k z}{dx^k}=\frac{d^k}{dx^k}\{P_l(x)\}$$

$$\Longrightarrow Q=\frac{d^k}{dx^k}\left\{c\frac{d^l(x^2-1)^l}{dx^l}\right\}=\frac{d^k}{dx^k}\left\{\frac{1}{2^l\cdot l!}\frac{d^l(x^2-1)^l}{dx^l}\right\}$$

BACKGROUND 2

Associated Legendre equation & Associated Legendre polynomial

Inserting Q in equation (A04) gives

$$(1-x^2)Q_2 - 2x(k+1)Q_1 + (l+k+1)(l-k)Q = 0 \qquad \text{(A05)}$$

$$\Rightarrow (1-x^2)\frac{d^2Q}{dx^2} - 2x(k+1)\frac{dQ}{dx} + (l+k+1)(l-k)Q = 0$$

Now suppose that,

$$Q = U(1-x^2)^{-\frac{|k|}{2}}$$

The first derivative is

$$Q_1 = U_1(1-x^2)^{-\frac{|k|}{2}} + U\left(-\frac{k}{2}\right)(1-x^2)^{-\frac{|k|}{2}-1}(-2x)$$

$$\Rightarrow Q_1 = U_1(1-x^2)^{-\frac{|k|}{2}} + Ukx(1-x^2)^{-\frac{|k|}{2}-1}$$

BACKGROUND 2

Associated Legendre equation & Associated Legendre polynomial

The second derivative is

$$Q_2 = U_2(1-x^2)^{-\frac{|k|}{2}} + 2\left(-\frac{k}{2}\right)(1-x^2)^{-\frac{|k|}{2}-1}(-2x)U_1 + U_1 kx(1-x^2)^{-\frac{|k|}{2}-1}$$

$$+\left[kx\left(-\frac{k}{2}-1\right)(1-x^2)^{-\frac{|k|}{2}-2}(-2x) + k(1-x^2)^{-\frac{|k|}{2}-1}\right]U$$

$$\Rightarrow Q_2 = U_2(1-x^2)^{-\frac{|k|}{2}} + 2U_1 kx(1-x^2)^{-\frac{|k|}{2}-1}$$

$$+U\left[k(k+2)x^2(1-x^2)^{-\frac{|k|}{2}-2} + k(1-x^2)^{-\frac{|k|}{2}-1}\right]$$

Now ,

$$(1-x^2)Q_2 = U_2(1-x^2)^{1-\frac{|k|}{2}} + 2U_1 kx(1-x^2)^{-\frac{|k|}{2}}$$

$$+U\left[x^2 k(k+2)(1-x^2)^{-\frac{|k|}{2}-1} + k(1-x^2)^{-\frac{|k|}{2}}\right]$$

BACKGROUND 2

Associated Legendre equation & Associated Legendre polynomial

$$-2x(k+1)Q_1 = -2x(k+1)(1-x^2)^{-\frac{|k|}{2}}U_1 - 2k(k+1)x^2(1-x^2)^{-\frac{|k|}{2}-1}U$$

$$(k+l+1)(l-k)Q = (k+l+1)(l-k)(1-x^2)^{-\frac{|k|}{2}}U$$

Now equation (A05) becomes,

$$(1-x^2)^{1-\frac{|k|}{2}}U_2 + \left[2kx(1-x^2)^{-\frac{|k|}{2}} - 2x(k+1)(1-x^2)^{-\frac{|k|}{2}}\right]U_1 +$$

$$\left[x^2k(k+2)(1-x^2)^{-\frac{|k|}{2}-1} + k(1-x^2)^{-\frac{|k|}{2}} - 2k(k+1)x^2(1-x^2)^{-\frac{|k|}{2}-1}\right.$$

$$\left. + (k+l+1)(l-k)(1-x^2)^{-\frac{|k|}{2}}\right]U = 0$$

BACKGROUND 2

Associated Legendre equation & Associated Legendre polynomial

On simplification

$$(1-x^2)U_2 + [2kx - 2x(k+1)]U_1$$

$$+\left[\frac{x^2k(k+2)}{(1-x^2)} + k - \frac{2k(k+1)x^2}{(1-x^2)} + (k+l+1)(l-k)\right]U = 0$$

$$\Rightarrow (1-x^2)U_2 - 2xU_1$$

$$+\left[\frac{x^2(k^2+2k-2k^2-2k)}{(1-x^2)} + k + kl + l^2 + l - k^2 - kl - k\right]U = 0$$

$$\Rightarrow (1-x^2)U_2 - 2xU_1 + \left[\frac{-x^2k^2}{(1-x^2)} + l(l+1) - k^2\right]U = 0$$

$$\Rightarrow (1-x^2)U_2 - 2xU_1 + \left[l(l+1) + \frac{-x^2k^2 - k^2 + x^2k^2}{(1-x^2)}\right]U = 0$$

BACKGROUND 2

Associated Legendre equation & Associated Legendre polynomial

$$\Rightarrow (1-x^2)U_2 - 2xU_1 + \left[l(l+1) - \frac{k^2}{(1-x^2)}\right]U = 0$$

$$\Rightarrow (1-\mathrm{x}^2)\frac{\mathrm{d}^2\mathrm{U}}{dx^2} - 2x\frac{dU}{dx} + \left[l(l+1) - \frac{k^2}{1-x^2}\right]U = 0 \qquad \text{(A06)}$$

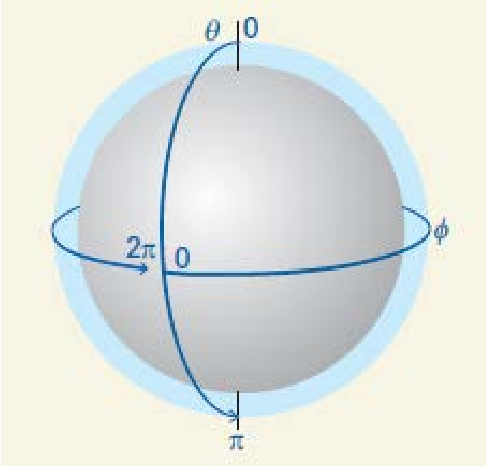
$$\Rightarrow \frac{d}{dx}\left[(1-\mathrm{x}^2)\frac{dU}{dx}\right] + \left[l(l+1) - \frac{k^2}{1-x^2}\right]U = 0 \qquad \text{(A07)}$$

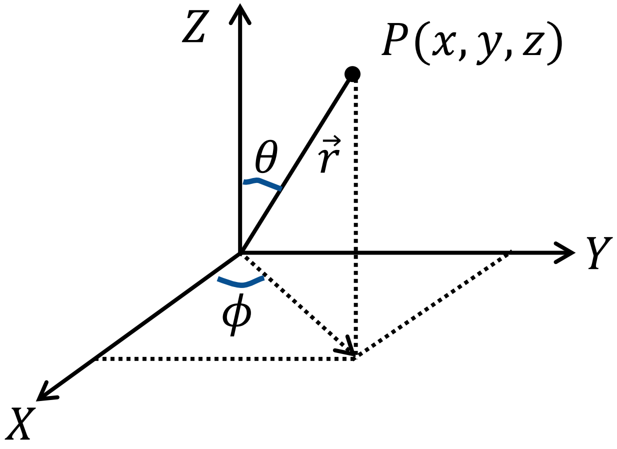
The equations (A06) & (A07) both are called associated Legendre equations and the solution U usually written as $P_l^{|k|}(x)$ is called associated Legendre polynomial in x of degree l and order k where $l \geq |k|$. Thus,

$$\mathrm{P_l^{|k|}(x)} = \mathrm{U} = (1-\mathrm{x}^2)^{\frac{|k|}{2}}Q = (1-x^2)^{\frac{|k|}{2}}\frac{d^{|k|}}{dx^{|k|}}P_l(x) \qquad \text{(A08)}$$

ROTATIONAL MOTION

Free Particle moving on Sphere:





The Hamiltonian operator for motion in three dimensions is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V\ ; \quad \text{where}, \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad (1)$$

The Laplacian, ∇^2 (read 'del squared'), is a convenient abbreviation for the sum of the three second derivatives. For the particle confined to a spherical surface, V = 0 wherever it is free to travel and Hamiltonian operator becomes,

ROTATIONAL MOTION

Free Particle moving on Sphere:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 \qquad (2)$$

To take advantage of the symmetry of the problem and the fact that *r* is a constant for a particle on a sphere, we use **spherical polar coordinates**, the radius *r*, the colatitude θ, and the azimuth φ as shown in Fig. 1, with

$$x = r\sin\theta\cos\phi, \qquad y = r\sin\theta\sin\phi, \qquad z = r\cos\theta \qquad (3)$$

And the Laplacian in the spherical polar coordinate is

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2\partial}{r\partial r} + \frac{1}{r^2}\Lambda^2; \;\; \Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right] \qquad (4)$$

ROTATIONAL MOTION

Free Particle moving on Sphere:

Because *r* is constant, we can discard the part of the Laplacian that involves differentiation with respect to *r*, and so write the Schrödinger equation as

$$-\frac{\hbar^2}{2mr^2}\Lambda^2\psi = E\psi \qquad (5)$$

The moment of inertia, $\mathrm{I} = \mathrm{mr}^2$, has appeared. This expression can be rearranged into

$$\Lambda^2\psi = -\beta\psi \qquad \beta = \frac{2IE}{\hbar^2} \qquad (6)$$

ROTATIONAL MOTION

Free Particle moving on Sphere:

Inserting Langarian, Λ^2 in the above equation leads

$$\frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right]\psi+\beta\psi=0 \qquad (7)$$

In equation (7), the wavefunction, ψ depends on both θ and ϕ variables. To separate variable, we try to substitute $\psi=\mathrm{T}(\theta)\mathrm{F}(\phi)$ in equation (7)

$$\frac{1}{\sin^2\theta}\frac{\partial^2\mathrm{TF}}{\partial\phi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right]\mathrm{TF}+\beta\mathrm{TF}=0 \qquad (8)$$

Which gives

$$\frac{\mathrm{T}}{\sin^2\theta}\frac{\partial^2\mathrm{F}}{\partial\phi^2}+\frac{\mathrm{F}}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial\mathrm{T}}{\partial\theta}\right]+\beta\mathrm{TF}=0 \qquad (9)$$

ROTATIONAL MOTION

Free Particle moving on Sphere:

Division through by PF, multiplication by $\sin^2\theta$, and minor rearrangement give

$$\frac{1}{\mathrm{F}}\frac{\partial^2\mathrm{F}}{\partial\phi^2}+\frac{\sin\theta}{\mathrm{T}}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial\mathrm{T}}{\partial\theta}\right]+\beta\sin^2\theta=0 \qquad (10)$$

The first term on the left depends only on ϕ and the remaining two terms depend only on θ. The argument used is that each term is equal to a constant. Thus, if we set the first term equal to the numerical constant $-m_l^2$, the separated equations are

$$\frac{1}{\mathrm{F}}\frac{\partial^2\mathrm{F}}{\partial\phi^2}=-\mathrm{m_l^2} \qquad (11)$$

$$\frac{\sin\theta}{\mathrm{T}}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial\mathrm{T}}{\partial\theta}\right]+\beta\sin^2\theta=\mathrm{m_l^2} \qquad (12)$$

ROTATIONAL MOTION

Free Particle moving on Sphere:

Rearrangement of equation (12) leads

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial \mathrm{T}}{\partial\theta}\right]+\left[\beta-\frac{\mathrm{m}_{\mathrm{l}}^{2}}{\sin^{2}\theta}\right]\mathrm{T}=0 \qquad (13)$$

The equation (11) is the same as the Schrodinger equation of a particle moving of a circular path and has the normalized solution of the form

$$\mathrm{F}_{\mathrm{m}_{\mathrm{l}}}=\frac{1}{\sqrt{2\pi}}e^{im_l\phi}, \qquad m_l=0,\pm1,\pm2\cdots(14)$$

where, m_l is the *magnetic quantum number*.

Solution of equation (13)

Let

$$x=\cos\theta$$

$$\frac{dT}{d\theta}=\frac{dT}{dx}\frac{dx}{d\theta}=-\sin\theta\frac{dT}{dx}, \qquad \text{Therefore,} \qquad \frac{d}{d\theta}=-\sin\theta\frac{d}{dx}$$

ROTATIONAL MOTION

Free Particle moving on Sphere:

Now the equation (13) becomes,

$$-\frac{d}{\partial x}\left[-(1-x^2)\frac{d}{dx}\right]+\left[\beta-\frac{\mathrm{m}_\mathrm{l}^2}{1-x^2}\right]\mathrm{T}=0$$

$$\Longrightarrow (1-x^2)\frac{d^2T}{\partial x^2}-2x\frac{dT}{dx}+\left[\beta-\frac{\mathrm{m}_\mathrm{l}^2}{1-x^2}\right]\mathrm{T}=0 \qquad (14)$$

The eq. (14) becomes Associated Legendre equation (see eq. A06) if

$$\beta = l(l+1), \qquad\qquad m_l^2 = k^2$$

The solutions of eq. (13) are, thus, Associated Legendre's polynomials, $P_l^{|m_l|}(x)$ of degree l and order $|m_l|$, where l is either zero or a positive integer and $l \geq |m_l|$. The solutions are given by

$$\mathrm{T}(x)=\mathrm{T}_{lm_l}(x)=\mathrm{P}_l^{|m_l|}(\mathrm{x})=(1-x^2)^{\frac{|m_l|}{2}}\frac{d^{|m_l|}}{dx^{|m_l|}}P_l(x) \qquad (15)$$

where, $$P_l(x)=\frac{1}{2^l\cdot l!}\frac{d^l(x^2-1)^l}{dx^l}$$

ROTATIONAL MOTION

Free Particle moving on Sphere:

In terms of $\cos\theta$

$$\mathrm{P}_l^{|m_l|}(\cos\theta) = \sin^{|m_l|}\theta \frac{d^{|m_l|}}{d(\cos\theta)^{|m_l|}} P_l(\cos\theta) \qquad (16)$$

where, $$P_l(\cos\theta) = \frac{(-1)^l}{2^l\, l!} \frac{d^l}{d(\cos\theta)^l} \sin^{2l}\theta$$

The normalized solutions are given by

$$\mathrm{T}(\theta) = \sqrt{\frac{2l+1}{2} \cdot \frac{(l-|m_l|)!}{(l+|m_l|)!}}\, P_l^{|m_l|}(\cos\theta) \qquad (17)$$

ROTATIONAL MOTION

Free Particle moving on Sphere:

The product of $\mathrm{T}(\theta)$ and $\mathrm{F}(\phi)$ is denoted by $Y_{lm_l}(\theta,\phi)$.

For a given values of l and m_l,the normalized wave

functions, $Y_{lm_l}(\theta,\phi)$ are called the **spherical harmonics**

and given by

$$Y_{lm_l}(\theta,\phi) = \frac{(-1)^{l+|m_l|}}{2^l l!}\sqrt{\frac{2l+1}{4\pi}\cdot\frac{(l-|m_l|)!}{(l+|m_l|)!}} \times \left[\sin^{|m_l|}\theta \frac{d^{l+|m_l|}}{d(\cos\theta)^{l+|m_l|}}\sin^{2l}\theta\right]e^{im_l\phi} \quad (18)$$

ROTATIONAL MOTION

Free Particle moving on Sphere:

Example: Evaluate $Y_{2,\pm 2}$

Soln: If $l = 2$ then $m_l = 0, \pm 1, \pm 2$

For $l = 2$ and $m_l = \pm 2$

$$N = \frac{(-1)^{2+2}}{2^2 \cdot 2!}\sqrt{\frac{2\cdot 2+1}{4\pi}\cdot\frac{(2-2)!}{(2+2)!}} = \frac{1}{32}\sqrt{\frac{5}{6\pi}}$$

$$P_2^2(\cos\theta) = \sin^2\theta \boxed{\frac{d^4}{d(\cos\theta)^4}\sin^4\theta} = 24\sin^2\theta$$

$x = \cos\theta$

$y = \sin^4\theta$

$\Rightarrow y = (1-x^2)^2$

$\Rightarrow y = 1 - 2x^2 + x^4$

$y_1 = -4x + 4x^3$

$y_2 = -4 + 12x^2$

$y_3 = 24x$

$y_4 = 24$

$$Y_{2,\pm 2} = \frac{1}{32}\sqrt{\frac{5}{6\pi}}\cdot 24\sin^2\theta\, e^{\pm 2i\phi} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi}$$

ROTATIONAL MOTION

Free Particle moving on Sphere:

The $Y_{lm_l}(\theta,\phi)$ for some l and m_l are given in Table1.

$$Y_{lm_l}(\theta,\phi) = \frac{(-1)^{l+|m_l|}}{2^l l!}\sqrt{\frac{2l+1}{4\pi}\cdot\frac{(l-|m_l|)!}{(l+|m_l|)!}}\left[\sin^{|m_l|}\theta\,\frac{d^{l+|m_l|}}{d(\cos\theta)^{l+|m_l|}}\sin^{2l}\theta\right]e^{im_l\phi}$$

$\boldsymbol{l}$	$\boldsymbol{m_l}$	$P_l(\cos\theta)$	N	$P_l^{\vert m_l\}}(\cos\theta)$	$e^{im_l\phi}$	$\boldsymbol{Y_{lm_l}(\theta,\phi)}$
0	0	1	$\left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$	1	1	$\left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$
1	0	$-\cos\theta$	$\left(\frac{3}{4\pi}\right)^{\frac{1}{2}}$	$\cos\theta$	1	$\left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\cos\theta$
	±1					
2	0					
	±1					
	±2					

ROTATIONAL MOTION

Graphical Representation of Spherical Harmonics:

The spherical harmonics are delt, so far, in complex forms except $m_l = 0$, which can not be represented graphically. The latter requires in real forms.

The linear combination of degenerate functions, $Y_{l,+m_l}$ and $Y_{l,-m_l}$ provides real functions.

$$Y_{l+} = \frac{1}{\sqrt{2}}\left(Y_{l,+m_l} + Y_{l,-m_l}\right) \quad \text{and} \quad Y_{l-} = \frac{1}{i\sqrt{2}}\left(Y_{l,+m_l} - Y_{l,-m_l}\right)$$

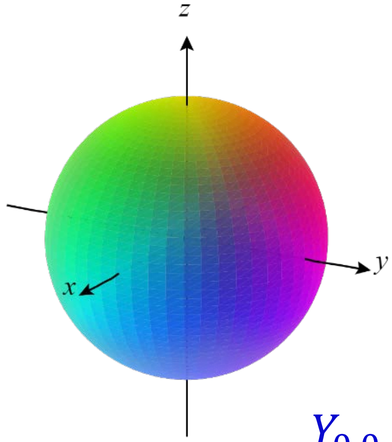
For example, $Y_{1+} = \frac{1}{\sqrt{2}}\left(Y_{1,+1} + Y_{1,-1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \cos\phi$

In real forms, l is retained but m_l is underdetermined.

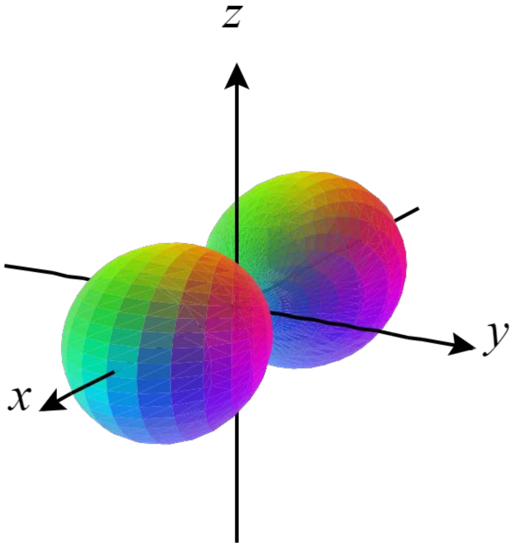
$$Y_{1-} = \frac{1}{i\sqrt{2}}\left(Y_{1,+1} - Y_{1,-1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \sin\phi$$

ROTATIONAL MOTION

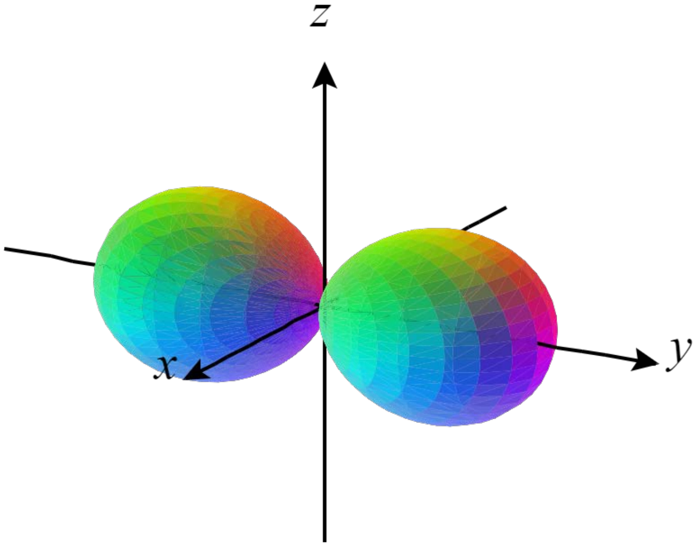
Graphical Representation of Spherical Harmonics:



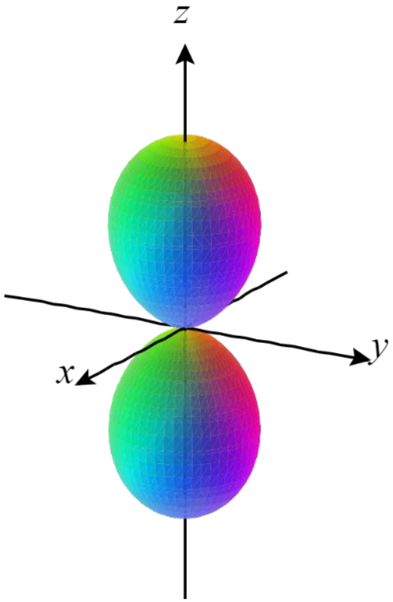
$Y_{0,0}$



$Y_{1,1} + Y_{1,-1} \rightarrow Y_{1+}$



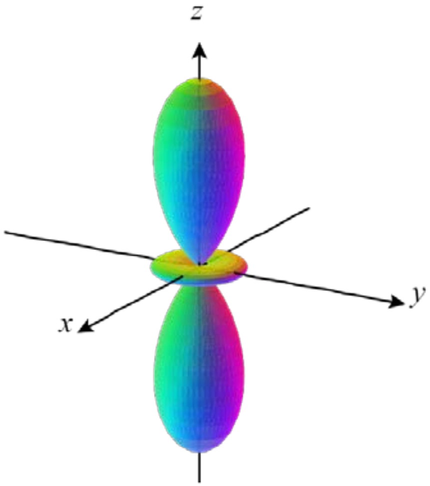
$Y_{1,1} - Y_{1,-1} \rightarrow Y_{1-}$



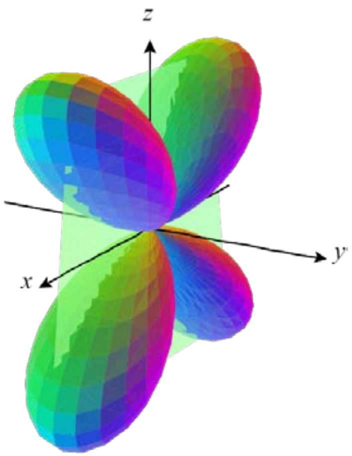
$Y_{1,0}$

ROTATIONAL MOTION

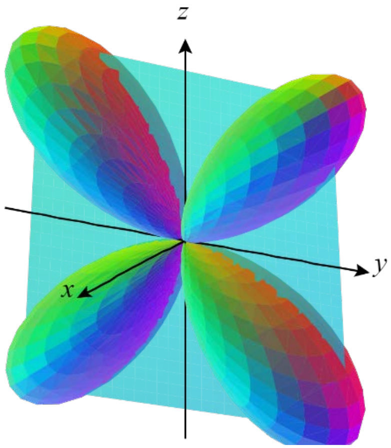
Graphical Representation of Spherical Harmonics:



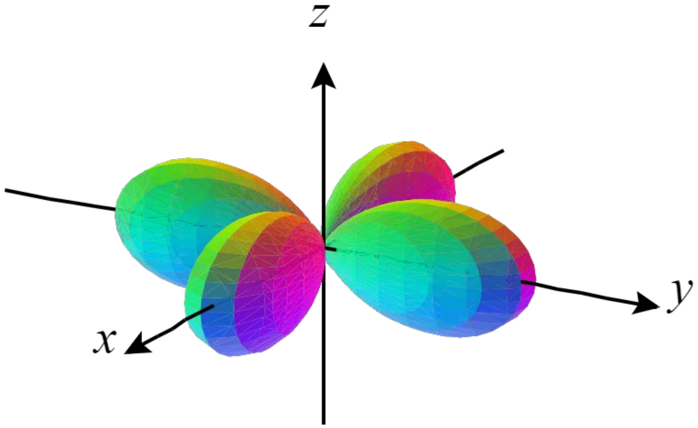
$Y_{2,0}$



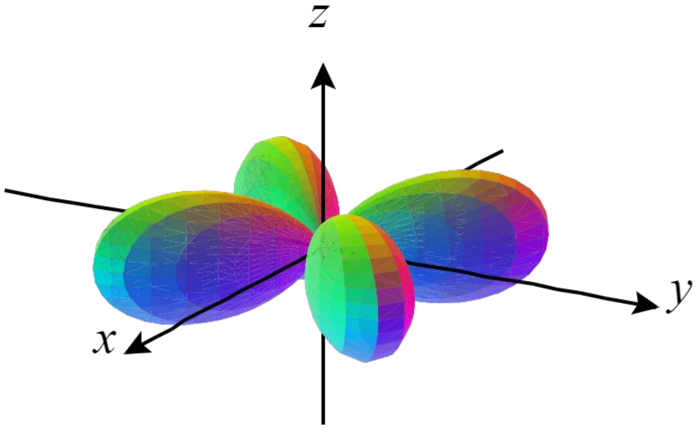
$Y_{2,1} + Y_{2,-1} \rightarrow Y_{2+}$



$Y_{2,1} - Y_{2,-1} \rightarrow Y_{2-}$



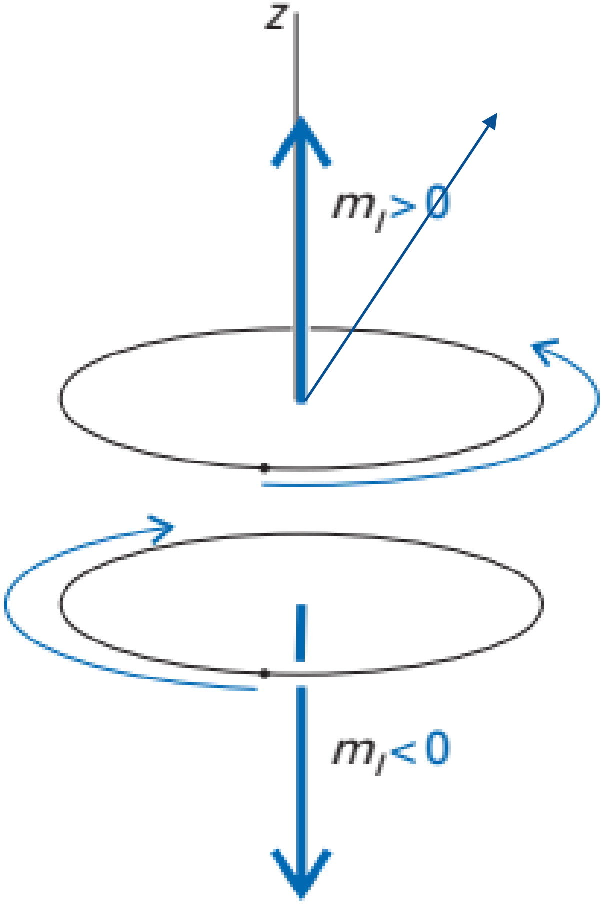
$Y_{2,2} + Y_{2,-2} \rightarrow Y_{2+}$



$Y_{2,2} - Y_{2,-2} \rightarrow Y_{2-}$

BACKGROUND 3

Angular momentum



The classical expression of angular momentum, $\vec{l}$

$$\vec{l} = \vec{r} \times \vec{p} = \begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

Writing $\vec{l} = l_x\hat{\imath} + l_y\hat{\jmath} + l_z\hat{k}$

$$l_x = yp_z - zp_y$$

$$l_y = zp_x - xp_z$$

$$l_z = xp_y - yp_x$$

BACKGROUND 3

Angular momentum

$$\hat{l}_z = x\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right) - y\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \quad \text{and} \quad L^2 = L_x^2 + L_y^2 + L_z^2$$

Converting to polar coordinates,

$$\hat{L}_x = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\phi\frac{\partial}{\partial\theta}\right)$$

$$\hat{L}_y = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\phi\frac{\partial}{\partial\theta}\right)$$

$$\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

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

ROTATIONAL MOTION

In case of particle on ring

Applying $\hat{H}$ and $\hat{L}_z$ to $\Phi_{m_l} = \frac{1}{\sqrt{2\pi}} e^{im_l\phi}$

$$\hat{H}\Phi_{m_l} = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2}\left(\frac{1}{\sqrt{2\pi}}e^{im_l\phi}\right) = \frac{m_l^2\hbar^2}{2I}\left(\frac{1}{\sqrt{2\pi}}e^{im_l\phi}\right) = \frac{m_l^2\hbar^2}{2I}\Phi_{m_l}$$

$$\hat{L}_z\Phi_{m_l} = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\left(\frac{1}{\sqrt{2\pi}}e^{im_l\phi}\right) = m_l\hbar\left(\frac{1}{\sqrt{2\pi}}e^{im_l\phi}\right) = m_l\hbar\Phi_{m_l}$$

Note that,

- Φ_{m_l} is the wavefunction of both $\hat{H}$ and $\hat{L}_z$.
- E and L_z can be determined simultaneously from Φ_{m_l}.

ROTATIONAL MOTION

However, the eigenfunction of $\widehat{H}$ in real form is not eigenfunction of $\hat{L}_z$

$$\hat{L}_z\Phi_{m_l} = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\left(\frac{1}{\sqrt{\pi}}\sin m_l\phi\right) = \frac{m_l\hbar}{i}\left(\frac{1}{\sqrt{\pi}}\cos \mathrm{m}_l\phi\right)$$

Note that,

- The eigenvalue of $\hat{L}_z$ is $m_l\hbar$

where $m_l = 0, \pm1, \pm2, \pm3, \cdots$

If $m_l > 0$; $\hat{L}_z$ is positive,

If $m_l < 0$; $\hat{L}_z$ is negative.

ROTATIONAL MOTION

In case of particle on sphere

Applying $\hat{H}$, $\hat{L}^2$ and $\hat{L}_z$ to $\psi_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta = N\cos\theta$

$$\hat{H}\psi_{1,0} = -\frac{\hbar^2}{2I}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left\{\sin\theta\frac{\partial}{\partial\theta}(N\cos\theta)\right\} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}(N\cos\theta)\right]$$

$$= -\frac{\hbar^2}{2I}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(-N\sin^2\theta\ ) + 0\right] = \frac{\hbar^2}{I}(N\cos\theta) = \frac{\hbar^2}{I}\psi_{1,0}$$

$$\hat{L}^2\psi_{1,0} = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left\{\sin\theta\frac{\partial}{\partial\theta}(N\cos\theta)\right\} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}(N\cos\theta)\right]$$

$$= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(-N\sin^2\theta\ ) + 0\right] = \hbar^2(N\cos\theta) = \hbar^2\psi_{1,0}$$

ROTATIONAL MOTION

But

$$\hat{L}_z \psi_{1,0} = \frac{\hbar}{i} \frac{\partial}{\partial \phi} (N \cos \theta) = 0$$

- $\psi_{1,0}$ is not wavefunction of $\hat{L}_z$.

However, $\psi_{1,0}$ can be written as $\psi_{1,0} = N \cos \theta \; e^{i \cdot 0 \cdot \phi}$

Now,

$$\hat{L}_z \psi_{1,0} = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \left(N \cos \theta \; e^{i \cdot 0 \cdot \phi} \right) = 0 \cdot N \cos \theta \; e^{i \cdot 0 \cdot \phi} = 0 \cdot \psi_{1,0}$$

- $\psi_{1,0}$ in complex form is a wavefunction of $\hat{L}_z$ with zero eigenvalue.

ROTATIONAL MOTION

The eigenvalue equations for $\hat{H}$, $\hat{L}^2$ and $\hat{L}_z$ can be written in the general form as,

$$\hat{H}\psi_{lm_l} = \frac{\beta\hbar^2}{2I}\psi_{lm_l} = l(l+1)\frac{\hbar^2}{2I}\psi_{lm_l}$$

$$\hat{L}^2\psi_{lm_l} = \beta\hbar^2\psi_{lm_l} = l(l+1)\hbar^2\psi_{lm_l}$$

$$\hat{L}_z\psi_{lm_l} = m_l\hbar\psi_{lm_l}$$

Quantization of Energy and angular momentum:

$$E_l = l(l+1)\frac{\hbar^2}{2I}$$

$$L^2 = l(l+1)\hbar^2 \qquad \Longrightarrow L = \sqrt{l(l+1)}\hbar$$

$$L_z = m_l\hbar$$

ROTATIONAL MOTION

Eigenvalues of particle rotating on ring vs sphere

Particle of ring:

$$\hat{H} = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} \;\&\; \psi_{m_l} = \frac{1}{\sqrt{2\pi}}e^{im_l\phi}$$

$$m_l^2 = \frac{2IE}{\hbar^2} \implies E = \frac{m_l^2\hbar^2}{2I} \qquad m_l = 0, \pm1, \pm2, \cdots$$

Note that both eigenfunction and eigenvalue depend on m_l.

Particle of sphere:

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

$$Y_{lm_l}(\theta,\phi) = N\left[\sin^{|m_l|}\theta\frac{d^{l+|m_l|}}{d(\cos\theta)^{l+|m_l|}}\sin^{2l}\theta\right]e^{im_l\phi}$$

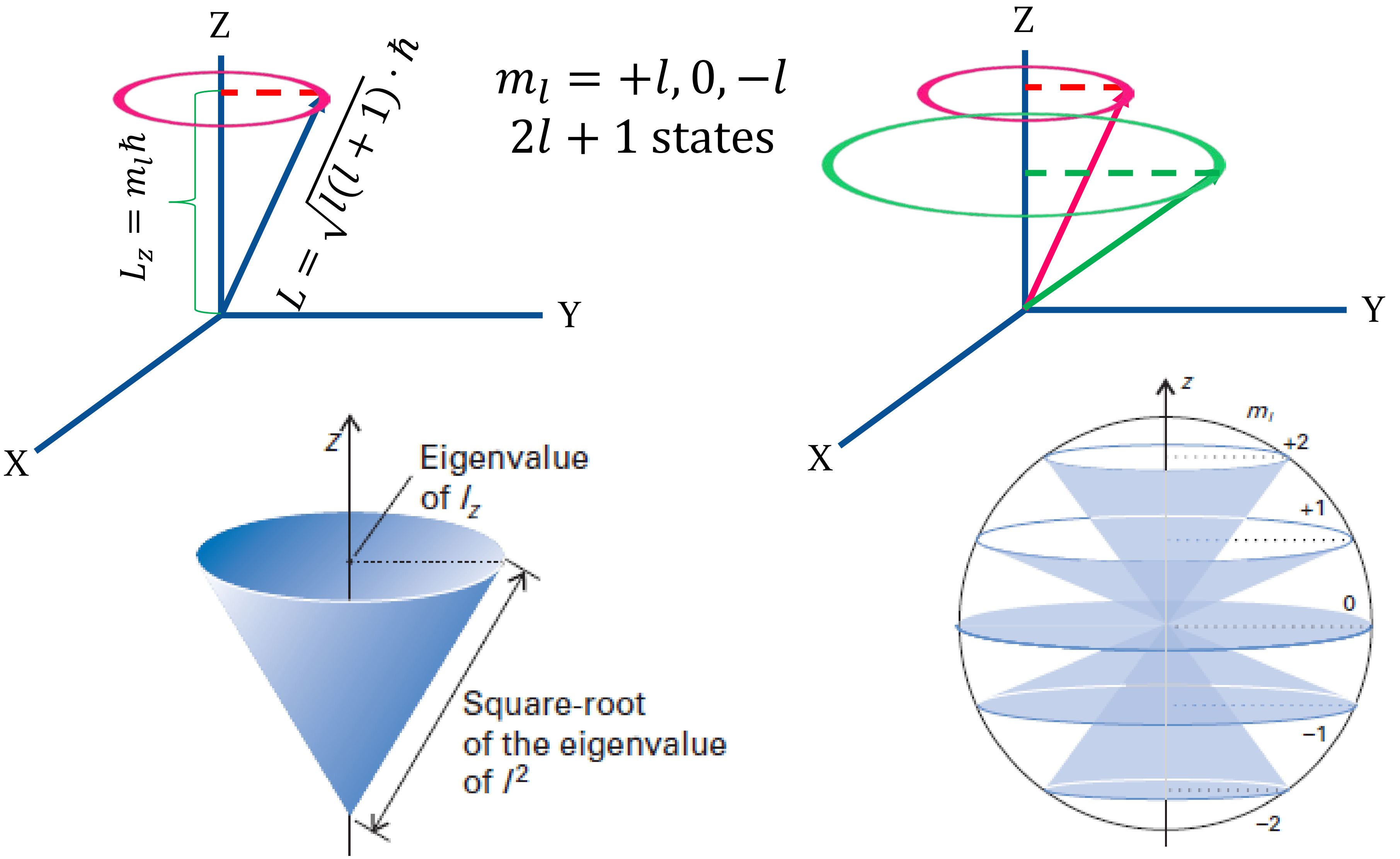
$$Where, \qquad N = \frac{(-1)^{l+|m_l|}}{2^l l!}\sqrt{\frac{2l+1}{4\pi}\cdot\frac{(l-|m_l|)!}{(l+|m_l|)!}}$$

$$\beta = \frac{2IE}{\hbar^2} \implies E = \frac{\beta\hbar^2}{2I} \qquad \text{where } \beta = l(l+1) \;\&\; m_l = +l \; to \; -l \; with \; 0$$

Note that only eigenfunction depends on both m_l & l, whereas eigenvalue depend on only l, why?

ROTATIONAL MOTION

Representation of Angular Momentum

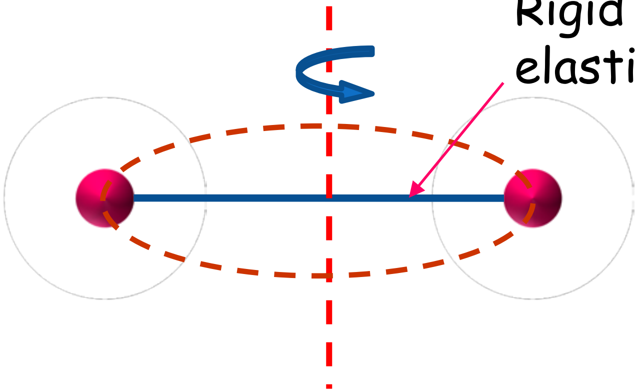


$$m_l = +l, 0, -l$$

$$2l + 1 \text{ states}$$

ROTATIONAL MOTION

Rigid Rotator

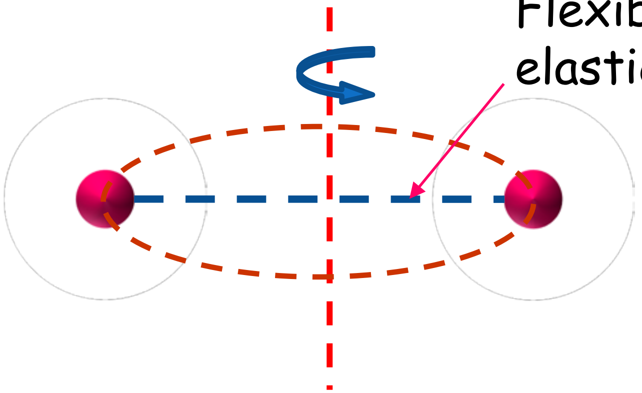


Rigid and non-elastic connector

A system consisting of two particles attached by a rigid and non-elastic connector is know as rigid rotator.

- ✓ It is imaginary and has no real sense.
- ✓ Its mathematics is simple.
- ✓ Its results help to build up the base for understanding real rotator (diatomic molecule).

Non-rigid Rotator



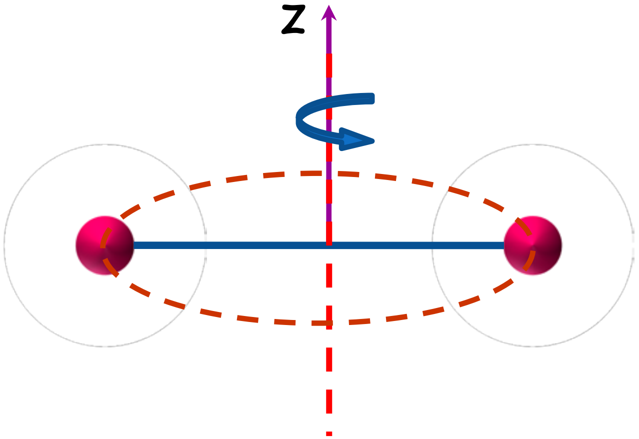
Flexible and elastic connector

A system consisting of two particles attached by a flexible and elastic connector is know as non-rigid rotator.

- ✓ It has real sense, for instance, diatomic molecules.
- ✓ Its mathematics is difficult.
- ✓ Its results help to understand rotational spectra of molecules

ROTATIONAL MOTION

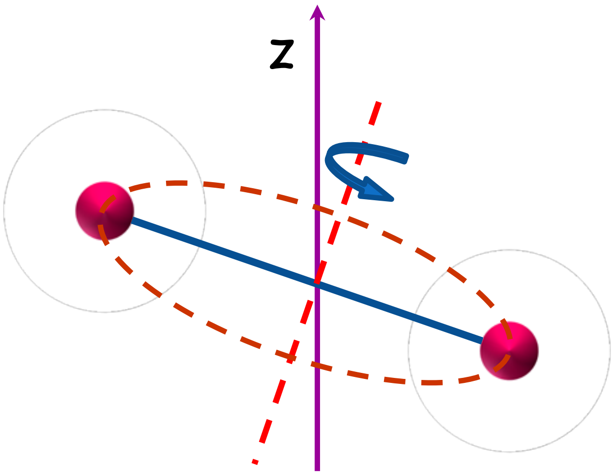
2D Rigid Rotator



If the rotation axis of rigid rotator aligns with any of x, y or z axes, then it is 2D rotator.

- ✓ Angular momentum L is equal to its L_z
- ✓ It is very similar to particle rotating on ring.

3D Rigid Rotator



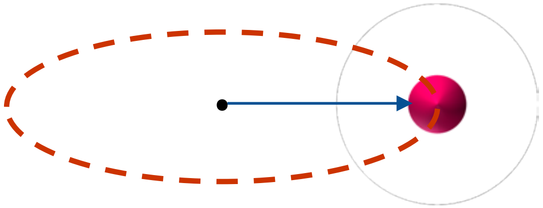
If the rotation axis of rigid rotator does not align to any of x, y or z axes, then it is 3D rotator.

- ➢ Angular momentum L is not equal to its L_z and $L^2 = L_x^2 + L_y^2 + L_z^2$
- ➢ It is very similar to particle rotating on sphere.

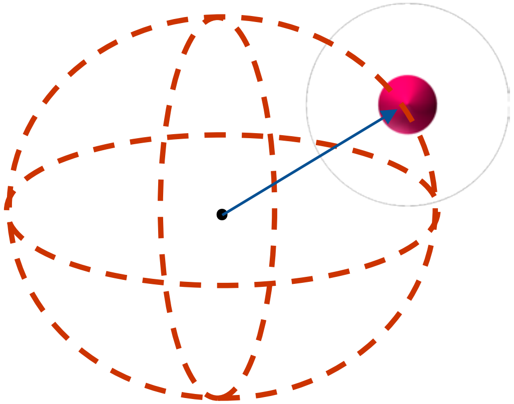
ROTATIONAL MOTION

Reduce two-bodies problems to one-body problems

One-body problems

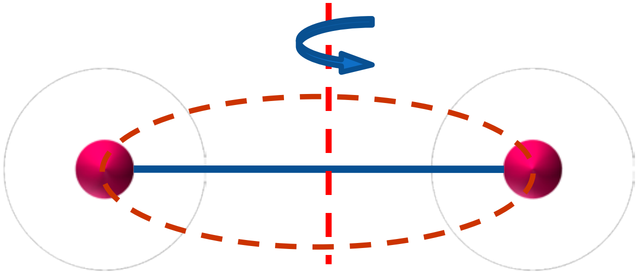


Particle on ring

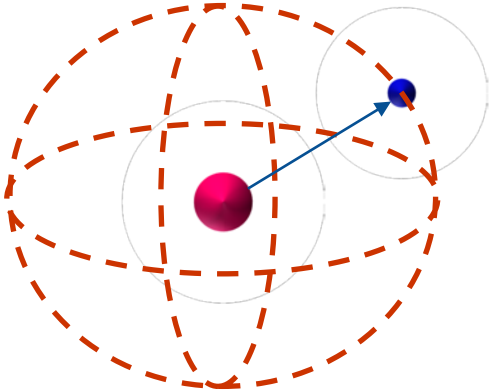


Particle on Sphere

Two-body problems



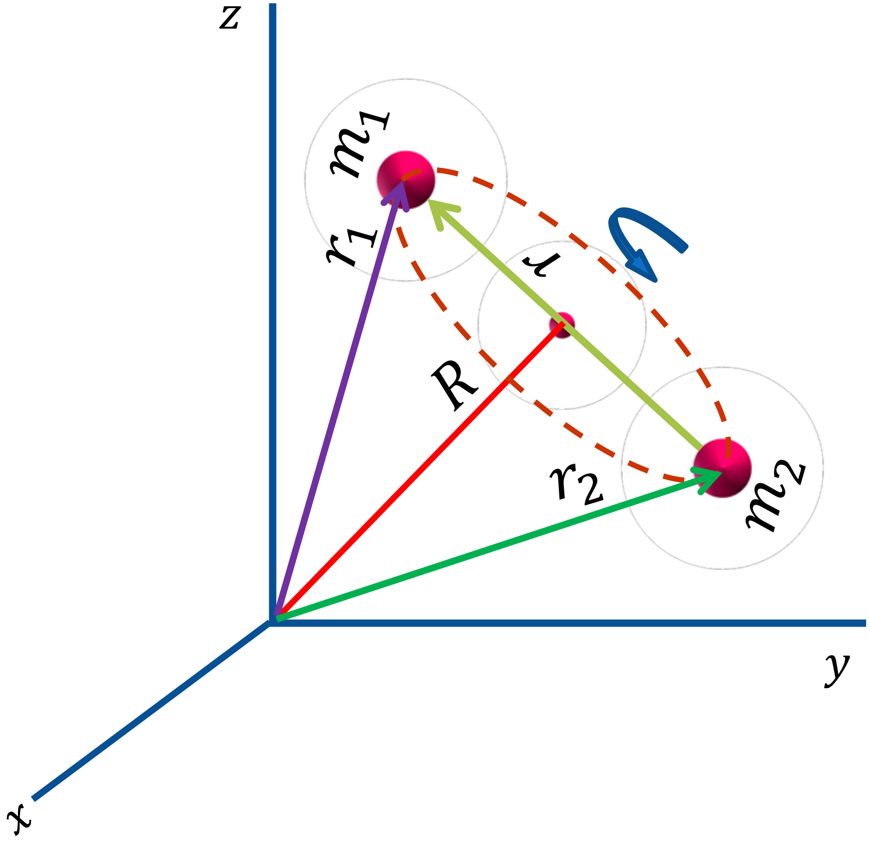
Rigid rotator



Hydrogen atom

ROTATIONAL MOTION

Reduce two-bodies problems to one-body problems



$$r = r_1 - r_2 \qquad (1)$$

$$M = m_1 + m_2$$

$$R = \frac{m_1 r_1 + m_2 r_2}{M} \qquad (2)$$

From Eq. (1) & (2)

$$r_1 = R - \frac{m_2 r}{m_1 + m_2} = R - \frac{\mu r}{m_1}$$

$$r_2 = R + \frac{m_1 r}{m_1 + m_2} = R + \frac{\mu r}{m_2}$$

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

ROTATIONAL MOTION

Reduce two-bodies problems to one-body problems

Total kinetic energy of system

$$T = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_2 v_2^2 = \frac{1}{2}m_1\left(\frac{dr_1}{dt}\right)^2 + \frac{1}{2}m_2\left(\frac{dr_2}{dt}\right)^2$$

$$\left(\frac{dr_1}{dt}\right)^2 = \frac{dr_1}{dt}\cdot\frac{dr_1}{dt} = \left(\frac{dR}{dt} - \frac{\mu}{m_1}\frac{dr}{dt}\right)\cdot\left(\frac{dR}{dt} - \frac{\mu}{m_1}\frac{dr}{dt}\right) = \left(\frac{dR}{dt}\right)^2 + \frac{\mu^2}{m_1^2}\left(\frac{dr}{dt}\right)^2$$

$$\left(\frac{dr_2}{dt}\right)^2 = \frac{dr_2}{dt}\cdot\frac{dr_2}{dt} = \left(\frac{dR}{dt} + \frac{\mu}{m_2}\frac{dr}{dt}\right)\cdot\left(\frac{dR}{dt} + \frac{\mu}{m_2}\frac{dr}{dt}\right) = \left(\frac{dR}{dt}\right)^2 + \frac{\mu^2}{m_2^2}\left(\frac{dr}{dt}\right)^2$$

$$T = \frac{1}{2}(m_1 + m_2)\left(\frac{dR}{dt}\right)^2 + \frac{\mu^2}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\left(\frac{dr}{dt}\right)^2 = \frac{1}{2}M\left(\frac{dR}{dt}\right)^2 + \frac{\mu^2}{2}\cdot\frac{1}{\mu}\left(\frac{dr}{dt}\right)^2$$

$$T = \frac{p_M^2}{2M} + \frac{p_\mu^2}{2\mu}$$

Translation energy

Internal kinetic energy

If center of mass is fixed then translational energy becomes zero, hence total kinetic energy is internal kinetic energy

$$T = \frac{p_\mu^2}{2\mu}$$

ROTATIONAL MOTION

Classical treatment of Rigid Rotator

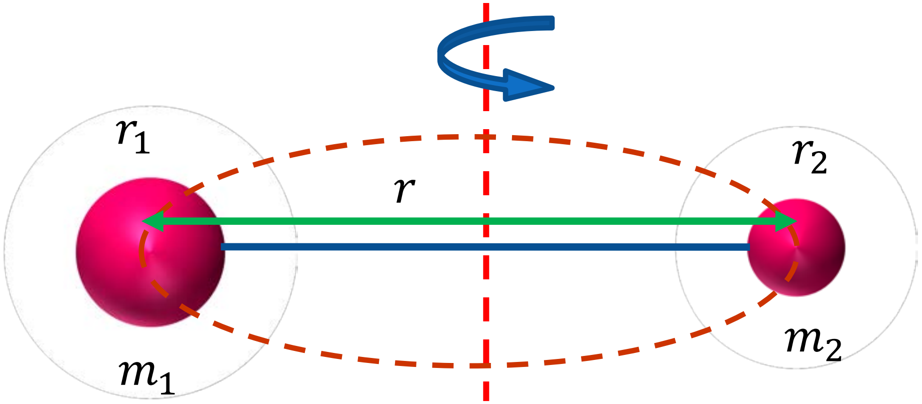


Fig. A rigid rotator consisting of two point masses m_1 and m_2 connected by weightless string of fixed length, r which is independent of time. The center of mass is fixed.

From results of reducing two-bodies problem with fixed center of mass to one-particle problem, the total kinetic energy is given by

$$T = \frac{p_\mu^2}{2\mu} = \frac{\left(\frac{I\omega}{r}\right)^2}{2\mu} = \frac{I^2\omega^2}{2\mu r^2} = \frac{L^2}{2I}$$

$$\boxed{T = \frac{L^2}{2I}}$$

Classical energy expression

Since, there are no restriction on I and ω, so, the classical energy of rigid rotator is continuous.

ROTATIONAL MOTION

Quantum mechanical treatment of Rigid Rotator

From results of reducing two-bodies problem with fixed center of mass to one-particle problem, the total kinetic energy is given by

$$T = \frac{p_\mu^2}{2\mu}$$

Hamiltonian operator,

$$\hat{H} = -\frac{p_\mu^2}{2\mu} + V(r)$$

The rigid rotator free of external force has $V(r) = 0$.

$$\hat{H} = -\frac{p_\mu^2}{2\mu} = -\frac{\hbar^2}{2\mu}\nabla_r^2$$

∇_r^2 or simply ∇^2 in spherical coordinate for 2D and 3D rigid rotator:

$$2D: \quad \nabla^2 = \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}$$

$$3D: \quad \nabla^2 = \frac{1}{r^2}\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]$$

ROTATIONAL MOTION

Quantum mechanical treatment of Rigid Rotator

If ψ is the wavefunction of rigid rotator then SE

$$2D: -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2}\psi = E\psi \quad (I = \mu r^2) \tag{4}$$

$$3D: -\frac{\hbar^2}{2I}\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]\psi = E\psi \quad (I = \mu r^2) \tag{5}$$

The eq. (4) & (5) are similar to SE of particle rotating on ring and sphere from where m is replaced by μ in eq. (4) & (5).

2D:

$$\Phi_{m_l} = \frac{1}{\sqrt{2\pi}}e^{im_l\phi}$$

$$E = \frac{m_l^2\hbar^2}{2I}$$

$$L = L_z = m_l\hbar$$

3D

$$Y_{lm_l}(\theta,\phi) = N\left[\sin^{|m_l|}\theta\frac{d^{l+|m_l|}}{d(\cos\theta)^{l+|m_l|}}\sin^{2l}\theta\right]e^{im_l\phi}$$

where, $$N = \frac{(-1)^{l+|m_l|}}{2^l l!}\sqrt{\frac{2l+1}{4\pi}\cdot\frac{(l-|m_l|)!}{(l+|m_l|)!}}$$

$$E_l = l(l+1)\frac{\hbar^2}{2I} \qquad L_z = m_l\hbar$$

$$L^2 = l(l+1)\hbar^2 \qquad \Rightarrow L = \sqrt{l(l+1)}\hbar$$

ROTATIONAL MOTION

Classical vs quantum mechanical energy of Rigid Rotator

Classical energy

$$T = \frac{L^2}{2I}$$

Since, there are no restriction on I and ω, so, the classical energy of rigid rotator is continuous.

Quantum mechanical energy

$$2D: \quad E = \frac{m_l^2 \hbar^2}{2I} \quad \& \quad 3D: \quad E_l = l(l+1)\frac{\hbar^2}{2I}$$

Where $m_l = +l \text{ to } -l$ including zero and $l = 0, 1, 2, \cdots$

It is obvious that quantum mechanical energy of both 2D & 3D rigid rotators depend on m_l or l which renders the quantized energy of rigid rotator.

ROTATIONAL MOTION

Problem 1:

Suppose two points of different masses rotate freely on different spheres of radius r_1 and r_2. A rigid rotator was made by touching those spheres.

(a) Write the classical energy expressions for rotating masses on spheres and rigid rotator.

(b) Write the quantum energy expressions for rotating masses on spheres and rigid rotator

(c) Show that quantum energy of rigid rotator is the sum of quantum energy of two mases rotating on different spheres.

(d) Compare the features of classical and quantum energies.

ROTATIONAL MOTION

Problem 2:

Suppose two particles A and B of masse m_1 and m_2 rotate freely on locus of radius r_1 and r_2 respectively. Radius vector of A makes constant angle with z-axis while B does not.

(a) Define the path of rotation of particle A and B.

(b) Write Hamiltonian operator for A and B

(c) Show that exited state of A is doubly degenerate whereas it is $(2l+1)$-fold degenerate for particle B.

(d) The angular momentum of B is given by $\sqrt{l(l+1)}\hbar$

(e) Represent angular momentum of B schematically when $l = 2$

(f) List all the spherical harmonics for $l = 2$ in real and imaginary forms.

(g) Draw spherical harmonics listed in (f).