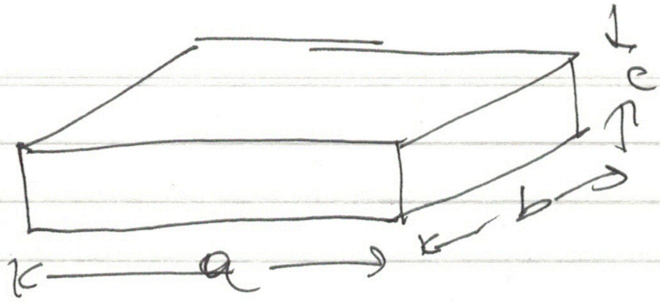


$$E = \frac{\hbar^2}{2m}\left[\left(\frac{n_x \pi}{a}\right)^2 + \left(\frac{n_y \pi}{b}\right)^2 + \left(\frac{n_z \pi}{c}\right)^2\right]$$

$$\Psi(x,y,z) = \text{cte} \times \sin\left[\frac{n_x \pi}{a} x\right] \sin\left[\frac{n_y \pi}{b} y\right] \sin\left[\frac{n_z \pi}{c} z\right]$$

<u>Potenciales con simetría esférica</u>: $V(\vec{r}) = V(|\vec{r}|)$

fuerzas centrales: $\vec{F} = -\vec{\nabla} V(|\vec{r}|)$

p. ej. potencial Coulombiano, gravitacional.

→ conviene re-expresar todo en <u>coords. esféricas</u>

(o) $r^2 = x^2 + y^2 + z^2$

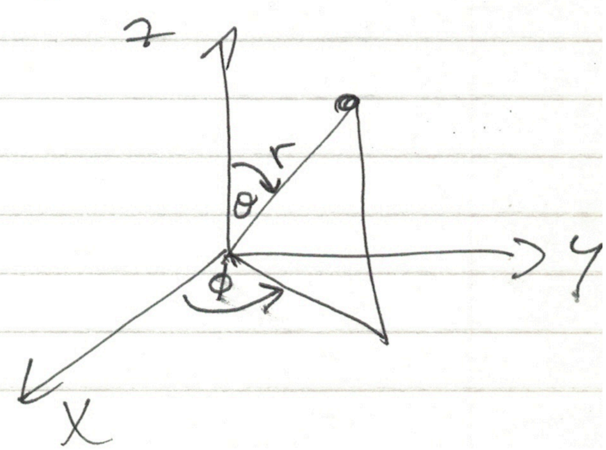
(*) $\cos\theta = \frac{z}{r} = \frac{z}{\sqrt{x^2+y^2+z^2}}$

(*) $\tan\phi = \frac{y}{x}$

$x = r \sin\theta \cos\phi$

$y = r \sin\theta \sin\phi$

$z = r \cos\theta$



objetivo: re-expresar la E. de S. en coords. esféric

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

$$(0) \Rightarrow 2r\frac{\partial r}{\partial x} = 2x \Rightarrow \frac{\partial r}{\partial x} = \frac{x}{r} = \boxed{\sin\theta\cos\phi} \quad (1)$$

$$(*) \Rightarrow -\sin\theta\frac{\partial\theta}{\partial x} = -\frac{1}{2}z(x^2+y^2+z^2)^{-3/2}\cdot 2x = -\frac{z}{r}\cdot\frac{x}{r^2} = -\frac{\cos\theta}{r}\sin\theta\cos\phi$$

$$\Rightarrow \boxed{\frac{\partial\theta}{\partial x} = \frac{1}{r}\cos\theta\cos\phi} \quad (2)$$

$$(*) \Rightarrow (1+\tan^2\phi)\frac{\partial\phi}{\partial x} = \frac{-y}{x^2} = \frac{-y}{x}\cdot\frac{1}{x} = -\tan\phi\cdot\frac{1}{r\sin\theta\cos\phi}$$

$$\frac{1}{\cos^2\phi}\cdot\frac{\partial\phi}{\partial x} = -\frac{\tan\phi}{r\sin\theta\cos\phi} \Rightarrow \frac{\partial\phi}{\partial x} = -\frac{\cos^2\phi\tan\phi}{r\sin\theta\cos\phi} = -\frac{\sin\phi}{r\sin\theta}$$

$$\therefore \boxed{\frac{\partial\phi}{\partial x} = -\frac{1}{r}\frac{\sin\phi}{\sin\theta}}$$

$$\therefore \frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\phi\frac{\partial}{\partial\theta} - \frac{1}{r}\frac{\sin\phi}{\sin\theta}\frac{\partial}{\partial\phi} \quad (3)$$

After "some" algebra:

$$\Rightarrow \nabla^2\Psi = \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\Psi) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2} \quad (4)$$

y la ec. de S. looks like:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi = E\Psi \quad (5)$$

ó $$\nabla^2 \Psi = \frac{2m}{\hbar^2}(V(r)-E)\Psi \qquad (6)$$

tomar $$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi) \qquad (7)$$

$$\frac{Y}{r}\frac{\partial^2}{\partial r^2}(rR) + \frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} = \frac{2m}{\hbar^2}(V(r)-E)RY$$

multip. por $r^2/(RY)$:

$$\underbrace{\frac{r}{R}\frac{\partial^2}{\partial r^2}(rR)}_{\text{sólo dep. de } r} + \frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = \underbrace{\frac{2mr^2}{\hbar^2}(V(r)-E)}_{\text{sólo dep. de } r}$$

$$\therefore \quad \frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = -\alpha \qquad (8)$$

$$\frac{r}{R}\frac{\partial^2}{\partial r^2}(rR) - \frac{2mr^2}{\hbar^2}(V(r)-E) = +\alpha \qquad (9)$$

$Y(\theta,\phi)$ en (8) describe la dependencia angular.

(8) puede escribirse como $\check{\Omega} Y = +\alpha Y$ (8')

Significado físico de $\check{\Omega}$

$$\underset{\substack{\text{energía}\\ \text{cinética}}}{K} = \frac{P_r^2}{2m} + \frac{L^2}{2mr^2}$$, donde $P_r = mv_r = m\,dr/dt$

→ La ec. de S. debería ser de la forma

$$\left[\frac{\check{P}_r^2}{2m} + \frac{\check{L}^2}{2mr^2}\right]u = (E-V)u$$

Comparando, vemos que $\check{P}_r^2 u = \frac{-\hbar^2}{r}\frac{\partial^2}{\partial r^2}(ru)$

y $$\check{L}^2 u = \frac{-\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) - \frac{\hbar^2}{\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2}$$

<u>Ej:</u> a partir de
$$L_x = yP_z - zP_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$L_y = zP_x - xP_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$
$$L_z = xP_y - yP_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

dem. que se obtiene:

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

De aquí se halla $L^2 = \check{L}_x^2 + \check{L}_y^2 + \check{L}_z^2 = \hbar^2\check{\Omega}$

Autovalores de $\check{\Omega}$: $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$

$$\Rightarrow \frac{\Phi}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + \frac{\Theta}{\sin^2\theta}\frac{d^2\Phi}{d\phi^2} = -\alpha\,\Theta\Phi \quad / \sin^2\theta/\Theta\Phi$$

$$\underbrace{\frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)}_{-\alpha - cte} + \underbrace{\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}}_{cte.} = -\alpha\sin^2\theta$$

Imponiendo $\Phi(\phi+2\pi) = \Phi(\phi) \Rightarrow cte = -m^2$, $m \to$ entero

$$\Phi'' = -m^2\Phi \implies \Phi = A e^{im\phi}$$

Notar que $\Phi(\phi)$ es autofunción de $\check{L}_z$:

$$L_z\Phi = -i\hbar\frac{\partial}{\partial\phi}(\Phi(\phi)) = -i\hbar\frac{\partial}{\partial\phi}\left(Ae^{im\phi}\right) = m\hbar\Phi$$

$\Rightarrow$ El resultado de medir L_z es siempre un multiplo <u>entero</u> de $\hbar$.

Por otro lado, $\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = +m^2 - \alpha\sin^2\theta$

$$\Rightarrow \quad \sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + (\alpha\sin^2\theta - m^2)\Theta = 0$$

Se ve complicado. Def: $x = \cos\theta$

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

Resolviendo por medio de una serie en x, se halla que la solución es finita $\forall\, \theta$ $(-1 < x < 1)$ sólo cuando

$$\alpha = l(l+1) \quad \text{donde } l \text{ entero}$$
$$y \quad l \geq |m|$$

$$\Rightarrow \boxed{\check{\Omega} Y = l(l+1) Y} \qquad y \text{ como } \check{L}^2 = \hbar^2 \Omega$$

$$\Rightarrow \boxed{\check{L}^2 Y(\theta,\phi) = \hbar^2 l(l+1) Y(\theta,\phi)} \qquad l = 0,1,2,\ldots$$

Autofunciones de $\check{L}^2$: $Y(\theta,\phi) = \Theta(\theta)\,\Phi(\phi)$

$$\underbrace{Y_{lm}(\theta,\phi)}_{\text{Armónicos esféricos}} = P_l^{|m|}(\cos\theta)\, e^{im\phi} \qquad (|m| \leq l)$$

$P_l^{|m|}$ → Pols. Asociados de Legendre

$$Y_{00} = \sqrt{1/4\pi}$$

$$Y_{11} = -\sqrt{3/8\pi}\,\sin\theta\, e^{i\phi}$$

$$Y_{10} = \sqrt{3/4\pi}\,\cos\theta$$

$$Y_{1,-1} = (3/8\pi)\,\sin\theta\, e^{-i\phi}$$

$$Y_{22} = \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\, e^{2i\phi}$$

$$Y_{21} = -\sqrt{\frac{15}{8\pi}}\,\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_{20} = \sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta - 1)$$

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

$$Y_{2,-2} = \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\, e^{-2i\phi}$$

$$Y_{33} = -\frac{1}{4}\sqrt{\frac{35}{4\pi}}\sin^3\theta\, e^{3i\phi}$$

$$Y_{32} = \frac{1}{4}\sqrt{\frac{105}{2\pi}}\sin^2\theta\cos\theta\, e^{2i\phi}$$

$$Y_{31} = -\frac{1}{4}\sqrt{\frac{21}{4\pi}}\sin\theta\,(5\cos^2\theta - 1)\, e^{i\phi}$$

$$Y_{30} = \sqrt{\frac{7}{4\pi}}\left(\frac{5}{2}\cos^3\theta - \frac{3}{2}\cos\theta\right)$$

$$Y_{l,-m}(\theta,\phi) = (-1)^m\, Y^*_{lm}(\theta,\phi)$$

$$Y_{lm}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\; P_l^m(\cos\theta)\, e^{im\phi} \qquad (1)$$

donde $$P_l^m(x) = (-1)^m (1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l \qquad (2)$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\; Y^*_{l'm'}(\theta,\phi)\, Y_{lm}(\theta,\phi) = \delta_{l'l}\,\delta_{m'm} \qquad (3)$$

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y^*_{lm}(\theta',\phi')\, Y_{lm}(\theta,\phi) = \delta(\phi-\phi')\,\delta(\cos\theta - \cos\theta')$$

$$g(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_{lm}\, Y_{lm}(\theta,\phi)$$

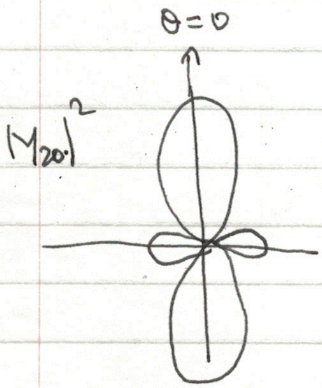
$$\Rightarrow A_{lm} = \int d\Omega\; Y^*_{lm}(\theta,\phi)\, g(\theta,\phi)$$

Notar que $Y_{l,-m} = (-1)^m Y_{lm}^*$

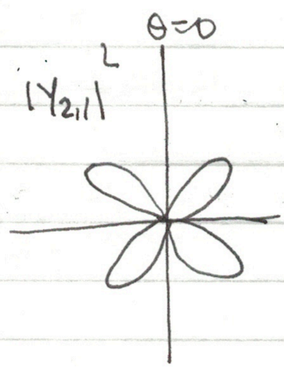
<u>Normalización</u> $\displaystyle\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \, |Y_{lm}(\theta,\phi)|^2 = 1$

$|Y_{lm}(\theta,\phi)|^2$ = densidad de probabilidad para las coords. angulares.

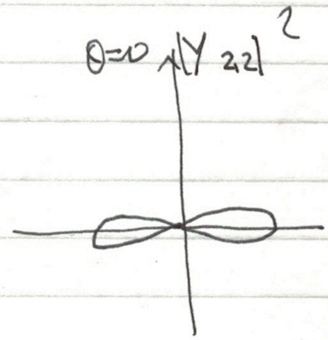
$\Rightarrow \displaystyle\int_{\phi_1}^{\phi_2} d\phi \int_{\theta_1}^{\theta_2} d\theta \, |Y_{lm}|^2 \sin\theta$ = prob. de hallar la partícula en $\phi_1 < \phi < \phi_2$ y $\theta_1 < \theta < \theta_2$



$\frac{5}{16\pi}(3\cos^2\theta - 1)^2$



$\frac{15}{8\pi}\sin^2\theta\cos^2\theta$



$\frac{15}{32\pi}\sin^4\theta$