Eq. de Schrödinger 3D
& Momento Angular (parte 1)

Já vimos isso brevemente antes..

Momento angular

$$\mathbf{L} = \mathbf{r} \times \mathbf{p},$$

$$L_x = y p_z - z p_y, \quad L_y = z p_x - x p_z, \quad L_z = x p_y - y p_x.$$

$$p_x \rightarrow -i\hbar\partial/\partial x, p_y \rightarrow -i\hbar\partial/\partial y, p_z \rightarrow -i\hbar\partial/\partial z.$$

Momento angular

Já vimos isso brevemente antes..

$$\mathbf{L} = \mathbf{r} \times \mathbf{p},$$

$$L_x = yp_z - zp_y, \quad L_y = zp_x - xp_z, \quad L_z = xp_y - yp_x.$$

$$p_x \to -i\hbar\partial/\partial x, p_y \to -i\hbar\partial/\partial y, p_z \to -i\hbar\partial/\partial z.$$

Os operadores L_x e L_y não comutam

$$[L_x, L_y] = [yp_z - zp_y, zp_x - xp_z]$$
$$= [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z].$$

$$[L_x, L_y] = yp_x[p_z, z] + xp_y[z, p_z] = i\hbar(xp_y - yp_x) = i\hbar L_z.$$

$$[L_x, L_y] = i\hbar L_z; \quad [L_y, L_z] = i\hbar L_x; \quad [L_z, L_x] = i\hbar L_y.$$

Spin

A teoria *algébrica* de spin é inspirada na teoria do momento angular orbital, a começar pelas relações de comutação fundamental:

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y.$$

Segue-se que (como antes) os autovetores de S^2 e S_z satisfazem

$$S^2 |sm\rangle = \hbar^2 s(s+1) |sm\rangle; \quad S_z |sm\rangle = \hbar m |sm\rangle;$$

e

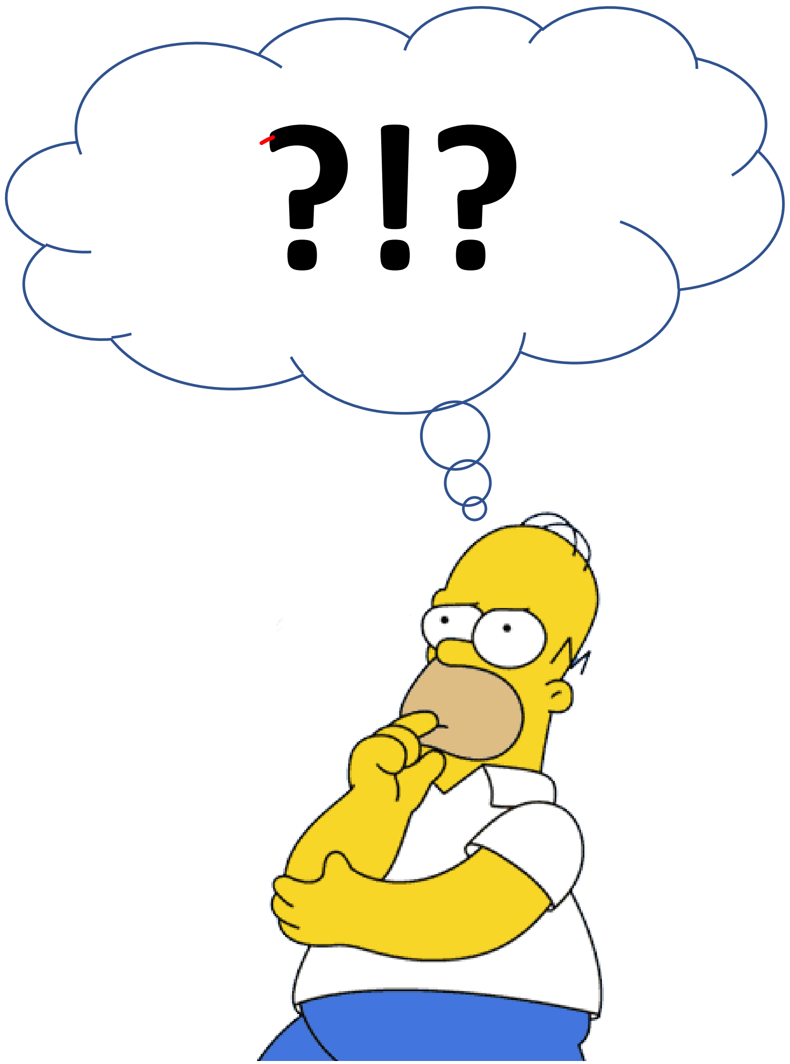
$$S_\pm |sm\rangle = \hbar \sqrt{s(s+1) - m(m \pm 1)}\, |s(m \pm 1)\rangle,$$

$$s = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots; \quad m = -s, -s+1, \ldots, s-1, s.$$

Momento angular

Toda a álgebra do Momento Angular deriva disso(!!)

$$[L_x, L_y] = i\hbar L_z ; \quad [L_y, L_z] = i\hbar L_x ; \quad [L_z, L_x] = i\hbar L_y .$$



Mecânica quântica em três dimensões...

Equação de Schrödinger em 3D

A generalização para três dimensões é simples: $i\hbar\frac{\partial\Psi}{\partial t}=H\Psi;$

pela receita-padrão: $p_x\rightarrow\frac{\hbar}{i}\frac{\partial}{\partial x},\quad p_y\rightarrow\frac{\hbar}{i}\frac{\partial}{\partial y},\quad p_z\rightarrow\frac{\hbar}{i}\frac{\partial}{\partial z},$

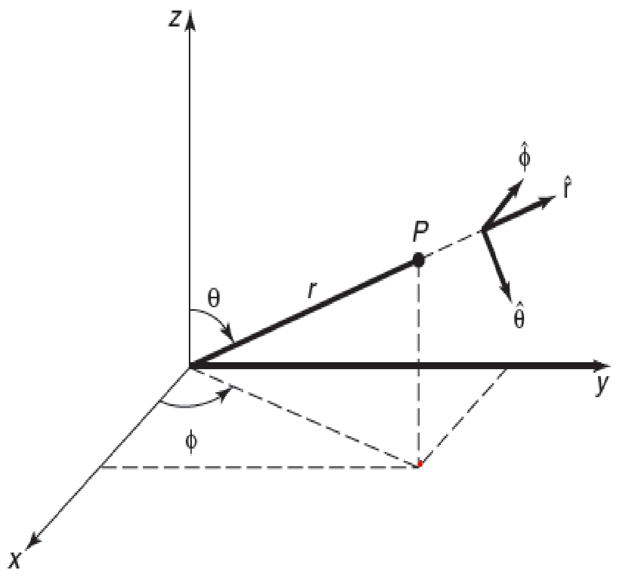
ou $\mathbf{p}\rightarrow\frac{\hbar}{i}\nabla,$. Assim $i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\Psi+V\Psi,$

em que

$$\nabla^2\equiv\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$

é o **Laplaciano**, em coordenadas cartesianas.

Equação de Schrödinger em coordenadas esféricas



Nas **coordenadas esféricas**, o Laplaciano toma a forma de

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \operatorname{sen}\theta}\frac{\partial}{\partial \theta}\left(\operatorname{sen}\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2\operatorname{sen}^2\theta}\left(\frac{\partial^2}{\partial \phi^2}\right).$$

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

Separação de variáveis

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

A equação angular

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

$$\frac{1}{Y}\left\{\frac{1}{\text{sen}\theta}\frac{\partial}{\partial\theta}\left(\text{sen}\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\text{sen}^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\}=-l(l+1)$$

dependência de ψ em θ e ϕ; multiplicando por Y sen^2 θ, torna-se

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

Tentamos a separação de variáveis: $Y(\theta,\phi)=\Theta(\theta)\Phi(\phi).$

Substituindo isso na equação e dividindo-a por $\Theta\Phi$, encontramos:

$$\left\{\frac{1}{\Theta}\left[\text{sen}\theta\frac{d}{d\theta}\left(\text{sen}\theta\frac{d\Theta}{d\theta}\right)\right]+l(l+1)\text{sen}^2\theta\right\}+\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=0.$$

Os primeiros polinômios de Legendre, $P_l(x)$: (a) forma funcional, (b) gráficos.

$P_0 = 1$

$P_1 = x$

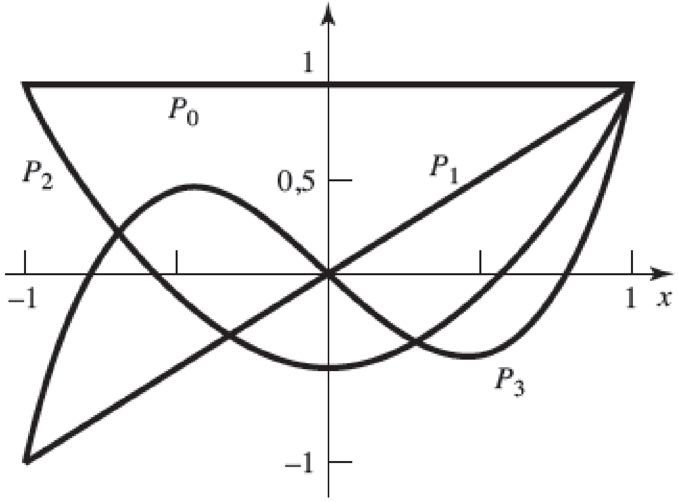
$P_2 = \frac{1}{2}(3x^2 - 1)$

$P_3 = \frac{1}{2}(5x^3 - 3x)$

$P_4 = \frac{1}{8}(35x^4 - 30x^2 + 3)$

$P_5 = \frac{1}{8}(63x^5 - 70x^3 + 15x)$

(a)

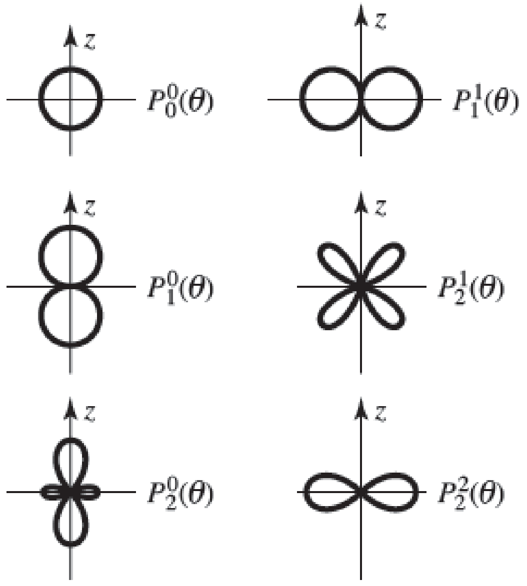


(b)

TABELA 4.2 Algumas funções associadas de Legendre, $P_l^m(\cos\theta)$: (a) forma funcional, (b) gráficos de $r = P_l^m(\cos\theta)$ (nesses gráficos, r diz qual a magnitude da função na direção θ; as figuras deveriam ser rotacionadas sobre o eixo z).

$P_0^0 = 1$	$P_2^0 = \frac{1}{2}(3\cos^2\theta - 1)$
$P_1^1 = \text{sen}\,\theta$	$P_3^3 = 15\,\text{sen}\,\theta(1 - \cos^2\theta)$
$P_1^0 = \cos\theta$	$P_3^2 = 15\,\text{sen}^2\theta\cos\theta$
$P_2^2 = 3\,\text{sen}^2\theta$	$P_3^1 = \frac{3}{2}\,\text{sen}\,\theta(5\cos^2\theta - 1)$
$P_2^1 = 3\,\text{sen}\,\theta\cos\theta$	$P_3^0 = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$

(a)



(b)

a condição de normalização se torna

$$\int |\psi|^2 \, r^2 \text{sen}\theta \, dr \, d\theta \, d\phi = \int |R|^2 \, r^2 \, dr \int |Y|^2 \, \text{sen}\theta \, d\theta \, d\phi = 1.$$

É conveniente que *R* e *Y* sejam normalizados separadamente:

$$\int_0^{\infty} |R|^2 \, r^2 \, dr = 1 \quad e \quad \int_0^{2\pi} \int_0^{\pi} |Y|^2 \, \text{sen}\theta \, d\theta \, d\phi = 1.$$

Harmônicos esféricos:

$$Y_l^m(\theta, \phi) = \epsilon \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} e^{im\phi} P_l^m(\cos\theta),$$

são automaticamente ortogonais, portanto

$$\int_0^{2\pi} \int_0^{\pi} [Y_l^m(\theta, \phi)]^* [Y_{l'}^{m'}(\theta, \phi)] \, \text{sen}\theta \, d\theta \, d\phi = \delta_{ll'} \delta_{mm'}.$$

Os primeiros harmônicos esféricos, $Y_l^m(\theta, \phi)$.

$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$	$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \mathrm{sen}^2\,\theta e^{\pm 2i\phi}$
$Y_1^0 = \left(\frac{3}{4\mathrm{p}}\right)^{1/2} \cos\theta$	$Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$
$Y_1^{\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2} \mathrm{sen}\,\theta e^{\pm i\phi}$	$Y_3^{\pm 1} = \mp\left(\frac{21}{64\pi}\right)^{1/2} \mathrm{sen}\,\theta\,(5\cos^2\theta - 1) e^{\pm i\phi}$
$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$	$Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2} \mathrm{sen}^2\,\theta\cos\theta e^{\pm 2i\phi}$
$Y_2^{\pm 1} = \mp\left(\frac{15}{8\pi}\right)^{1/2} \mathrm{sen}\,\theta\cos\theta e^{\pm i\phi}$	$Y_3^{\pm 3} = \mp\left(\frac{35}{64\pi}\right)^{1/2} \mathrm{sen}^3\,\theta e^{\pm 3i\phi}$

$$L_x = \frac{\hbar}{i}\left(-\mathrm{sen}\,\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right),$$

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

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

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

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

To be continued ...

... até a próxima aula.

Boa semana !!