Road to spherical harmonics

1. Hamiltonian in central field $H = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r}$
2. separate r and θ, ϕ $\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}\Lambda^2$
3. Laplacian in polar coordinate $\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$

4. Legendre differential equation is part of Laplacian equation
5. Rodrigues formula is solution Leibniz rule
6. full Laplacian equation is associated Legendre differential equation
7. Derivative of Rodrigues formula is solution

→ spherical harmonics

Why it is worthwhile taking time for spherical harmonics?

1. it is a wave function — but, of what ?
2. rotational energy — $E = Bh\,J(J+1)$
3. angular momentum — J, K, Ka, Kc
4. symmetry — $(-1)^J$
5. selection rule — $\Delta J = 0, \pm 1, 0 \nleftrightarrow 0$
6. (vanishing integral) — expansion

Hamiltonian in central field

$$p_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$H = \frac{p^2}{2m} + V(x)$$

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

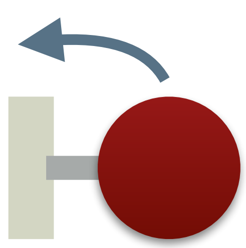
$$= \sum_{i}^{n} \frac{p_i^2}{2m_i} + \sum_{i<j}^{n} \frac{Z_i Z_j e^2}{r_{ij}}$$

kinetic | potential

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

$$= -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r}$$

we have shown



all that rotates

Laplacian

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{1}{r^2}\Lambda^2$$

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

Legendrian

$$H\Psi = E\Psi$$

goal: to know wavefunction

if $\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$

radial angular

$$HRY = -\frac{\hbar^2}{2\mu}\nabla^2(RY) - \frac{Ze^2}{r}RY$$

$$= -\frac{\hbar^2}{2\mu}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}\Lambda^2\right)RY - \frac{Ze^2}{r}RY$$

$$= -\frac{\hbar^2}{2\mu}\left(Y\frac{1}{r}\frac{\partial^2}{\partial r^2}rR + R\frac{1}{r^2}\Lambda^2 Y\right) - \frac{Ze^2}{r}RY$$

if $\Lambda^2 Y = c_1 Y$ equation involves Y only

$$Y\frac{1}{r}\frac{\partial^2}{\partial r^2}rR + \frac{R}{r^2}c_1 Y - V(r)RY = -\frac{2\mu}{\hbar^2}ERY$$

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}rR + \frac{R}{r^2}c_1 - V(r)R = -\frac{2\mu}{\hbar^2}ER$$

equation involves R only

Road to spherical harmonics

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➡ spherical harmonics

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

so we will look for solution of

(or better if there is)

if $\Lambda^2 Y = c_1 Y$ **equation involves Y only**

Legendre differential equation

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

$$\frac{d}{dx}\left[(1-x^2)\frac{dy}{dx}\right] + n(n+1)\,y = 0 \quad \text{1}$$

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

Rodrigues formula

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

satisfies 1

so we will look for solution of

(or better if there is)

if $\Lambda^2 Y = c_1 Y$ **equation involves Y only**

One more thing

Legendrian

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

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

$$\Lambda^2 Y = c_1 Y$$

$$y = P_n(x)$$

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

do not look same.

$$\Lambda_1^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

θ part of Λ^2

$$x = \cos\theta$$

$$dx = -\sin\theta\, d\theta$$

$$g(\theta) = g\left(\theta(x)\right) = f(x)$$

$$\Lambda_1^2 g = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial g}{\partial\theta}\right]$$

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

$$\Lambda_1^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

$$x = \cos\theta$$

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$$\Lambda_1^2 g = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial g}{\partial\theta}\right]$$

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

$$\frac{dg}{d\theta} = \frac{df}{dx}\frac{dx}{d\theta} = \frac{df}{dx}(-\sin\theta)$$

$$\frac{d^2 g}{d\theta^2} = \frac{d}{d\theta}\left[\frac{df}{dx}(-\sin\theta)\right]$$

$$= \frac{d^2 f}{dx^2}\frac{dx}{d\theta}(-\sin\theta) + \frac{df}{dx}(-\cos\theta)$$

$$= \frac{d^2 f}{dx^2}\sin^2\theta - \frac{df}{dx}\cos\theta$$

$$= (1-x^2)\frac{d^2 f}{dx^2} - x\frac{df}{dx}$$

$$\Lambda_1^2 g = \frac{\cos\theta}{\sin\theta} \cdot \frac{df}{dx}(-\sin\theta) + (1-x^2)\frac{d^2 f}{dx^2} - x\frac{df}{dx}$$

$$= -\cos\theta \frac{df}{dx} + (1-x^2)\frac{d^2 f}{dx^2} - x\frac{df}{dx}$$

$$= -x\frac{df}{dx} + (1-x^2)\frac{d^2 f}{dx^2} - x\frac{df}{dx}$$

$$= -2x\frac{df}{dx} + (1-x^2)\frac{d^2 f}{dx^2}$$

$$\Lambda_1^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

$$x = \cos\theta$$

$$dx = -\sin\theta\, d\theta$$

$$g(\theta) = g(\theta(x)) = f(x)$$

$$\Lambda_1^2 g = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial g}{\partial\theta}\right]$$

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

$$\frac{dg}{d\theta} = \frac{df}{dx}\frac{dx}{d\theta} = \frac{df}{dx}(-\sin\theta)$$

$$\frac{d^2 g}{d\theta^2} = \frac{d}{d\theta}\left[\frac{df}{dx}(-\sin\theta)\right]$$

$$= \frac{d^2 f}{dx^2}\frac{dx}{d\theta}(-\sin\theta) + \frac{df}{dx}(-\cos\theta)$$

$$= \frac{d^2 f}{dx^2}\sin^2\theta - \frac{df}{dx}\cos\theta$$

$$= (1-x^2)\frac{d^2 f}{dx^2} - x\frac{df}{dx}$$

Legendre differential equation

$$\frac{d}{dx}\left[(1-x^2)\frac{dy}{dx}\right] + n(n+1)\,y = 0 \quad [1]$$

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

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

$$\Lambda^2 y = -n(n+1)\,y$$

$$\Lambda^2 Y = c_1 Y$$

What to do with ϕ

polar azimuthal

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

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

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

$$\Lambda^2\,Y = \left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right]Y$$

$$\Lambda^2\,\Theta\Phi = \left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right]\Theta\Phi$$

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

equation ϕ only

2 find ϕ

$$\Lambda^2\,\Theta\Phi = \left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right]\Theta\Phi$$

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

$$= -\frac{m^2}{\sin^2\theta}\Theta\Phi + \Phi\Lambda_1^2\Theta$$

$$\Lambda^2\Theta = -\frac{m^2}{\sin^2\theta}\Theta + \Lambda_1^2\Theta$$

equation θ only

$$\Lambda^2\Theta = -\frac{m^2}{\sin^2\theta}\Theta + \Lambda_1^2\Theta$$

$$\Lambda_1^2 g = -2x\,\frac{df}{dx} + (1-x^2)\,\frac{d^2 f}{dx^2}$$

Legendre differential equation

$$\Theta(\theta) = \tilde{\Theta}(x)$$

$$x = \cos\theta$$

$$\Lambda^2\tilde{\Theta} = -\frac{m^2}{1-x^2}\tilde{\Theta} + \Lambda_1^2\tilde{\Theta}$$

$$\Lambda^2\tilde{\Theta}\Phi = -\frac{m^2}{1-x^2}\tilde{\Theta}\Phi + \Phi\Lambda_1^2\tilde{\Theta}$$

$$\Lambda^2\tilde{\Theta} = -\frac{m^2}{1-x^2}\tilde{\Theta}(x) - 2x\,\frac{d\tilde{\Theta}(x)}{dx} + (1-x^2)\,\frac{d^2\tilde{\Theta}(x)}{dx^2}$$

$$= -n(n+1)\,\tilde{\Theta}(x)$$

$$\Lambda^2\Theta = -\frac{m^2}{\sin^2\theta}\Theta + \Lambda_1^2\Theta$$

$$\Lambda_1^2 g = -2x\,\frac{df}{dx} + (1-x^2)\,\frac{d^2 f}{dx^2}$$

Legendre differential equation

$$\Theta(\theta) = \tilde{\Theta}(x)$$

$$x = \cos\theta$$

$$\Lambda^2\tilde{\Theta} = -\frac{m^2}{1-x^2}\tilde{\Theta} + \Lambda_1^2\tilde{\Theta}$$

$$\Lambda^2\tilde{\Theta}\Phi = -\frac{m^2}{1-x^2}\tilde{\Theta}\Phi + \Phi\Lambda_1^2\tilde{\Theta}$$

$$\Lambda^2\tilde{\Theta} = -\frac{m^2}{1-x^2}\tilde{\Theta}(x) - 2x\,\frac{d\tilde{\Theta}(x)}{dx} + (1-x^2)\,\frac{d^2\tilde{\Theta}(x)}{dx^2}$$

$$= -n(n+1)\,\tilde{\Theta}(x)$$

<u>associated</u> Legendre differential equation

Legendre differential equation

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

$$\frac{d}{dx}\left[(1-x^2)\frac{dy}{dx}\right] + n(n+1)\,y = 0 \quad \text{1}$$

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

Rodrigues formula

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

satisfies 1

$$f = (x^2-1)^n$$ **is enough**

$$f' = n(x^2-1)^{n-1}\cdot 2x$$

$$f'' = n(n-1)\,(x^2-1)^{n-2}\cdot 4x^2 + 2n(x^2-1)^{n-1}$$

$$= 2x(n-1)\,\frac{f'}{x^2-1} + 2n\,\frac{f}{x^2-1}$$

Rodrigues formula

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} \left[(x^2-1)^n\right]$$

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

$$f = (x^2-1)^n$$

$$f' = n(x^2-1)^{n-1} \cdot 2x$$

$$f'' = n(n-1)\,(x^2-1)^{n-2} \cdot 4x^2 + 2n(x^2-1)^{n-1}$$

$$= 2x(n-1)\,\frac{f'}{x^2-1} + 2n\,\frac{f}{x^2-1}$$

$$(x^2-1)\,f'' = 2x(n-1)f' + 2nf$$

differentiate both sides

n times

Leibniz rule

$$\frac{d}{dx}(f \cdot g) = f^{(1)}g^{(0)} + f^{(0)}g^{(1)}$$

$$\frac{d^n}{dx^n}(f \cdot g) = \frac{d^{n-1}}{dx^{n-1}}\left(f^{(1)}g^{(0)} + f^{(0)}g^{(1)}\right)$$

$$= \frac{d^{n-2}}{dx^{n-2}}\left(f^{(2)}g^{(0)} + f^{(1)}g^{(1)} + f^{(1)}g^{(1)} + f^{(0)}g^{(2)}\right)$$

$$= \ldots$$

$$(f \cdot g)^{(n)} = \sum_{k=0}^{n} \binom{n}{k} f^{(k)} g^{(n-k)}$$

remember binomial theorem?

$$(x+y)^2 = x^2 + 2xy + y^2$$

$$(x+y)^3 = x^3 + 3x^2y + 3xy^2 + y^3$$

$$(x+y)^n = x^n + n \cdot x^{n-1}y + \ldots + n \cdot xy^{n-1} + y^n$$

.....

$$(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^k y^{n-k}$$

Rodrigues formula

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

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

$$f = (x^2-1)^n$$

$$f' = n(x^2-1)^{n-1}\cdot 2x$$

$$f'' = n(n-1)\,(x^2-1)^{n-2}\cdot 4x^2 + 2n(x^2-1)^{n-1}$$

$$= 2x(n-1)\,\frac{f'}{x^2-1} + 2n\,\frac{f}{x^2-1}$$

$$(x^2-1)\,f'' = 2x(n-1)f' + 2nf$$

differentiate both sides

n times

$$(x^2-1)f^{(n+2)} + n\cdot 2xf^{(n+1)} + \frac{n(n-1)}{2}\cdot 2f^{(n)} = 2x(n-1)f^{(n+1)} + 2n(n-1)f^{(n)} + 2nf^{(n)}$$

$$(x^2-1)f^{(n+2)} + [2nx - 2(n-1)x]\,f^{(n+1)} + [n(n-1) - 2n(n-1) - 2n]\,f^{(n)} = 0$$

Leibniz rule

$$(f\cdot g)^{(n)} = \sum_{k=0}^{n}\binom{n}{k} f^{(k)}g^{(n-k)}$$

$$(x^2-1)\,f''$$

g f

$g^{(1)} = 2x$

$g^{(2)} = 2$

$g^{(3)} = 0$

max k=2 is enough

$$2x(n-1)f'$$

g f

$g^{(1)} = 2$

$g^{(2)} = 0$

max k=1 is enough

Rodrigues formula

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

satisfies $\frac{d}{dx}\left[(1-x^2)\frac{dy}{dx}\right] + n(n+1)\,y = 0$

$$f = (x^2-1)^n$$

$$f' = n(x^2-1)^{n-1}\cdot 2x$$

$$f'' = n(n-1)\,(x^2-1)^{n-2}\cdot 4x^2 + 2n(x^2-1)^{n-1}$$

$$= 2x(n-1)\frac{f'}{x^2-1} + 2n\frac{f}{x^2-1}$$

$$(x^2-1)\,f'' = 2x(n-1)f' + 2nf$$

differentiate both sides

n times

$$(x^2-1)f^{(n+2)} + n\cdot 2xf^{(n+1)} + \frac{n(n-1)}{2}\cdot 2f^{(n)} = 2x(n-1)f^{(n+1)} + 2n(n-1)f^{(n)} + 2nf^{(n)}$$

$$(x^2-1)f^{(n+2)} + [2nx - 2(n-1)x]\,f^{(n+1)} + [n(n-1) - 2n(n-1) - 2n]\,f^{(n)} = 0$$

Leibniz rule

$$(f\cdot g)^{(n)} = \sum_{k=0}^{n}\binom{n}{k} f^{(k)}g^{(n-k)}$$

$$(x^2-1)f^{(n+2)} + 2xf^{(n+1)} - n(n+1)f^{(n)} = 0$$

$$(1-x^2)f^{(n+2)} - 2xf^{(n+1)} + n(n+1)f^{(n)} = 0$$

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

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

Rodrigues is the solution of Legendre

$$y = \frac{d^n}{dx^n}(x^2-1)^n$$

1. Hamiltonian in central field
2. separate r and θ, φ
3. Laplacian in polar coordinate
4. Legendre differential equation is part of Laplacian
5. Rodrigues formula is solution
6. **full Laplacian is associated Legendre differential equation**
7. **Derivative of Rodrigues formula is solution**

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

$$\Lambda^2=\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

$$\frac{d}{dx}\left[(1-x^2)\frac{dy}{dx}\right]+n(n+1)\,y=0$$

Show

$$v=(1-x^2)^{\frac{m}{2}}y^{(m)}$$

is the solution of $\boxed{2}$

$$y=P_n(x)$$

$$P_n(x)=\frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

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

$$\frac{d}{dx}\left[(1-x^2)\frac{dy}{dx}\right] + n(n+1)\,y = 0 \quad (1)$$

$y = P_n(x)$

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

y was solution of Legendre

Leibniz rule

$$(f\cdot g)^{(n)} = \sum_{k=0}^{n}\binom{n}{k} f^{(k)} g^{(n-k)}$$

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

differentiate both sides

m times

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

$$\frac{d^m}{dx^m}\left[(1-x^2)\frac{d^2y}{dx^2}\right] = (1-x^2)y^{(m+2)} - 2mx\,y^{(m+1)} - 2\cdot\frac{m(m-1)}{2}\,y^{(m)}$$

$$= (1-x^2)y^{(m+2)} - 2mx\,y^{(m+1)} - m(m-1)\,y^{(m)}$$

$$(1-x^2)\frac{d^2y}{dx^2}$$

g f

$$\frac{d^m}{dx^m}\left[2x\frac{dy}{dx}\right] = 2x\,y^{(m+1)} + 2m\,y^{(m)}$$

$g^{(1)} = -2x$

$g^{(2)} = -2$

$g^{(3)} = 0$

max k=2 is enough

$$n(n+1)\frac{d^m y}{dx^m} = n(n+1)\,y^{(m)}$$

$$\frac{d^m}{dx^m}\left[(1-x^2)\frac{d^2y}{dx^2}\right] - \frac{d^m}{dx^m}\left[2x\frac{dy}{dx}\right] + n(n+1)\frac{d^my}{dx^m} = 0$$ 3

$$\frac{d^m}{dx^m}\left[(1-x^2)\frac{d^2y}{dx^2}\right] = (1-x^2)y^{(m+2)} - 2mx\,y^{(m+1)} - 2\cdot\frac{m(m-1)}{2}\,y^{(m)}$$

$$= (1-x^2)y^{(m+2)} - 2mx\,y^{(m+1)} - m(m-1)\,y^{(m)}$$

$$\frac{d^m}{dx^m}\left[2x\frac{dy}{dx}\right] = 2x\,y^{(m+1)} + 2m\,y^{(m)}$$

$$n(n+1)\frac{d^my}{dx^m} = n(n+1)\,y^{(m)}$$

3 $$(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} + [-m(m-1) - 2m + n(n+1)]\,y^{(m)} = 0$$

$$(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - [m(m+1) + n(n+1)]\,y^{(m)} = 0$$ 4

$$\frac{d^m}{dx^m}\left[(1-x^2)\frac{d^2y}{dx^2}\right] - \frac{d^m}{dx^m}\left[2x\frac{dy}{dx}\right] + n(n+1)\frac{d^my}{dx^m} = 0 \quad \mathbf{3}$$

$$\frac{d^m}{dx^m}\left[(1-x^2)\frac{d^2y}{dx^2}\right] = (1-x^2)y^{(m+2)} - 2mx\,y^{(m+1)} - 2\cdot\frac{m(m-1)}{2}\,y^{(m)}$$

$$= (1-x^2)y^{(m+2)} - 2mx\,y^{(m+1)} - m(m-1)\,y^{(m)}$$

$$\frac{d^m}{dx^m}\left[2x\frac{dy}{dx}\right] = 2x\,y^{(m+1)} + 2m\,y^{(m)}$$

$$n(n+1)\frac{d^my}{dx^m} = n(n+1)\,y^{(m)}$$

associated Legendre

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

Show $v = (1-x^2)^{\frac{m}{2}}y^{(m)}$

is the solution

$$\mathbf{3} \quad (1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - [-m(m-1) - 2m + n(n+1)]\,y^{(m)} = 0$$

$$(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - [m(m+1) + n(n+1)]\,y^{(m)} = 0 \quad \mathbf{4}$$

preparation finished

associated Legendre

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

Show $v=(1-x^2)^{\frac{m}{2}}y^{(m)}$ is the solution

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

$$\left[-mx\,(1-x^2)^{\frac{m}{2}-1}\right]'$$

$$=-m\,(1-x^2)^{\frac{m}{2}-1}-mx\left(\frac{m}{2}-1\right)(1-x^2)^{\frac{m}{2}-2}\cdot(-2x)$$

$$=\left[-m(1-x^2)+2mx^2\cdot\left(\frac{m}{2}-1\right)\right](1-x^2)^{\frac{m}{2}-2}$$

$$=\left[mx^2-m+mx^2\cdot(m-2)\right](1-x^2)^{\frac{m}{2}-2}$$

$$=m\left[x^2-1+x^2\cdot(m-2)\right](1-x^2)^{\frac{m}{2}-2}$$

$$=m\left[(m-1)\,x^2-1\right](1-x^2)^{\frac{m}{2}-2}$$

$$\frac{dv}{dx}=\frac{m}{2}(1-x^2)^{\frac{m}{2}-1}\cdot(-2x)\,y^{(m)}+(1-x^2)^{\frac{m}{2}}y^{(m+1)}$$

$$=-mx\,(1-x^2)^{\frac{m}{2}-1}\,y^{(m)}+(1-x^2)^{\frac{m}{2}}\,y^{(m+1)}$$

$$\frac{d^2v}{dx^2}=m\left[(m-1)\,x^2-1\right](1-x^2)^{\frac{m}{2}-2}y^{(m)}-mx\,(1-x^2)^{\frac{m}{2}-1}\,y^{(m+1)}$$

$$-mx\,(1-x^2)^{\frac{m}{2}-1}\,y^{(m+1)}+(1-x^2)^{\frac{m}{2}}\,y^{(m+2)}$$

$$=m\left[(m-1)\,x^2-1\right](1-x^2)^{\frac{m}{2}-2}y^{(m)}-2mx\,(1-x^2)^{\frac{m}{2}-1}\,y^{(m+1)}+(1-x^2)^{\frac{m}{2}}\,y^{(m+2)}$$

and here our preparation

$$(1-x^2)y^{(m+2)}-2(m+1)x\,y^{(m+1)}-\left[m(m+1)+n(n+1)\right]y^{(m)}=0 \quad \mathbf{4}$$

associated Legendre

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

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

Show $v = (1-x^2)^{\frac{m}{2}} y^{(m)}$ **is the solution**

$$\left[-mx\,(1-x^2)^{\frac{m}{2}-1}\right]'$$

$$= -m\,(1-x^2)^{\frac{m}{2}-1} - mx\left(\frac{m}{2}-1\right)(1-x^2)^{\frac{m}{2}-2}\cdot(-2x)$$

$$= \left[-m(1-x^2) + 2mx^2\cdot\left(\frac{m}{2}-1\right)\right](1-x^2)^{\frac{m}{2}-2}$$

$$= \left[mx^2 - m + mx^2\cdot(m-2)\right](1-x^2)^{\frac{m}{2}-2}$$

$$= m\left[x^2 - 1 + x^2\cdot(m-2)\right](1-x^2)^{\frac{m}{2}-2}$$

$$= m\left[(m-1)\,x^2 - 1\right](1-x^2)^{\frac{m}{2}-2}$$

$$\frac{dv}{dx} = \frac{m}{2}(1-x^2)^{\frac{m}{2}-1}\cdot(-2x)\,y^{(m)} + (1-x^2)^{\frac{m}{2}}y^{(m+1)}$$

$$= -mx\,(1-x^2)^{\frac{m}{2}-1}\,y^{(m)} + (1-x^2)^{\frac{m}{2}}\,y^{(m+1)}$$

$$\frac{d^2 v}{dx^2} = m\left[(m-1)\,x^2 - 1\right](1-x^2)^{\frac{m}{2}-2}y^{(m)} - mx\,(1-x^2)^{\frac{m}{2}-1}\,y^{(m+1)}$$
$$- mx\,(1-x^2)^{\frac{m}{2}-1}\,y^{(m+1)} + (1-x^2)^{\frac{m}{2}}\,y^{(m+2)}$$

$$= m\left[(m-1)\,x^2 - 1\right](1-x^2)^{\frac{m}{2}-2}y^{(m)} - 2mx\,(1-x^2)^{\frac{m}{2}-1}\,y^{(m+1)} + (1-x^2)^{\frac{m}{2}}\,y^{(m+2)}$$

and here our preparation

$$(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - \left[m(m+1) + n(n+1)\right]y^{(m)} = 0 \quad \boxed{4}$$

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

$$v = (1-x^2)^{\frac{m}{2}} y^{(m)}$$

Show ________ = 0

$$\textbf{5} \quad \frac{dv}{dx} = -mx\,(1-x^2)^{\frac{m}{2}-1}\, y^{(m)} + (1-x^2)^{\frac{m}{2}}\, y^{(m+1)}$$

$$\textbf{6} \quad \frac{d^2 v}{dx^2} = m\,\left[(m-1)\,x^2 - 1\right](1-x^2)^{\frac{m}{2}-2} y^{(m)} - 2mx\,(1-x^2)^{\frac{m}{2}-1}\, y^{(m+1)} + (1-x^2)^{\frac{m}{2}}\, y^{(m+2)}$$

$$(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - [m(m+1) + n(n+1)]\, y^{(m)} = 0 \quad \textbf{4}$$

from "non-associated" Legendre differential equation

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

$$v = (1-x^2)^{\frac{m}{2}}\, y^{(m)}$$

Show ________ = 0

$$\boxed{5} \quad \frac{dv}{dx} = -mx\,(1-x^2)^{\frac{m}{2}-1}\, y^{(m)} + (1-x^2)^{\frac{m}{2}}\, y^{(m+1)}$$

$$\boxed{6} \quad \frac{d^2v}{dx^2} = m\,\left[(m-1)\,x^2 - 1\right](1-x^2)^{\frac{m}{2}-2} y^{(m)} - 2mx\,(1-x^2)^{\frac{m}{2}-1} y^{(m+1)} + (1-x^2)^{\frac{m}{2}} y^{(m+2)}$$

$$(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - [m(m+1) + n(n+1)]\,y^{(m)} = 0 \quad \boxed{4}$$

from “non-associated” Legendre differential equation

$$(1-x^2)\frac{d^2v}{dx^2} = m\,\left[(m-1)\,x^2 - 1\right](1-x^2)^{\frac{m}{2}-1} y^{(m)} - 2mx\,(1-x^2)^{\frac{m}{2}} y^{(m+1)} + (1-x^2)^{\frac{m}{2}+1} y^{(m+2)}$$

$$-2x\frac{dv}{dx} = 2mx^2\,(1-x^2)^{\frac{m}{2}-1}\, y^{(m)} - 2x\,(1-x^2)^{\frac{m}{2}}\, y^{(m+1)}$$

$$-\frac{m^2}{1-x^2}\,v = -\frac{m^2}{1-x^2}(1-x^2)^{\frac{m}{2}}\, y^{(m)}$$

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

$$v = (1-x^2)^{\frac{m}{2}} y^{(m)}$$ **Show** ______ **= 0**

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

$$-2x\frac{dv}{dx} = 2mx^2(1-x^2)^{\frac{m}{2}-1} y^{(m)} - 2x(1-x^2)^{\frac{m}{2}} y^{(m+1)}$$

$$-\frac{m^2}{1-x^2} v = -\frac{m^2}{1-x^2}(1-x^2)^{\frac{m}{2}} y^m$$

$$-2mx - 2x = -2(m+1)x \quad \times(1-x^2)^{\frac{m}{2}}$$

$$\begin{aligned} & m\left[(m-1)x^2 - 1\right] + 2mx^2 - m^2 \\ &= m(m+1)x^2 - m^2 - m \\ &= m(m+1)x^2 - m(m+1) \\ &= m(m+1)(x^2-1) \\ &= -m(m+1)(1-x^2) \end{aligned}$$

$$\times(1-x^2)^{\frac{m}{2}-1}$$

+ +

$$\begin{aligned} &= (1-x^2)(1-x^2)^{\frac{m}{2}} y^{(m+2)} - 2(m+1)x(1-x^2)^{\frac{m}{2}} y^{(m+1)} - m(m+1)(1-x^2)^{\frac{m}{2}} y^{(m)} \\ &= (1-x^2)^{\frac{m}{2}}\left[(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - m(m+1)y^{(m)}\right] \\ &= (1-x^2)^{\frac{m}{2}}\left[-n(n+1)y^{(m)}\right] \\ &= -n(n+1)\,v \end{aligned}$$

4

$$(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - \left[m(m+1) + n(n+1)\right] y^{(m)} = 0 \quad \mathbf{4}$$

"non-associated" Legendre differential equation

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

$$v = (1-x^2)^{\frac{m}{2}} y^{(m)}$$ **Show** ______ **= 0**

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

$$-2x\frac{dv}{dx} = 2mx^2(1-x^2)^{\frac{m}{2}-1}y^{(m)} - 2x(1-x^2)^{\frac{m}{2}}y^{(m+1)}$$

$$-\frac{m^2}{1-x^2}v = -\frac{m^2}{1-x^2}(1-x^2)^{\frac{m}{2}}y^m$$

$$-2mx - 2x = -2(m+1)x \quad \times(1-x^2)^{\frac{m}{2}}$$

$$m\left[(m-1)x^2 - 1\right] + 2mx^2 - m^2$$
$$= m(m+1)x^2 - m^2 - m$$
$$= m(m+1)x^2 - m(m+1)$$
$$= m(m+1)(x^2-1)$$
$$= -m(m+1)(1-x^2)$$

$$\times(1-x^2)^{\frac{m}{2}-1}$$

$$= (1-x^2)(1-x^2)^{\frac{m}{2}}y^{(m+2)} - 2(m+1)x(1-x^2)^{\frac{m}{2}}y^{(m+1)} - m(m+1)(1-x^2)^{\frac{m}{2}}y^{(m)}$$
$$= (1-x^2)^{\frac{m}{2}}\left[(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - m(m+1)y^{(m)}\right]$$
$$= (1-x^2)^{\frac{m}{2}}\left[-n(n+1)y^{(m)}\right]$$
$$= -n(n+1)\,v$$

4

$$(1-x^2)y^{(m+2)} - 2(m+1)x\,y^{(m+1)} - \left[m(m+1) + n(n+1)\right]y^{(m)} = 0$$ **4**

"non-associated" Legendre differential equation

So what did we do?

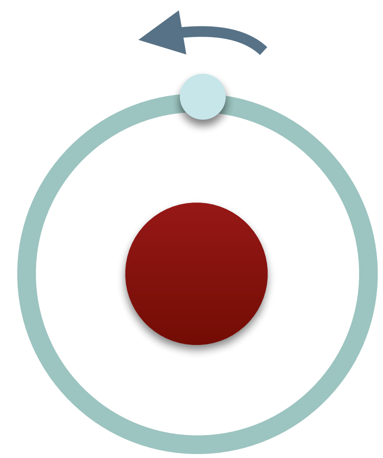
started from here

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r}$$

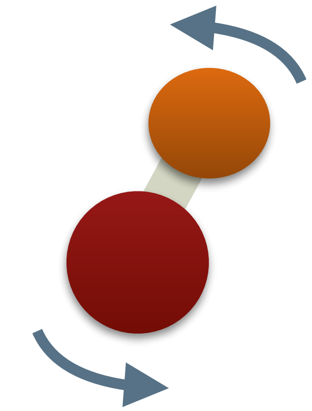
$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}\Lambda^2$$

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

we had this in mind



but this is exactly same



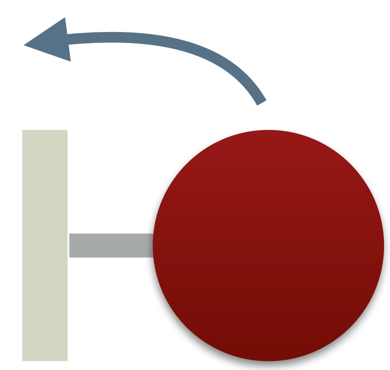
convinced angular wavefunction is solution of associated Legendre differential equation

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

$$\Lambda^2 Y(\theta,\phi) = -l(l+1)Y(\theta,\phi)$$

$$Y_{l,m}(x,\phi) = \frac{1}{2^l\, l!}(1-x^2)^{\frac{m}{2}}\frac{d^{l+m}}{dx^{l+m}}\left[(x^2-1)^l\right]$$

$$x = \cos\theta$$



1 find μ

both of them are this

except

1 Rigid rotor with r fixed.

2 central field is not explicit.

Road to **spherical harmonics**

1. Hamiltonian in central field $H = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r}$
2. separate r and θ, ϕ $\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}\Lambda^2$
3. Laplacian in polar coordinate $\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$

---

4. Legendre differential equation is part of Laplacian
5. Rodrigues formula is solution   Leibniz rule
6. full Laplacian is associated Legendre differential equation
7. Derivative of Rodrigues formula is solution

➡ **spherical harmonics**

$$v = (1-x^2)^{\frac{m}{2}} y^{(m)}$$

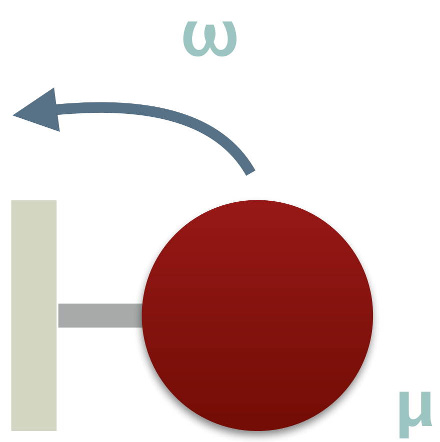
$$y = P_n(x)$$

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

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

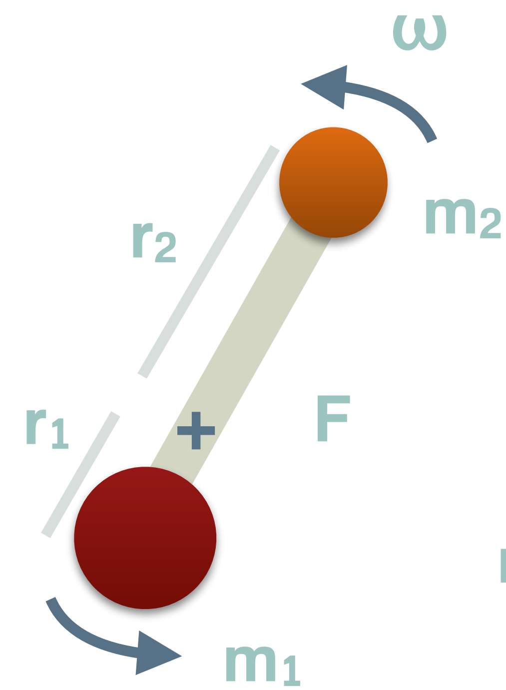
Exercise today

1. find μ



2. find ϕ

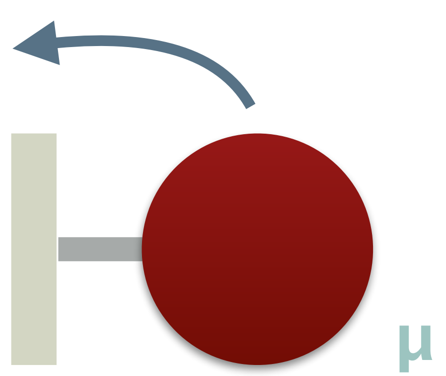
if $$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi$$



$m_1 r_1 \omega_1^2 = F$

Exercise today

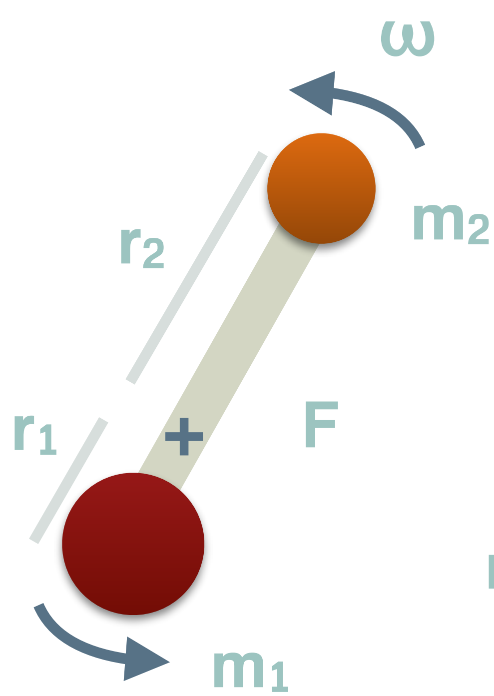
1 find μ



2 find ϕ

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

$\Phi = \exp(-im\phi)$



$m_1 r_1 \omega_1^2 = F$

because $\omega = \omega_1 = \omega_2$

$m_1 r_1 = m_2 r_2$

rigid rotor $r = r_1 + r_2$

$= r_1 + \dfrac{m_1}{m_2} r_2$

$= \dfrac{m_1 + m_2}{m_1} r_2$

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

$\mu r \omega^2 = F$