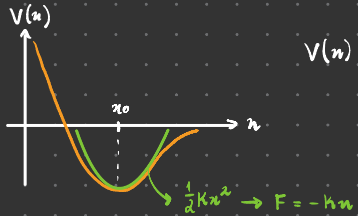
20/11/23

# Oscilador Harmônico




$$V(x) = V(x_0) + \cancel{V'(x_0)(x-x_0)} + \underbrace{\frac{V''(x_0)}{2}}_{>0:\ \text{estável}}(x-x_0)^2 + \cdots$$

Equilíbrio

$$m\ddot{x} = -kx \Rightarrow \ddot{x} + \omega^2 x = 0$$
$$\omega^2 = k/m$$

→ $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$

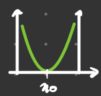
→ $\phi_n = A e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right)$

→ $\phi_n(x) = \langle x|n\rangle, \quad P = |\phi_n|^2$

* Densidade de probabilidade:

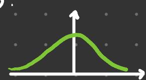
Clássica:

$P \sim \frac{1}{v} \rightarrow$

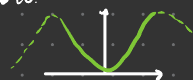



Quântica:

$n \to 0$:



$n \to \infty$:



* Método algébrico: sem representações

→ $H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2$ } Positivo definido: $A^\dagger = A \rightarrow \langle\psi|A|\psi\rangle \geq 0$ | $[X,P] = i\hbar$

→ $H|\phi_n\rangle = E_n|\phi_n\rangle \rightarrow E_n = \langle\phi_n|H|\phi_n\rangle > 0$ (excluindo solução trivial)

↳ $\left\langle\psi\right|\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2\left|\psi\right\rangle$ $\quad m>0, \ \omega^2>0$

↳ $\langle\psi|PP|\psi\rangle = \langle\psi|P^\dagger P|\psi\rangle = \langle\chi|\chi\rangle \geq 0$

→ $a^2 + b^2 = (a-ib)(a+ib)$

$P^2 + X^2 = (P-iX)(P+iX) = P^2 - iPX + iXP + X^2 = P^2 + X^2 + i\overbrace{[X,P]}^{i\hbar} = P^2 + X^2 - \hbar$ → H é fatorável

→ $H = A^\dagger A + cI, \quad A = \text{cte}\cdot\hat{a}$

↳ $\hat{a} \equiv \frac{1}{\sqrt{2\hbar m\omega}}(m\omega X + iP)$ ↳ $\hat{a}^\dagger \equiv (\hat{a})^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega X - iP)$

$$\hat{a}^\dagger\hat{a} = \frac{1}{2\hbar m\omega}(m\omega X - iP)(m\omega X + iP) = \frac{1}{2\hbar m\omega}\left(m^2\omega^2X^2 + im\omega XP - im\omega PX + P^2\right)$$
$$= \frac{1}{2\hbar m\omega}\left(m^2\omega^2X^2 + P^2 + i\hbar m\omega\underbrace{[X,P]}_{i\hbar}\right) = \frac{1}{2\hbar m\omega}\left(m^2\omega^2X^2 + P^2 - m\omega\hbar\right)$$
$$= \frac{1}{2}\frac{m\omega}{\hbar}X^2 + \frac{P^2}{2\hbar m\omega} - \frac{1}{2} = \frac{1}{\hbar\omega}\left(\frac{1}{2}m\omega^2X^2 + \frac{P^2}{2m}\right) - \frac{1}{2}$$

$\boxed{H = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)}$ $\quad N \equiv \hat{a}^\dagger\hat{a} \Rightarrow$ $\boxed{H = \hbar\omega\left(N + \frac{1}{2}\right)}$

$$\rightarrow [\hat{a}, \hat{a}^\dagger] = \frac{1}{2\hbar\omega m}\left[m\omega X + iP,\ m\omega X - iP\right] = \frac{1}{2\hbar m\omega}\left([m\omega X,\ m\omega X - iP] + i[P,\ m\omega X - iP]\right)$$

$$= \frac{1}{2\hbar\omega m}\left(m\omega(-i)i\hbar + im\omega(-i\hbar)\right) = 1$$

$$\rightarrow \begin{cases} H = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) = \hbar\omega\left(N + \frac{1}{2}\right) \\ [\hat{a}, \hat{a}^\dagger] = 1 \end{cases}$$

$\rightarrow N^\dagger = (\hat{a}^\dagger\hat{a})^\dagger = \hat{a}^\dagger\hat{a} \rightarrow N = N^\dagger$

$N|n\rangle = n|n\rangle \Rightarrow n \in \mathbb{R}$ pois $N^\dagger = N$ e $n \geq 0$ pois $N$ é positivo definido

$$\rightarrow H|n\rangle = \hbar\omega\left(N + \tfrac{1}{2}\right)|n\rangle = E_n|n\rangle \Rightarrow \hbar\omega\left(n + \tfrac{1}{2}\right)|n\rangle = E_n|n\rangle \Rightarrow \boxed{E_n = \hbar\omega\left(n + \tfrac{1}{2}\right)}$$

$\rightarrow n \in \mathbb{R}^+ \rightarrow n \in \mathbb{N}$? $\quad \langle n'|n\rangle = \delta_{nn'}$

$$aa^\dagger a|n\rangle = na|n\rangle \Rightarrow (I + a^\dagger a)a|n\rangle = na|n\rangle$$

$aa^\dagger - a^\dagger a = I$

$aa^\dagger = I + a^\dagger a$

$$a|n\rangle + (a^\dagger a)a|n\rangle = n\,a|n\rangle$$

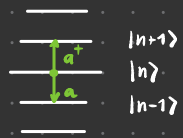
$$N(a|n\rangle) = (n-1)(a|n\rangle)$$

$$a^\dagger a^\dagger a|n\rangle = na^\dagger|n\rangle \Rightarrow a^\dagger(aa^\dagger - 1)|n\rangle = na^\dagger|n\rangle$$

$$-a^\dagger|n\rangle + (a^\dagger a)a^\dagger|n\rangle = na^\dagger|n\rangle$$

$$N(a|n\rangle) = (n+1)(a^\dagger|n\rangle)$$

$$\boxed{\begin{aligned} a|n\rangle &= c|n-1\rangle \\ a^\dagger|n\rangle &= d|n+1\rangle \end{aligned}}$$




Operador escada

$$\rightarrow \langle n|N|n\rangle = n\overbrace{\langle n|n\rangle}^{1} = n$$

$$\langle n|a^\dagger a|n\rangle = n \Rightarrow \langle n-1|c^* c|n-1\rangle = |c|^2\overbrace{\langle n-1|n-1\rangle}^{n} = n$$

$$c \in \mathbb{R} \rightarrow c = \sqrt{n}$$

$$\langle n|aa^\dagger|n\rangle = \langle n|I + a^\dagger a|n\rangle = (n+1)\langle n|n\rangle = n+1$$

$$= \langle n+1|d^* d|n+1\rangle = |d^2|\langle n+1|n+1\rangle = n+1 \rightarrow d \in \mathbb{R} \rightarrow d = \sqrt{n+1}$$

$\rightarrow n = 0, 1, 2, \ldots \longrightarrow a|0\rangle = 0$ Ground state $\quad |0\rangle \neq 0 \quad$ $a^\dagger|0\rangle = |1\rangle$, $a^\dagger|1\rangle = \sqrt{2}|2\rangle$, $\vdots$

$$\boxed{|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle} \qquad \boxed{\begin{aligned} a|n\rangle &= \sqrt{n}\,|n-1\rangle \\ a^\dagger|n\rangle &= \sqrt{n+1}\,|n+1\rangle \end{aligned}}$$

* Solução:

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right)$$

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle, \quad \hat{a}|0\rangle = 0$$

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega X + iP)$$

$$\hat{a}^\dagger = (\hat{a})^\dagger$$

* Representação $|x\rangle$:

$$\langle x|a|0\rangle = 0$$

$$\langle x|m\omega X + iP|0\rangle = 0$$

$$m\omega\underbrace{\langle x|X|0\rangle}_{x\phi_0(x)} + i\underbrace{\langle x|P|0\rangle}_{-i\hbar\frac{\partial}{\partial x}\phi_0(x)} = 0$$

$$m\omega x\phi_0(x) + \hbar\frac{d}{dx}\phi_0(x)$$

$$\frac{d}{dx}\phi_0(x) = -\frac{m\omega x}{\hbar}\phi_0(x)$$

$$\phi_0(x) = Ae^{-\frac{m\omega}{2\hbar}x^2}$$

$$|1\rangle = a^\dagger|0\rangle$$

$$\langle x|1\rangle = \langle x|a^\dagger|0\rangle$$

$$\phi_1(x) = \frac{1}{\sqrt{2\hbar m\omega}}\langle x|m\omega X - iP|0\rangle$$

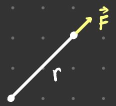
$$= \frac{1}{\sqrt{2\hbar m\omega}}\left(m\omega x\phi_0(x) - \hbar\frac{d}{dx}\phi_0(x)\right)$$

$$= \frac{1}{\sqrt{2\hbar m\omega}}\left(2m\omega x\phi_0(x)\right)$$

$$\phi_1(x) = 2\sqrt{\frac{m\omega}{\hbar}}\,x\,\phi_0(x)$$

$$\begin{cases} H_0(\xi) = I \\ H_1(\xi) = 2\xi \end{cases}$$

# Soluções da Eq. Schrödinger independente do tempo em 3D para potenciais centrais



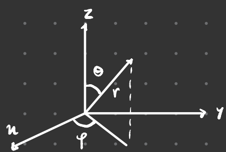

→ $V = V(r)$
→ $\vec{F} \parallel \vec{r}$
→ $\vec{r} \times \vec{F} = 0$
→ Conservação da energia e do momento angular

* Potencial central: simétrico em relação a rotações

→ $H|\psi\rangle = E|\psi\rangle$

→ $H = \dfrac{P^2}{2M} + V(R)$ $\begin{cases} \vec{R} = X\hat{i} + Y\hat{j} + Z\hat{k} \\ \vec{P} = P_x\hat{i} + P_y\hat{j} + P_z\hat{k} \end{cases}$

$x = r\,\text{sen}\,\theta \cos\varphi \qquad 0 \leq \theta \leq \pi$
$y = r\,\text{sen}\,\theta\,\text{sen}\,\varphi \qquad 0 \leq \varphi \leq 2\pi$
$z = r\cos\theta \qquad 0 < r < \infty$




→ $\langle \vec{r}|H|\psi\rangle = E\langle \vec{r}|\psi\rangle$

→ $\begin{cases} -\dfrac{\hbar^2}{2M}\nabla^2\psi(\vec{r}) + V(r)\psi(\vec{r}) = E\psi(\vec{r}) \\ \text{c.c.} \end{cases}$

$r = \sqrt{x^2+y^2+z^2}$

$\theta = \text{arctg}\left(\dfrac{z}{\sqrt{x^2+y^2}}\right) \quad \Big| \quad \varphi = \text{arctg}\left(\dfrac{y}{x}\right)$

→ $\nabla^2\psi = \dfrac{1}{r^2}\dfrac{\partial}{\partial r}\left(r^2\dfrac{\partial\psi}{\partial r}\right) + \dfrac{1}{r^2\,\text{sen}\,\theta}\dfrac{\partial}{\partial\theta}\left(\text{sen}\,\theta\dfrac{\partial\psi}{\partial\theta}\right) + \dfrac{1}{r^2\,\text{sen}^2\theta}\dfrac{\partial^2\psi}{\partial\varphi^2}$

$d^3r = dx\,dy\,dz = r^2 dr\,\text{sen}\,\theta\,d\theta\,d\varphi$

→ Separação de variáveis: $\psi(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi)$

$$\frac{1}{R}\left[\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\right] - \frac{2Mr^2}{\hbar^2}\left[V(r)-E\right] = -\frac{1}{Y}\left[\frac{1}{\text{sen}\,\theta}\frac{\partial}{\partial\theta}\,\text{sen}\,\theta\frac{\partial Y}{\partial\theta} + \frac{1}{\text{sen}^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right] = \ell(\ell+1)$$

↳ $\dfrac{d}{dr}\left(r^2\dfrac{dR}{dr}\right) - \dfrac{2Mr^2}{\hbar^2}\left[V(r)-E\right]R = \ell(\ell+1)R \qquad (1)$

↳ $\text{sen}\,\theta\dfrac{\partial}{\partial\theta}\left(\text{sen}\,\theta\dfrac{\partial Y}{\partial\theta}\right) + \dfrac{\partial^2 Y}{\partial\varphi^2} = -\ell(\ell+1)\,\text{sen}^2\theta\,Y \qquad (2)$

$Y(\theta,\varphi) = F(\theta)\,G(\varphi)$

$\begin{cases} \text{sen}\,\theta\dfrac{d}{d\theta}\left(\text{sen}\,\theta\dfrac{dF}{d\theta}\right) + \ell(\ell+1)\,\text{sen}^2\theta\,F = m^2F \qquad (2a) \\ \dfrac{d^2G}{d\varphi^2} = -m^2G \qquad (2b) \quad \rightarrow G(\varphi+2\pi) = G(\varphi) \end{cases}$

↳ Resolvendo (2b):

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

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

$\displaystyle\int_{-1}^{1} dx\,P_\ell(x)\,P_{\ell'}(x) = \frac{2}{(2\ell+1)}\delta_{\ell\ell'}$

$\left.\begin{array}{l} G(\varphi) = e^{im\varphi} \\ G(\varphi+2\pi) = e^{im\varphi}e^{im2\pi} \end{array}\right\} e^{im2\pi} = 1 \rightarrow m = 0, \pm1, \pm2, \ldots$

polinômios associados de Legendre

↳ Resolvendo (2a): $x = \cos\theta$ → Legendre $\begin{cases} \text{regular} \rightarrow \ell = 0, 1, 2, \ldots,\ m = -\ell, \ldots, \ell \rightarrow F(\theta) = P_\ell^{|m|}(\cos\theta) \\ \text{não regular} \end{cases}$

Harmônicos Esféricos: $\boxed{Y_\ell^m(\theta,\varphi) = A\,P_\ell^{|m|}(\cos\theta)\,e^{im\varphi}}$ $\quad \ell = 0, 1, 2, \ldots \quad |m| \leq \ell$

↳ ortonormal: $A = \varepsilon\sqrt{\dfrac{(2\ell+1)}{4\pi}\dfrac{(\ell-|m|)!}{(\ell+|m|)!}}$, $\varepsilon = \begin{cases} (-1)^m, & m \geq 0 \\ 1, & m < 0 \end{cases}$

$$\int_0^{2\pi}\int_0^{\pi} \underbrace{\text{sen}\,\theta\,d\theta\,d\varphi}_{d\Omega}\; Y_\ell^{m\,*}(\theta,\varphi)\,Y_{\ell'}^{m'}(\theta,\varphi) = \delta_{\ell\ell'}\delta_{mm'} \rightarrow \int d\Omega\; Y_\ell^{m\,*}(\Omega)\,Y_{\ell'}^{m'}(\Omega) = \delta_{\ell\ell'}\delta_{mm'}$$

# * Propriedades dos Harmônicos Esféricos:

1) Ortonormais: $\int d\Omega \, Y_\ell^{m*}(\Omega)\, Y_{\ell'}^{m'}(\Omega) = \delta_{\ell\ell'}\delta_{mm'}$

2) Base $g(\theta,\varphi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_{\ell m} Y_\ell^m(\theta,\varphi)$

↳ Clausura: $\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\Omega)\, Y_\ell^m(\Omega') = \delta(\Omega-\Omega')$

3) Conjugação complexa: $\left(Y_\ell^m(\theta,\varphi)\right)^* = Y_\ell^{-m}(\theta,\varphi)\,(-1)^m$

4) Paridade: $\Omega \to -\Omega$

$(\theta,\varphi) \to (\pi-\theta,\ \varphi+\pi)$

$Y_\ell^m(-\Omega) = (-1)^\ell\, Y_\ell^m(\Omega)$

5) Teorema da adição: $P_\ell(\cos\alpha) = \frac{4\pi}{(2\ell+1)} \sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\Omega)\, Y_\ell^m(\Omega')$


6) Momento angular: $\vec{L} = \vec{R}\times\vec{P}$

↳ $L_x = Y P_z - Z P_y$

↳ $L_y = Z P_x - X P_z$

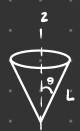
↳ $L_z = X P_y - Y P_x$

$\left.\begin{matrix}[X, P_x] \\ [Y, P_y] \\ [Z, P_z]\end{matrix}\right\} = i\hbar \rightarrow$ $[L_x, L_y] = i\hbar L_z$, $[L_z, L_x] = i\hbar L_y$, $[L_y, L_z] = i\hbar L_x$

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

$[L^2, L_i] = 0, \quad i = x, y, z$

$\{L_z, L^2\}$




$|x, y, z\rangle$

$|p_x, p_y, p_z\rangle$

$|L_x, \cancel{L_y}, L_z\rangle$

→ Representar em posição: $L_z = X P_y - Y P_x$

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

$\vec{P} \to -i\hbar\left(\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}\right)$

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

$$L_z Y_\ell^m(\Omega) = -i\hbar\frac{\partial}{\partial\varphi}\left[A P_\ell^{|m|}(\cos\theta)\, e^{im\varphi}\right] = \hbar m Y_\ell^m \rightarrow L_z Y_\ell^m(\Omega) = \overbrace{\hbar m}^{\text{autovalores de } L_z} Y_\ell^m(\Omega)$$

$m = 0, \pm 1, \pm 2, \dots \rightarrow 0, \pm\hbar m, \pm 2\hbar m, \dots$

$$L^2 = -\hbar^2\left[\frac{1}{\operatorname{sen}\theta}\frac{\partial}{\partial\theta}\left(\operatorname{sen}\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\operatorname{sen}^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \overset{(2a)}{=} \hbar^2\ell(\ell+1)\, Y_\ell^m(\Omega) \rightarrow L^2 Y_\ell^m(\Omega) = \overbrace{\hbar^2\ell(\ell+1)}^{\text{autovalores de } L^2} Y_\ell^m(\theta,\varphi)$$

$\ell = 0, 1, \dots$

$\rightarrow 0, 2\hbar^2, 6\hbar^2, \dots$

$\rightarrow 0, \sqrt{2}\hbar, \sqrt{6}\hbar, \dots$

$|\ell\, m\rangle$ ($m \to L_z$, $\ell \to L^2$)

$\begin{cases} m \rightarrow \text{projeção do momento angular} \\ \ell \rightarrow \text{módulo do momento angular} \end{cases}$

* C.C.O.C.: $\{H, L^2, L_z\} \rightarrow \{|k\,\ell\, m\rangle\}$

* 29/11/23

→ Equação radial: $\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2Mr^2}{\hbar^2}\left[V(R) - E\right]R = \ell(\ell+1)R$

$\langle \vec{r}|k\ell m\rangle = \frac{\mu_{k\ell}(r)}{r} Y_\ell^m(\theta,\varphi)$

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

$r^2\frac{dR}{dr} = r\frac{du}{dr} - u$

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

$$\rightarrow r\frac{d^2u}{dr^2} - \frac{2Mr^2}{\hbar^2}\left[V(r) - E\right]\frac{u}{r} = \ell(\ell+1)\frac{u}{r} \Rightarrow -\frac{\hbar^2}{2M}\frac{d^2\mu}{dr^2} + \left[\underbrace{V(r) + \frac{\hbar^2\ell(\ell+1)}{2Mr^2}}_{V_{eff}(r)}\right]\mu(r) = E\mu(r)$$

$$\left\{ \begin{array}{l} \boxed{-\frac{\hbar^2}{2M}\frac{d^2\mu_{k\ell}}{dr^2} + V_{eff}(r)\,\mu_{k\ell} = E_{k\ell}\,\mu_{k\ell}} \\ \mu_{k\ell}(0) = 0, \quad r \in [0,\infty] \end{array} \right.$$

$E \rightarrow k$

$$\rightarrow \int |\psi|^2 d^3r = 1 \rightarrow \int |R(r)|^2 |Y_\ell^m(\theta,\varphi)|^2 r^2 dr \underbrace{\operatorname{sen}\theta\, d\theta\, d\varphi}_{d\Omega} = 1$$

$$\hookrightarrow \int_0^\infty |R(r)|^2 r^2 dr = 1 \rightarrow \int_0^\infty |\mu(r)|^2 dr = 1$$

$$\hookrightarrow \int d\Omega\, |Y_\ell^m(\theta,\varphi)|^2 = 1 \rightarrow Y_\ell^{m*}(\Omega)\, Y_\ell^m(\Omega) = \delta_{mm}\delta_{\ell\ell} = 1$$

| Polinômios ortogonais | Peso | Intervalo |
|---|---|---|
| Legendre | $\operatorname{sen}\theta$ | $[-1, 1]$ |
| Hermite | gaussiana | $(-\infty, \infty)$ |
| Laguerre | exponencial | $[0, \infty)$ |

* Exemplos
- i) Átomo de Hidrogênio: $V(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$
- ii) Oscilador harmônico isotrópico: $V(r) = \frac{1}{2}m\omega^2 r^2$
- iii) Partícula livre: $V(r) = 0$

## i) Átomo de H

$$\begin{cases} -\frac{\hbar^2}{2M}\frac{d^2\mu}{dr^2} + \left(-\frac{e^2}{4\pi\varepsilon_0 r} + \frac{\hbar^2 \ell(\ell+1)}{2Mr^2}\right)\mu = E\mu \\ \mu(0)=0 \\ \mu(r\to\infty)\to 0 \quad \text{(estados ligados)} \end{cases}$$

↳ "mais rápido" que $\frac{1}{r}$

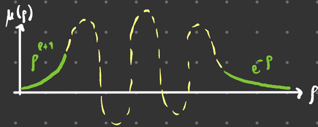
$$\alpha \equiv \sqrt{\frac{-2ME}{\hbar^2}}, \quad \alpha \in \mathbb{R} \rightarrow E = -\frac{\hbar^2}{2M}\alpha^2$$

$$\rho \equiv \alpha r, \quad \rho_0 = \frac{Me^2}{2\pi\varepsilon_0 \hbar^2 \alpha}$$

$$\therefore \boxed{\frac{d^2\mu}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right]\mu}$$

→ Assintótico: $\rho \to \infty \rightarrow \frac{d^2\mu}{d\rho^2} = \mu \; \Big\{ \mu = e^{-\rho}$ ou $\cancel{\mu = e^{\rho}}$

→ Na origem: $\rho \to 0 \rightarrow \frac{d^2\mu}{d\rho^2} = \frac{\ell(\ell+1)}{\rho^2}\mu \; \Big\{ \mu = \rho^{\ell+1}$ ou $\cancel{\mu = \rho^{-\ell}}$




$$\therefore \boxed{\mu(\rho) = \rho^{\ell+1} e^{-\rho} v(\rho)}$$

$$\rightarrow \rho \frac{d^2 v}{d\rho^2} + 2(\ell+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(\ell+1)]v = 0$$

↳ $v(\rho) = c_0 + c_1\rho + c_2\rho^2 + \dots = \sum_{j=0}^{\infty} c_j \rho^j$

↳ $\sum_j [\dots]\rho^j = 0 \Rightarrow [\dots] = 0 \Rightarrow c_{j+1}(j+1)(j+2\ell+2) - (2(j+\ell+1) - \rho_0)c_j = 0 \Rightarrow c_{j+1} = \frac{2(j+\ell+1) - \rho_0}{(j+1)(j+2\ell+2)} c_j$

↳ $j \gg 1$: $c_{j+1} = \frac{2j}{j^2} c_j = \frac{2}{j+1} c_j \rightarrow c_{j+1} = \frac{2}{(j+1)} \cdot \frac{2}{j} \cdot \frac{2}{j-1} = \frac{2^{j+1}}{(j+1)!} \rightarrow v(\rho) \rightarrow \sum_j \frac{2^j}{j!}\rho^j = \sum_j \frac{(2\rho)^j}{j!} = \cancel{e^{2\rho}}$

⇒ a série tem uma potência máxima $j_{max}$ (grau do polinômio) → $c_{j_{max}+1} = 0$

↳ $2(j_{max} + \ell + 1) - \rho_0 = 0 \rightarrow \rho_0 = 2\underbrace{(j_{max} + \ell + 1)}_{n}$

$n$: nº quântico principal → $n = 1, 2, \dots$

↳ $\rho_0 = 2n \Rightarrow \rho_0^2 = 4n^2 \Rightarrow \frac{M^2 e^4}{4\pi^2\varepsilon_0^2\hbar^4\alpha^2} = 4n^2 \Rightarrow -\left(\frac{M^2e^4}{4\pi^2\varepsilon_0^2\hbar^4}\right)\frac{\hbar^2}{2ME} = 4n^2 \Rightarrow \boxed{E_n = -\frac{Me^4}{32\pi^2\varepsilon_0^2\hbar^2}\frac{1}{n^2}} = -\frac{13.6\text{ eV}}{n^2}$

$g_n(E_n) = n^2 \times \underbrace{2}_{\text{spin}}$

## * Números quânticos

$\overset{K\;L\;M}{n = 1, 2, 3, \dots}$ → camada

$n = j_{max} + \ell + 1 \rightarrow \ell = n - j_{max} - 1 = \underset{s\;p\;d}{0, 1, 2, \dots} \quad \begin{cases} j_{max} = 0 \Rightarrow \ell_{max} = n-1 \\ j_{max} = n-1 \Rightarrow \ell_{min} = 0 \end{cases}$

K: $n=1$, $\ell=0 \rightarrow \mu = c_0 \rho e^{-\rho}$

L: $n=2$, $\ell = 0, 1 \rightarrow \mu = \rho e^{-\rho}(c_0 + c_1\rho)$

$$\boxed{\phi_{n\ell m}(r,\theta,\varphi) = \frac{\mu_{n\ell}(r)}{r} Y_\ell^m(\theta,\varphi) = R_{n\ell}(r) Y_\ell^m(\theta,\varphi)}$$

$$\phi_{n\ell m}(r,\theta,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}} \left(\frac{2r}{na_0}\right)^\ell L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right) e^{-\frac{r}{na_0}} Y_\ell^m(\theta,\varphi)$$

#01/12/23

$\rightarrow \{H, L^2, L_z\} \rightarrow |k\ell m\rangle \begin{cases} H|k\ell m\rangle = E_{k\ell}|k\ell m\rangle \\ L^2|k\ell m\rangle = \hbar^2 \ell(\ell+1)|k\ell m\rangle \\ L_z|k\ell m\rangle = m\hbar|k\ell m\rangle \end{cases}$

## i) Átomo de Hidrogênio:

$V(r) = -\dfrac{e^2}{4\pi\varepsilon_0 r}$ | $u_{k\ell}(r) = \rho^{\ell+1} e^{-\rho} v(\rho)$ $\begin{cases} \rho = \alpha r, \quad \alpha = \frac{1}{\hbar}\sqrt{-2ME_{k\ell}} \rightarrow E_{k\ell} = -\frac{\hbar^2\alpha^2}{2M} \\ v(\rho) \rightarrow \text{polinômio associado de Laguerre de grau máximo } g_{max} \end{cases}$

$$E_{j_{max}\ell} = -\frac{13{,}6\,eV}{(j_{max}+\ell+1)^2} \rightarrow E_n = -\frac{13{,}6\,eV}{n^2}$$

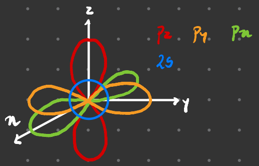
$\begin{cases} n = 1, 2, 3, \dots \\ \ell = 0, 1, \cdots n-1 \\ m = -\ell, \dots, \ell \end{cases}$ $\quad K, L, M, \dots \quad s, p, f, d, \dots \quad \rightarrow g_n = \sum_{\ell=0}^{n-1} (2\ell+1) = n^2$

$$\underbrace{p_{\substack{x \\ y}} = -\frac{(Y_1^1 \mp Y_1^{-1})}{\sqrt{2}} \qquad p_z \rightarrow Y_1^0}$$

$p_x = \sqrt{\frac{3}{4\pi}}\,\text{sen}\,\theta\cos\varphi = \sqrt{\frac{3}{4\pi}}\,\frac{x}{r}$

$p_y = \sqrt{\frac{3}{4\pi}}\,\text{sen}\,\theta\,\text{sen}\,\varphi = \sqrt{\frac{3}{4\pi}}\,\frac{y}{r}$

$p_z = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\,\frac{z}{r}$




$\rightarrow$ Densidade de probabilidade $\begin{cases} |\phi|^2(r,\theta,\varphi) \rightarrow 1/m^3 \\ r^2|R(r)|^2 \rightarrow 1/m \end{cases}$

$\rightarrow$ Hibridização: $\psi = \alpha Y_0^0 + \beta Y_1^{-1} + \gamma Y_1^0 + \delta Y_1^1$

## ii) Oscilador Harmônico Isotrópico

$\rightarrow H = -\dfrac{\hbar^2}{2M}\nabla^2 + \dfrac{1}{2}\mu\omega^2 r^2$

$\rightarrow \phi_{k\ell m}(r,\theta,\varphi) = \dfrac{\mu_{k\ell}(r)}{r} Y_\ell^m(\theta,\varphi)$

$-\dfrac{\hbar^2}{2M}\dfrac{d^2}{dr^2}\mu_{k\ell} + \left(\dfrac{1}{2}M\omega^2 r^2 + \dfrac{\hbar^2 \ell(\ell+1)}{2Mr^2}\right)\mu_{k\ell} = E_{k\ell}\mu_{k\ell}$

$\mu_{k\ell}(r\to\infty) \to 0$

$\mu_{k\ell}(0) = 0$

$\rightarrow r \to \xi$: $\mu_{k\ell}(\xi) = e^{-\frac{\xi^2}{2}} V(\xi)$

$\rightarrow E_{k\ell} = \hbar\omega(\overbrace{k+\ell}^{n} + \frac{3}{2})$ $\begin{cases} k = 0, 2, 4, \dots & \text{grau do polinômio} \\ \ell = 0, 1, 2, 3, \dots \end{cases}$ $\Rightarrow \boxed{E_n = \hbar\omega\left(n + \frac{3}{2}\right)}$

$\mu_{k\ell} \rightarrow$ tabelados

### → Degenerescência:

* $n = 0$: GS $\rightarrow E_0 = \frac{3}{2}\hbar\omega$
  $k=0, \ell=0 \rightarrow g_0 = 0$
* $n = 1 \rightarrow E_1 = \frac{5}{2}\hbar\omega$
  $k=0, \ell=1 \rightarrow m = -1, 0, 1 \rightarrow g_1 = 3$
* $n = 2 \rightarrow E_2 = \frac{7}{2}\hbar\omega$
  $k=2, \ell=0 \rightarrow 1$ | $k=0, \ell=2 \rightarrow 5 \rightarrow g_2 = 6$

### → Em coordenadas cartesianas:

$\rightarrow H = \left(-\dfrac{\hbar^2}{2M}\dfrac{\partial^2}{\partial x^2} + \dfrac{1}{2}m\omega^2 x^2\right) + \left(-\dfrac{\hbar^2}{2M}\dfrac{\partial^2}{\partial y^2} + \dfrac{1}{2}m\omega^2 y^2\right) + \left(-\dfrac{\hbar^2}{2M}\dfrac{\partial^2}{\partial z^2} + \dfrac{1}{2}m\omega^2 z^2\right) = H_x + H_y + H_z$

$\left.\begin{array}{l} \rightarrow \psi(x,y,z) = f(x)g(y)h(z) \\ \rightarrow E = E_x + E_y + E_z \end{array}\right\} \psi(x,y,z) = f_{n_x}(x) f_{n_y}(y) f_{n_z}(z) \rightarrow E_{n_i} = \hbar\omega\left(n_i + \frac{1}{2}\right), \quad i = x, y, z$

$$\boxed{E_{n_x n_y n_z} = \hbar\omega\left(\underbrace{n_x + n_y + n_z}_{\equiv n} + \frac{3}{2}\right)}$$

$\rightarrow \psi_{n_x n_y n_z}(x,y,z) = A_{n_x} H_{n_x}(\xi_x) e^{-\frac{\xi_x^2}{2}} A_{n_y} H_{n_y}(\xi_y) e^{-\frac{\xi_y^2}{2}} A_{n_z} H_{n_z} e^{-\frac{\xi_z^2}{2}}$

$$\therefore \boxed{\psi(x,y,z) = A_{n_x} A_{n_y} A_{n_z} H_{n_x}(\xi_x) H_{n_y}(\xi_y) H_{n_z}(\xi_z) e^{-\frac{m\omega}{2\hbar} r^2}}$$

* $|k\ell m\rangle \neq |n_x n_y n_z\rangle \rightarrow$ combinação linear $\rightarrow$ bases diferentes para o mesmo subespaço

$|k\ell m\rangle \downarrow \{H, L^2, L_z\}$ $\quad |n_x n_y n_z\rangle \downarrow \{H_x, H_y, H_z\}$

* 04/12/23

## iii) Partícula livre

$\rightarrow V = 0$

$\rightarrow \phi_{k\ell m}(r,\theta,\varphi) = R_{n\ell}(r)\, Y_\ell^m(\theta,\varphi) = \dfrac{u_{k\ell}}{r}\, Y_\ell^m(\theta,\varphi)$

$$\rightarrow \begin{cases} -\dfrac{\hbar^2}{2M}\dfrac{d^2}{dr^2}\mu(r) + \dfrac{\hbar^2 \ell(\ell+1)}{2\mu r^2}\mu(r) = E\mu(r) \\ \mu(0) = 0 \end{cases} \longrightarrow \mu(r) = A r \underbrace{j_\ell(kr)}_{\text{Esférica de Bessel}} + B r \underbrace{\eta_\ell(kr)}_{\text{Esférica de Neumann}}$$

$$\rightarrow x \to 0: \begin{cases} j_\ell(x) \sim x^\ell \ ✓ \\ \eta_\ell(x) \sim \dfrac{1}{x^{\ell+1}} \ ✗ \end{cases} \Rightarrow \boxed{\mu_{k\ell}(r) = r\, j_\ell(kr)} \quad \boxed{R_{k\ell}(r) = j_\ell(kr)}$$

$$\rightarrow j_\ell(x) = [\dots]\frac{\operatorname{sen} x}{x} + [\dots]\frac{\cos x}{x}$$

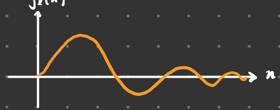
↳ polinômio de grau $\ell^{-1}$ em $x$

↳ polinômio de grau $\ell$ em $x^{-1}$

$$j_0(x) = \frac{\operatorname{sen} x}{x}$$

$$j_1(x) = \frac{\operatorname{sen} x}{x^2} - \frac{\cos x}{x}$$

$$\rightarrow x \to \infty: \begin{cases} j_\ell(x) \to \dfrac{1}{x}\operatorname{sen}\left(x - \dfrac{\ell\pi}{2}\right) \\ \eta_\ell(x) \to \dfrac{1}{x}\cos\left(x - \dfrac{\ell\pi}{2}\right) \end{cases}$$




$$\rightarrow \{H, L^2, L_z\}: |k\ell m\rangle \rightarrow \boxed{\phi_{k\ell m}(\vec{r}) = j_\ell(kr)\, Y_\ell^m(\theta,\varphi)}$$

$\rightarrow$ Mantendo $k$ (energia) fixo: $e^{i\vec{k}\cdot\vec{r}} = 4\pi \overset{?}{\square} \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} j_\ell(kr)\, Y_\ell^{m*}(\hat{k})\, Y_\ell^m(\hat{r})$

※ 06/12/23

# Momento Angular

→ $\vec{L} = \vec{R}\times\vec{P} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ X & Y & Z \\ P_x & P_Y & P_z \end{vmatrix} = (YP_z - ZP_Y)\hat{i} + (ZP_x - XP_z)\hat{j} + (XP_y - YP_x)\hat{k}$

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

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

$[A,B] = -[B,A]$

→ $[L_x, L_y] = [YP_z - ZP_Y,\ ZP_x - XP_z] = [YP_z,\ ZP_x - XP_z] - [ZP_Y,\ ZP_x - XP_z]$

$= [YP_z, ZP_x] - \overset{0}{\cancel{[YP_z, XP_z]}} - \overset{0}{\cancel{[ZP_Y, ZP_x]}} + [ZP_Y, XP_z]$

$= Y[P_z, ZP_x] + \overset{0}{\cancel{[Y, ZP_x]}}P_z + Z\overset{0}{\cancel{[P_Y, XP_z]}} + [Z, XP_z]P_Y$

$= Y\left(Z\overset{0}{\cancel{[P_Y, P_x]}} + \overset{-i\hbar}{\widetilde{[P_z, Z]}}P_x\right) + \left(X\overset{i\hbar}{\widetilde{[Z, P_z]}} + \overset{0}{\cancel{[Z, X]}}P_z\right)P_Y$

$= -i\hbar YP_x + i\hbar XP_Y = i\hbar(XP_y - YP_x)$

∴ $\boxed{[L_x, L_y] = i\hbar L_z \qquad [L_z, L_x] = i\hbar L_y \qquad [L_y, L_z] = i\hbar L_x}$ → álgebra do momento angular

$\boxed{[L^2, L_i] = 0}$ $\quad i = x, y, z$

## Momento Angular Generalizado ($\vec{J}$)

→ $\boxed{J_i^\dagger = J_i}$, $i = x, y, z$

→ $\boxed{[J_x, J_Y] = i\hbar J_z}$

* Autovalores e autovetores:

→ Representação padrão: $\{|j\,m\rangle\}$

→ $J^2|jm\rangle = \hbar^2 j(j+1)|jm$

→ $J_z|jm\rangle = m\hbar|jm\rangle$

→ $\langle\chi|J^2|\chi\rangle = \langle\chi|(J_x^2 + J_y^2 + J_z^2)|\chi\rangle = \overbrace{\langle\chi|J_x^\dagger J_x|\chi\rangle}^{\geq 0} + [\cdots]$ ⇒ $J^2$ positivo definido ⇒ $\hbar^2 j(j+1) \geq 0$

→ Operador escada: $\begin{cases} J_+ \equiv J_x + iJ_y \\ J_- \equiv J_x - iJ_y \end{cases}$ | $(J_+)^\dagger = J_-$, $(J_-)^\dagger = J_+$

↳ $[J^2, J_\pm] = 0$, $\quad [J_z, J_\pm] = \hbar J_\pm$

↳ $J_+J^2|jm\rangle = \hbar^2 j(j+1)J_+|jm\rangle$
$J_+J_z|jm\rangle = \hbar m J_+|jm\rangle$
$J_zJ_+ - J_+J_z = \hbar J_+$

→ $\left.\begin{array}{l} J^2(J_+|jm\rangle) = \hbar^2 j(j+1)(J_+|jm\rangle) \\ J_z(J_+|jm\rangle) = \hbar(m+1)(J_+|jm\rangle) \end{array}\right\}$ $J_+|jm\rangle$ é autovetor de $J^2$ com autovalor $\hbar^2 j(j+1)$ e autovetor de $J_z$ com autovalor $\hbar(m+1)$

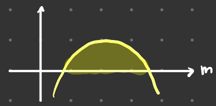
$\boxed{\begin{array}{l} J_+|jm\rangle = c|j, m+1\rangle \\ J_-|jm\rangle = d|j, m-1\rangle \end{array}}$ → $j$ fixo

→ Determinação de c e d:

$$J_+ J_- = (J_x + iJ_y)(J_x - iJ_y) = J_x^2 + J_y^2 - i\underbrace{[J_x, J_y]}_{i\hbar J_z} \Rightarrow J_+J_- = J_x^2 + J_y^2 + \hbar J_z + J_z^2 - J_z^2$$

$$\boxed{J_+J_- = J^2 + \hbar J_z - J_z^2}$$

$$\langle jm | J_+ J_- | jm \rangle \geq 0$$
$$\langle jm | (J^2 + \hbar J_z - J_z^2) | jm \rangle \geq 0$$
$$[\hbar^2 j(j+1) + \hbar^2 m - \hbar^2 m^2] \langle jm | jm \rangle \geq 0 \Rightarrow \boxed{j(j+1) + m - m^2 \geq 0}$$




$$\tilde{m} = \frac{-1 \pm \sqrt{1 + 4j(j+1)}}{-2} = \frac{1 \mp \sqrt{\overbrace{1 + 4j^2 + 4j}^{(2j+1)^2}}}{2} = \frac{1 \pm (2j+1)}{2} \quad \begin{cases} \tilde{m} = j+1 \\ \tilde{m} = -j \end{cases} \Rightarrow -j \leq m \leq j+1$$

$$\boxed{J_-J_+ = J^2 - \hbar J_z - J_z^2} \Rightarrow \boxed{j(j+1) - m - m^2 \geq 0} \Rightarrow -j-1 \leq m \leq j$$

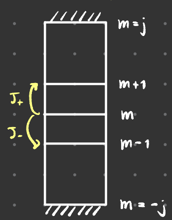
$$\therefore \boxed{-j \leq m \leq j}$$

$$\left.\begin{aligned} &\langle jm | J_+ J_- | jm \rangle \geq 0 \\ &\langle jm | d^* d | jm \rangle = |d|^2 \end{aligned}\right\} \; |d|^2 = \langle jm | J_+J_- | jm \rangle = \hbar^2 j(j+1) + \hbar^2 m - \hbar^2 m^2 \Rightarrow \boxed{d = \hbar\sqrt{j(j+1) - m(m-1)}}$$

$$|c|^2 = \langle jm | J_-J_+ | jm \rangle = \hbar^2 j(j+1) - \hbar^2 m - \hbar^2 m^2 \Rightarrow \boxed{c = \hbar\sqrt{j(j+1) - m(m+1)}}$$

* Resumindo:

$$J_+|jm\rangle = \hbar\sqrt{j(j+1) - m(m+1)}\,|j, m+1\rangle \qquad J_+|j, m=j\rangle = 0 \qquad -j \leq m \leq j$$
$$J_-|jm\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\,|j, m-1\rangle \qquad J_-|j, m=-j\rangle = 0$$




$2j$ passos → $2j+1$ degraus

$2j \in \mathbb{N} \Rightarrow \boxed{j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots}$

$j$ é inteiro ou semi-inteiro

※ 00/12/23

# Matrizes de Momento Angular

## Representação padrão

→ $\{|jm\rangle\}$

→ $\langle j'm'|A|jm\rangle \neq 0$ p/ $j'=j$

↳ $J^2, J_z, J_+, J_-, J_x, J_y$

| $j'm' \backslash jm$ | $j=0$, $m=0$ | $j=\frac{1}{2}$, $m=-\frac{1}{2},\frac{1}{2}$ | $j=1$, $m'=-1,0,1$ |
|---|---|---|---|
| $j'=0$, $m'=0$ | 1x1 | 0 | 0 |
| $j'=\frac{1}{2}$, $m'=-\frac{1}{2},\frac{1}{2}$ | 0 | 2x2 | 0 |
| $j'=1$, $m'=\ldots$ | 0 | 0 | 3x3 |
| $\vdots$ | | | |

$$\langle j'm'|J^2|jm\rangle = \hbar^2 j(j+1)\delta_{j'j}\delta_{m'm}$$

$$\langle j'm'|J_z|jm\rangle = \hbar m\,\delta_{j'j}\delta_{m'm}$$

$$\langle j'm'|J_\pm|jm\rangle = \hbar\sqrt{j(j+1)-m(m\pm1)}\,\delta_{j'j}\delta_{m'm\pm1}$$

→ $j=\frac{1}{2}$: $\langle \tfrac{1}{2}m'|A|\tfrac{1}{2}m\rangle$

$$A_{m'm} = \begin{pmatrix} A_{\frac12\frac12} & A_{\frac12-\frac12} \\ A_{-\frac12\frac12} & A_{-\frac12-\frac12} \end{pmatrix}$$

↳ $A=J^2$: $\langle j'm'|A|jm\rangle = \hbar^2 j(j+1)\delta_{j'j}\delta_{m'm} \Rightarrow \boxed{J^2 = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1\end{pmatrix}}$ → diagonal: comuta com todos

↳ $A=J_z$: $\langle j'm'|J_z|jm\rangle = \hbar m\,\delta_{j'j}\delta_{m'm} \Rightarrow \boxed{J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}}$

↳ $A=J_+$: $\langle j'm'|J_+|jm\rangle = \hbar\sqrt{j(j+1)-m(m+1)}\,\overbrace{\langle j'm'|j,m+1\rangle}^{\delta_{j'j}\delta_{m',m+1}} \Rightarrow J_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0\end{pmatrix}$, $J_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0\end{pmatrix}$

↳ $A=J_x$: $J_x = \frac{J_+ + J_-}{2} \Rightarrow \boxed{J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}}$

↳ $A=J_y$: $J_y = \frac{J_+ - J_-}{2i} \Rightarrow \boxed{J_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0\end{pmatrix}}$

→ $j=1$:

$$A_{m'm} = \begin{pmatrix} A_{11} & A_{10} & A_{1-1} \\ A_{01} & A_{00} & A_{0-1} \\ A_{-11} & A_{-10} & A_{-1-1} \end{pmatrix} \rightarrow$$

$$J^2 = 2\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1\end{pmatrix} \qquad J_x = \frac{\hbar}{\sqrt2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0\end{pmatrix}$$

$$J_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1\end{pmatrix} \qquad J_y = \frac{\hbar}{\sqrt2}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0\end{pmatrix}$$

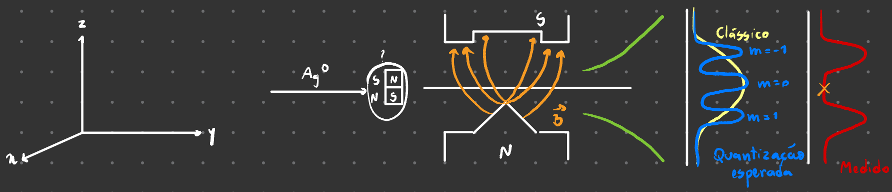
# Momento de dipolo magnético

→ Espira: 


fator giromagnético $\begin{cases} \text{Clássico: } g=1 \\ \text{Quântico: } g = 2{,}00\ldots \end{cases}$ p/ ē com spin

$$m = iA = \frac{q}{\tau}\pi R^2 = \frac{q}{\frac{2\pi R}{v}}\pi R^2 = \frac{q}{2} vR = \frac{q}{2M}\overbrace{MvR}^{L} \longrightarrow \boxed{\vec{m} = g\frac{q}{2M}\vec{L}}$$

# Experimento de Stern-Gerlach 1922




→ momento angular intrínseco (spin) quantizado em $\frac{1}{2}$

→ Evidências do spin $\begin{cases} \text{i) Exp. Stern-Gerlach} \\ \text{ii) Efeito Zeeman anômalo} \\ \text{iii) Teoria de momento angular (possibilidade de } j \text{ semi-inteiro)} \end{cases}$

* Postulados de Pauli:

$\left.\begin{array}{l} \vec{L}: \text{ orbital } (|lm_l\rangle) \\ \vec{S}: \text{ spin } (|sm_s\rangle) \end{array}\right\}$ $\vec{J}$: generalizado $(|jm_j\rangle)$

i) $\vec{S}$ é um momento angular que satisfaz

- $S_x^\dagger = S_x, \quad S_y^\dagger = S_y, \quad S_z^\dagger = S_z$ $\qquad [\vec{L}, \vec{S}] = 0$
- $[S_x, S_y] = i\hbar S_z$, permutações cíclicas
- $S^2|sm_s\rangle = \hbar^2 s(s+1)|sm_s\rangle$ → $s$ fixo $\forall$ partícula → "spin da partícula"

  $S_z|sm_s\rangle = \hbar m_s |sm_s\rangle$
- $N = 2s+1, \quad m_s = -s, s = \pm\frac{1}{2}$

$\vec{S}$: momento angular intrínseco
$s$: spin da partícula (fixo)
↳ número quântico

ii) Cada partícula da natureza tem um único valor de $s$

iii) Para um único elétron, $s = \frac{1}{2}$

11/12/23

# Spin

→ Momento angular intrínseco

→ $\vec{S}$ : $[S_x, S_y] = i\hbar S_z$ e permutações cíclicas

→ Momento de dipolo magnético $\begin{cases} \vec{m}_S = \overset{\sim 2}{g_S} \frac{q}{2M} \vec{S} \rightarrow \text{intrínseco} \\ \vec{m}_L = \underset{\sim 1}{g_L} \frac{q}{2M} \vec{L} \rightarrow \text{orbital} \end{cases}$

## * Postulados de Pauli:

1) $\exists\ \vec{S}$ como momento angular intrínseco

2) Cada partícula é caracterizada pelo spin, que é dado pelo número quântico $s$ (fino) → $\mathcal{E} = \mathcal{E}_L \otimes \mathcal{E}_S = 2s+1$ (N fino)

3) Para o elétron, $s = \frac{1}{2}$

## Partícula de $s = \frac{1}{2}$

→ $s = 1/2$, $m = -1/2,\ 1/2$

→ $|s = \tfrac{1}{2}, m_s = \tfrac{1}{2}\rangle = |m_s = 1/2\rangle = |\uparrow\rangle = |+\rangle$

$|s = \tfrac{1}{2}, m_s = -\tfrac{1}{2}\rangle = |m_s = -\tfrac{1}{2}\rangle = |\downarrow\rangle = |-\rangle$

## * Matrizes de Pauli:

$$\boxed{S_x = \frac{\hbar}{2}\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\sigma_x} \qquad S_y = \frac{\hbar}{2}\underbrace{\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}_{\sigma_y} \qquad S_z = \frac{\hbar}{2}\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\sigma_z} \qquad S^2 = \frac{3\hbar^2}{4}\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{I}}$$

→ $\boxed{S_i = \frac{\hbar}{2}\sigma_i}$ $\qquad \vec{S} = \frac{\hbar}{2}\vec{\sigma}$

### * Propriedades:

1) $\sigma_i^2 = I$
2) $\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}$
3) $[\sigma_i, \sigma_j] = 2\sigma_k$ e p.c.
4) $\mathrm{Tr}\,\sigma_i = 0$
5) $\mathrm{Det}\,\sigma_i = -1$

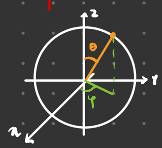
$\Big\}\ \lambda = \pm 1$

→ Escada: $m = \frac{1}{2}$ ↑, $m = -\frac{1}{2}$ ↓

$S_+|\uparrow\rangle = 0$
$S_-|\uparrow\rangle = \hbar|\downarrow\rangle$
$S_+|\downarrow\rangle = \hbar|\uparrow\rangle$
$S_-|\downarrow\rangle = 0$

→ $(S_\pm)^2\,|m_s = \pm\tfrac{1}{2}\rangle = 0$

### * Esfera de Block:




$|\chi\rangle = c_\uparrow|\uparrow\rangle + c_\downarrow|\downarrow\rangle$

$|c_\uparrow|^2 + |c_\downarrow|^2 = 1$

$c_\uparrow = \cos\left(\frac{\theta}{2}\right)$ $\quad 0 \leq \theta \leq \pi$

$c_\downarrow = e^{i\varphi}\,\mathrm{sen}\left(\frac{\theta}{2}\right)$ $\quad 0 \leq \varphi \leq 2\pi$

### * Mais spins:

$\underbrace{\overset{2}{\mathcal{E}_1} \otimes \overset{2}{\mathcal{E}_2}}_{N} \rightarrow 2^2 \longrightarrow \mathcal{E}_1 \otimes \cdots \otimes \mathcal{E}_N \rightarrow 2^N$

* Exemplo: $|\chi_i\rangle = |\uparrow\rangle$

$|m_x = \frac{1}{2}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \equiv |\rightarrow\rangle$

$|m_x = -\frac{1}{2}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \equiv |\leftarrow\rangle$

↳ Preparação: Stern-Gerlach

→ Medir $S_x$ { Quais valores? $\pm\frac{\hbar}{2}$ ; Qual probabilidade?

$P_x(\frac{\hbar}{2}) = |\langle\rightarrow|\chi_i\rangle|^2 = \left|\frac{1}{\sqrt{2}}(1\ \ 1)\begin{pmatrix}1\\0\end{pmatrix}\right|^2 = \frac{1}{2}$

$P_x(-\frac{\hbar}{2}) = |\langle\leftarrow|\chi_i\rangle|^2 = \left|\frac{1}{\sqrt{2}}(1\ -1)\begin{pmatrix}1\\0\end{pmatrix}\right|^2 = \frac{1}{2}$

→ Colapso $|\rightarrow\rangle$

→ Medir $S_z$ { Quais valores? $\pm\frac{\hbar}{2}$ ; Qual probabilidade?

$P_z(\frac{\hbar}{2}) = |\langle\uparrow|\rightarrow\rangle|^2 = \frac{1}{2}$

$P_z(\frac{\hbar}{2}) = |\langle\downarrow|\rightarrow\rangle|^2 = \frac{1}{2}$

* Exemplo: Orbital 2p

→ Estado inicial: $Y_1^1(\theta,\varphi) \rightarrow |\ell=1, m_\ell=1\rangle = |m_z=1\rangle$

→ Medir $L_z$ { Quais valores? $\hbar, 0, -\hbar$ ; Qual probabilidade?

→ Medir $L_x$ { Quais valores? ; Qual probabilidade?

→ $|m_z=1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}$, $|m_z=0\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}$, $|m_z=-1\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$

→ $L_z = \hbar\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}$, $L_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}$

→ $L_x$: $\begin{vmatrix}-\lambda&1&0\\1&-\lambda&1\\0&1&-\lambda\end{vmatrix} = 0 \rightarrow$ $-\lambda^3 + 2\lambda = 0 \rightarrow \lambda'_1 = 0$

$\lambda^2 = 2 \rightarrow \lambda' = \pm\sqrt{2}$

$\therefore \lambda = \hbar, 0, -\hbar$

→ $\lambda' = 0$: $\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = 0 \Rightarrow$ $b=0$, $a+c=0 \Rightarrow a=-c \rightarrow |0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}$

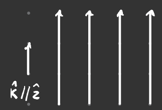
→ $\lambda' = \sqrt{2}$: $\begin{pmatrix}-\sqrt{2}&1&0\\1&-\sqrt{2}&1\\0&1&-\sqrt{2}\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = 0 \Rightarrow$ $-\sqrt{2}a + b = 0 \Rightarrow b = \sqrt{2}a$ ; $a - \sqrt{2}b + c = 0 \Rightarrow a = c$ ; $b - \sqrt{2}c = 0 \Rightarrow b = \sqrt{2}c$ $\rightarrow |\hbar\rangle = \frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix}$

→ $\lambda' = -\sqrt{2}$: $\begin{pmatrix}\sqrt{2}&1&0\\1&\sqrt{2}&1\\0&1&\sqrt{2}\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = 0 \Rightarrow$ $\left.\begin{matrix}\sqrt{2}a + b = 0\\ a+\sqrt{2}b+c = 0\\ b+\sqrt{2}c = 0\end{matrix}\right\}$ $a = c$, $b = -\sqrt{2}a$ $\rightarrow |-\hbar\rangle = \frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}$

$$\left.\begin{aligned}
P(\hbar) &= |\langle m_x=1|m_z=1\rangle|^2 = \left|\tfrac{1}{2}(1\ \sqrt{2}\ 1)\begin{pmatrix}1\\0\\0\end{pmatrix}\right|^2 = \tfrac{1}{4}\\
P(0) &= |\langle m_x=0|m_z=1\rangle|^2 = \left|\tfrac{1}{\sqrt{2}}(1\ 0\ -1)\begin{pmatrix}1\\0\\0\end{pmatrix}\right|^2 = \tfrac{1}{2}\\
P(-\hbar) &= |\langle m_x=-1|m_z=1\rangle|^2 = \left|\tfrac{1}{2}(1\ -\sqrt{2}\ 1)\begin{pmatrix}1\\0\\0\end{pmatrix}\right|^2 = \tfrac{1}{4}
\end{aligned}\right\} \Sigma P = 1$$

※ 13/12/23

# Precessão de Larmor




$\vec{B} = B_0 \hat{k}$

$\vec{m} = g \frac{q}{2m} \vec{S}$

$H = -\vec{m} \cdot \vec{B}$

$\rightarrow H = -g \frac{q}{2m} \vec{S} \cdot \vec{B} = -\underbrace{g \frac{q}{2m}}_{\gamma} B_0 S_z \Rightarrow H = -\gamma B_0 S_z$

$\rightarrow s = \frac{1}{2} : j = \frac{1}{2}, \; N = 2j + 1 = 2$

$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \{|\uparrow\rangle, |\downarrow\rangle\} \quad \{|m_s = \frac{1}{2}\rangle, |m_s = -\frac{1}{2}\rangle\} \longrightarrow H = -\frac{\gamma B_0 \hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Rightarrow E = \pm \frac{\gamma B_0 \hbar}{2} \begin{cases} E_\uparrow = -\frac{\gamma B_0 \hbar}{2} \rightarrow |\uparrow\rangle, |m_s = \frac{1}{2}\rangle, |+\rangle, |0\rangle \\ E_\downarrow = \frac{\gamma B_0 \hbar}{2} \rightarrow |\downarrow\rangle, |m_s = -\frac{1}{2}\rangle, |-\rangle, |1\rangle \end{cases}$

$\rightarrow |\chi\rangle = c_\uparrow |\uparrow\rangle + c_\downarrow |\downarrow\rangle \rightarrow c_\uparrow = \cos\frac{\theta}{2}, \; c_\downarrow = e^{i\varphi} \operatorname{sen}\frac{\theta}{2} \Rightarrow \langle \chi | \chi \rangle = 1$ (*)

$\rightarrow |\chi(t)\rangle = U(t,0)|\chi(0)\rangle$

$\quad \hookrightarrow U(t,0)|\uparrow\rangle = e^{-\frac{iE_\uparrow}{\hbar}t}|\uparrow\rangle = e^{i\frac{\gamma B_0}{2}t}|\uparrow\rangle$

$\quad \hookrightarrow U(t,0)|\downarrow\rangle = e^{-\frac{iE_\downarrow}{\hbar}t}|\downarrow\rangle = e^{-i\frac{\gamma B_0}{2}t}|\downarrow\rangle$

$\Big\} \; |\chi(t)\rangle = c_\uparrow U(t,0)|\uparrow\rangle + c_\downarrow U(t,0)|\downarrow\rangle \Rightarrow \boxed{|\chi(t)\rangle = c_\uparrow e^{\frac{i\gamma B_0}{2}t}|\uparrow\rangle + c_\downarrow e^{-\frac{i\gamma B_0}{2}t}|\downarrow\rangle}$

$\rightarrow \langle \vec{S} \rangle (t) = ?$

$\quad \hookrightarrow$ T. Ehrenfest: $\frac{d}{dt}\langle \vec{S} \rangle = \frac{1}{i\hbar}\langle [\vec{S}, \vec{H}] \rangle$

$\quad \hookrightarrow$ Explícito: $\langle S_x \rangle \hat{i} + \langle S_y \rangle \hat{j} + \langle S_z \rangle \hat{k}$

$\alpha \equiv \frac{\gamma B_0}{2}$

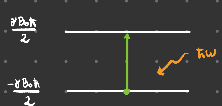
$\langle S_z \rangle = \langle \chi(t) | S_z | \chi(t) \rangle = \left(c_\uparrow^* e^{-i\alpha t} \quad c_\downarrow^* e^{i\alpha t}\right) \begin{pmatrix} 0 & -\frac{i\hbar}{2} \\ \frac{i\hbar}{2} & 0 \end{pmatrix} \begin{pmatrix} c_\uparrow e^{i\alpha t} \\ c_\downarrow e^{-i\alpha t} \end{pmatrix} = \frac{\hbar}{2}\left(|c_\uparrow|^2 - |c_\downarrow|^2\right) = \frac{\hbar}{2}\left(\cos^2\frac{\theta}{2} - \operatorname{sen}^2\frac{\theta}{2}\right) \Rightarrow \boxed{\langle S_z \rangle = \frac{\hbar}{2}\cos\theta}$

Analogamente, $\boxed{\langle S_y \rangle = \frac{\hbar}{2} \operatorname{sen}\theta \operatorname{sen}(\gamma B_0 t)}$ $\boxed{\langle S_x \rangle = \frac{\hbar}{2} \operatorname{sen}\theta \cos(\gamma B_0 t)}$

$\boxed{\begin{array}{c} \omega_L \equiv \gamma B_0 \\ \text{Frequência de Larmor} \end{array}}$


$\rightarrow \omega_L = \gamma B_0, \; \gamma = g \frac{q}{2m} \Rightarrow \boxed{\omega_L = g \frac{q}{2m} B_0}$

$\begin{cases} \omega_L \rightarrow \text{precessão do spin} \\ \omega_c \rightarrow \text{frequência do cíclotron} \rightarrow \omega_c = \frac{qB_0}{m} \rightarrow g \approx 2 \Rightarrow \omega_L \approx \omega_c \end{cases}$




$\omega = \frac{\Delta E}{\hbar} = \omega_L \sim MHz$

$B_0 \rightarrow B_0 + \tilde{B}(x, y, z)$

P/ próton: $\omega_L = 42{,}58 \frac{MHz}{T}$

P/ elétron: $\omega_L \sim \frac{GHz}{T}$

# Adição de Momento Angular

→ $\vec{J}_1$ é momento angular: $[J_{1x}, J_{1y}] = i\hbar J_{1z}$ e p.c.
$\vec{J}_2$ " " " : $[J_{2x}, J_{2y}] = i\hbar J_{2z}$ e p.c.
$\Big\}$ $[\vec{J}_1, \vec{J}_2] = 0 \Rightarrow \vec{J} = \vec{J}_1 + \vec{J}_2$ é momento angular

→ $|m_\ell, m_s\rangle$

* Exemplo: $\ell = 1$, $s = \frac{1}{2}$

$|m_\ell, m_s\rangle = |m_\ell\rangle \otimes |m_s\rangle \rightarrow \mathcal{E} = \mathcal{E}_{2\ell+1} \otimes \mathcal{E}_{2s+1} \rightarrow N = \overbrace{(2j_\ell+1)}^{3}\overbrace{(2j_s+1)}^{2} = 6$

→ $|j_1 m_1, j_2 m_2\rangle = \underbrace{|j_1 m_1\rangle}_{\mathcal{E}_{2j_1+1}} \otimes \underbrace{|j_2 m_2\rangle}_{\mathcal{E}_{2j_2+1}} \longrightarrow$ c.c.o.c.: $\{J_1^2, J_2^2, J_{1z}, J_{2z}\}$ → projeções de $\vec{J}_1$ e $\vec{J}_2$ bem definidas

↳ c.c.o.c.: $\{J_2^2, J_{2z}\}$

↳ c.c.o.c.: $\{J_1^2, J_{1z}\}$

→ Outra representação: $\{J^2, J_z, J_1^2, J_2^2\}$ → soma dos momentos angulares bem definida

※ 15/12/23

→ $\vec{J} = \vec{J}_1 + \vec{J}_2$

→ Duas bases: $|j_1, j_2, m_1, m_2\rangle$ ; $|j_1, j_2, J, m\rangle$ $\Bigg\{$ $J_z|j_1, j_2, m_1, m_2\rangle = \hbar\overbrace{(m_1+m_2)}^{\equiv m}|j_1, j_2, m_1, m_2\rangle$
$J_z|j_1, j_2, J, m\rangle = \hbar m|j_1, j_2, J, m\rangle$

$\Big\}$ $\overbrace{|j_1, j_2, \underline{m_1}, \underline{m_2}\rangle}^{\text{não é a.v. de } J^2} \neq \overbrace{|j_1, j_2, J, \underline{m}\rangle}^{\text{autovetor de } J^2}$

↳ Degenerescência ↵

* Exemplo: $j_1 = 2 \rightarrow m_1 = -2, -1, 0, 1, 2 \rightarrow 5$
$j_2 = 1 \rightarrow m_2 = -1, 0, 1 \rightarrow 3$

↳ Dimensão: $\dim(\mathcal{E}_{j_1} \otimes \mathcal{E}_{j_2}) = 5 \times 3 = 15$

→ Base 1: $|j_1, j_2, m_1, m_2\rangle$ → 15 estados

→ Base 2: $|J, m\rangle$, $m = m_1 + m_2$

Pelos extremos: $|J=3, m=3\rangle = |\overset{m_2}{+2}, \overset{m_1}{+1}\rangle$
$|J=3, m=-3\rangle = |-2, -1\rangle$ $\Big\}$ gerar demais estados: $J_\pm$

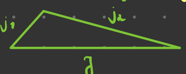
$J_- \longleftrightarrow J_+$

ortogonalidade
$J=3$: $m = -3, -2, -1, 0, 1, 2, 3 \rightarrow 7$
$J=2$: $m = -2, -1, 0, 1, 2 \rightarrow 5$
$J=1$: $m = -1, 0, 1 \rightarrow 3$
$\Bigg\}$ $5 \otimes 3 = 7 \oplus 5 \oplus 3$

* Dimensão de $\mathcal{E}$:

Base 1: $\{|j_1, j_2, m_1, m_2\rangle\} \longrightarrow N = (2j_1+1)(2j_2+1)$
Base 2: $\{|j_1, j_2, J, m\rangle\} \longrightarrow N = \sum_J (2J+1)$

Regra do triângulo: $\displaystyle\sum_{J=|j_1-j_2|}^{j_1+j_2} (2J+1) = (2j_1+1)(2j_2+1)$




$\boxed{|j_2 - j_1| \leq J \leq j_2 + j_1}$

*** Representações:** $j_1$ e $j_2$ fixos

$$\left.\begin{array}{l} J = j_1+j_2, \dots, |j_1-j_2| \\ m = -J, \dots, J \end{array}\right\} |J, m\rangle \quad \text{"+ física"}$$

$$\left.\begin{array}{l} m_1 = -j_1, \dots, j_1 \\ m_2 = -j_2, \dots, j_2 \end{array}\right\} |m_1, m_2\rangle \quad \text{"+ fácil"}$$

*** Ortonormalidade e clausura:**

$$\langle Jm|J'm'\rangle = \delta_{JJ'}\delta_{mm'} \qquad \Big| \qquad \langle j_1,j_2,m_1,m_2|j_1,j_2,m_1',m_2'\rangle = \delta_{m_1m_1'}\delta_{m_2m_2'}$$

$$\sum_{J=|j_1-j_2|}^{j_1+j_2}\sum_{m=-J}^{J} |Jm\rangle\langle Jm| = I \qquad \Big| \qquad \sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2} |j_1,j_2,m_1,m_2\rangle\langle j_1,j_2,m_1,m_2| = I$$

*** Relação entre as representações:**

$$|Jm\rangle = I|Jm\rangle = \sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2} |j_1,j_2,m_1,m_2\rangle\langle j_1,j_2,m_1,m_2|Jm\rangle \rightarrow C^{j_1j_2J}_{m_1m_2m}: \text{Coeficientes de Clebsch-Gordan}$$

$$\boxed{\begin{array}{l} |Jm\rangle = \displaystyle\sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2} C^{j_1j_2J}_{m_1m_2m}\,|j_1,j_2,m_1,m_2\rangle \\ |j_1,j_2,m_1,m_2\rangle = \displaystyle\sum_{J=|j_1-j_2|}^{j_1+j_2}\sum_{m=-J}^{J} C^{j_1j_2J}_{m_1m_2m}\,|Jm\rangle \end{array}}$$

*** Propriedades dos coeficientes de CG:**

1) $C^{j_1j_2J}_{m_1m_2m} \neq 0 \ \forall\ J = j_1+j_2, \dots, |j_1-j_2|$ e $m = m_1+m_2$

2) $|J=j_1+j_2, m=j_1+j_2\rangle = |j_1,j_2, m_1=j_1, m_2=j_2\rangle \rightarrow C^{j_1,j_2,j_1+j_2}_{j_1,j_2,j_1+j_2} = 1$

3) Relação de recorrência: Mesmo $J$: $J_\pm|J,m\rangle$
Outro $J$: ortogonalidade

*** Exemplo: Singleto e tripleto**

→ Duas partículas de spin $s = \frac{1}{2}$

→ $\vec{S} = \vec{S}_1 + \vec{S}_2 \rightarrow \mathcal{E}_{\frac{1}{2}} \otimes \mathcal{E}_{\frac{1}{2}}$
$|\uparrow\rangle_1 \quad |\uparrow\rangle_2$
$|\downarrow\rangle_1 \quad |\downarrow\rangle_2$

$|\uparrow\uparrow\rangle \rightarrow m_s = \frac{1}{2}+\frac{1}{2} = 1 \qquad |\uparrow\downarrow\rangle \rightarrow m_s = \frac{1}{2}-\frac{1}{2} = 0$

$|\downarrow\downarrow\rangle \rightarrow m_s = -\frac{1}{2}-\frac{1}{2} = -1 \qquad |\downarrow\uparrow\rangle \rightarrow m_s = -\frac{1}{2}+\frac{1}{2} = 0$

→ Base 1: $|m_1 m_2\rangle \rightarrow |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$

→ Base 2: $|S\, m_s\rangle$

a. operador escada
b. coef. CG
c. simetria

$S = |s_1-s_2|, \dots, s_1+s_2 \rightarrow S = 0, 1$

$$③\left\{\begin{array}{l} |S=1, m_s=1\rangle = |\uparrow\uparrow\rangle \\ |S=1, m_s=0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |S=1, m_s=-1\rangle = |\downarrow\downarrow\rangle \end{array}\right. \rightarrow \text{simétrico}$$

$$①\left\{ |S=0, m_s=0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \right. \rightarrow \text{anti-simétrico}$$

18/12/23

* Problema 4.55 Griffiths

$$R_{21}\left(\sqrt{\tfrac{1}{3}}\,Y_1^0\chi_+ + \sqrt{\tfrac{2}{3}}\,Y_1^1\chi_-\right) \rightarrow \text{Superposição na parte angular e de spin}$$

$n=2$, $l=1$; $m_l=0$, $m_s=\frac{1}{2}$; $m_l=1$, $m_s=-\frac{1}{2}$

$$|\psi\rangle = \sqrt{\tfrac{1}{3}}\,|l=1, m_l=0, m_s=\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}}\,|l=1, m_l=1, m_s=-\tfrac{1}{2}\rangle$$

a) $L^2$: $L^2|\psi\rangle = \hbar^2 l(l+1)|\psi\rangle \rightarrow 2\hbar^2,\ P=1 \rightarrow l=1$ não está em superposição

b) $L_z$: $0,\ P(0)=\frac{1}{3}$

$\hbar,\ P(\hbar)=\frac{2}{3}$

c) $S^2$: $\frac{3\hbar^2}{4},\ P=1 \rightarrow$ spin é intrínseco: não há superposição

d) $S_z$: $\frac{\hbar}{2},\ P(\frac{\hbar}{2})=\frac{1}{3}$

$-\frac{\hbar}{2},\ P(-\frac{\hbar}{2})=\frac{2}{3}$

e) $J^2$: $\vec{J}=\vec{L}+\vec{S}\ |\ j=|l-s|, \dots, l+s \Rightarrow j=\frac{1}{2}, \frac{3}{2}$

$\hookrightarrow l=1,\ s=\frac{1}{2}$

$\rightarrow \frac{3}{4}\hbar^2,\ P(\frac{3}{4}\hbar^2)=\frac{8}{9}$

$\rightarrow \frac{15}{4}\hbar^2,\ P(\frac{15}{4}\hbar^2)=\frac{1}{9}$

Troca de base: $m = m_l + m_s = \frac{1}{2}$

$$|m_l=0, m_s=\tfrac{1}{2}\rangle = \sqrt{\tfrac{2}{3}}\,|j=\tfrac{3}{2}, m=\tfrac{1}{2}\rangle - \sqrt{\tfrac{1}{3}}\,|j=\tfrac{1}{2}, m=\tfrac{1}{2}\rangle$$
$$|m_l=1, m_s=-\tfrac{1}{2}\rangle = \sqrt{\tfrac{1}{3}}\,|j=\tfrac{3}{2}, m=\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{3}}\,|j=\tfrac{1}{2}, m=\tfrac{1}{2}\rangle$$

⋮

f) $J_z$: $m=\frac{1}{2}$ em ambos os estados $\rightarrow \frac{\hbar}{2},\ P=1$

# Simetrias

→ Invariância frente a alguma transformação

→ Simetrias $\begin{cases} \text{discretas} & \text{ex.: rotação de quadrado} \\ \text{contínuas} & \text{ex.: rotação de círculo} \end{cases}$

→ Definem um grupo

| | $A_1$ | $A_2$ | $A_3$ |
|---|---|---|---|
| $A_1$ | $A_i$ | $A_j$ | $A_k$ |
| $A_2$ | ... | ... | ... |
| $A_3$ | ... | ... | ... |

Tabela de multiplicação

grupo: fechado sob multiplicação

→ Na MQ: transformações de simetria implementadas por transformações unitárias $S^{-1} = S^\dagger$

$$\boxed{S^\dagger H S = H \rightarrow [H,S] = 0}$$

Há simetria se a operação comutar com H

* Degenerescência:

$[H,S] = 0$

$H|\phi_n\rangle = E_n|\phi_n\rangle$

$SH|\phi_n\rangle = E_n S|\phi_n\rangle$

$HS|\phi_n\rangle = E_n S|\phi_n\rangle$

$|\phi_n\rangle$ e $S|\phi_n\rangle$: mesma energia

Se $|\phi_n\rangle$ e $S|\phi_n\rangle$ não L.I.: degenerescência

* Simetrias contínuas: $S(\varepsilon)$ — $\varepsilon = 0 \rightarrow I$

↳ Leis de conservação:

$S(\varepsilon) = e^{-\frac{i\varepsilon}{\hbar}G}$

$S(\varepsilon \rightarrow 0) = I - \frac{i\varepsilon}{\hbar} G$ → gerador do grupo → $G^\dagger = G$

infinitesimal

Operação

$[H,S] = 0 \rightarrow [H,G] = \frac{d\langle G\rangle}{dt} = 0 \Rightarrow \langle G\rangle$ é conservado

$G|g\rangle = g|g\rangle$

$U(t,t_0)|g\rangle = |\psi(t)\rangle$

$G|\psi(t)\rangle = GU(t,t_0)|g\rangle = U(t,t_0)G|g\rangle = g|\psi(t)\rangle$ → medida de g independente do tempo

* Exemplos:
- Translações espaciais → momento linear
- Translações temporais → energia
- Rotações espaciais → momento angular

✲ 20/12/23

$T(\lambda_1)\,T(\lambda_2) = T(\lambda_1+\lambda_2)$
$T(0) = I$

## ✲ Translação espacial $T(\lambda)$:

→ $T(\lambda)|x\rangle = |x+\lambda\rangle$
$XT(\lambda)|x\rangle = X|x+\lambda\rangle = (x+\lambda)|x+\lambda\rangle = (x+\lambda)\,T(\lambda)|x\rangle = T(\lambda)(x+\lambda)|x\rangle = T(\lambda)(X+\lambda I)|x\rangle$

$\therefore \boxed{[X, T(\lambda)] = \lambda T(\lambda)}$

→ $[X,P] = i\hbar \Rightarrow [X, F(P)] = i\hbar F'(P)$

→ $T = F(P) \Rightarrow [X, T(\lambda)] = \lambda T(\lambda) = i\hbar T'(P) \Rightarrow \frac{d}{dP} T(P) = -\frac{i\lambda}{\hbar} T(P)$

$\therefore T(\lambda) = e^{-\frac{i\lambda}{\hbar}P} \longrightarrow \boxed{T(\vec{\lambda}) = e^{-\frac{i}{\hbar}\vec{\lambda}\cdot\vec{P}}}$

→ $\vec{P}$ é o gerador da operação de translação espacial $T(\lambda)$

→ apenas a partícula livre apresenta simetria de translação espacial (para $\forall \lambda \in \mathbb{R}$)

↳ Teorema de Bloch → simetria translacional discreta

→ $[T(a), H] = 0$

$T(a)|x\rangle = (x+a)|x\rangle$
$T(a)^\dagger|x\rangle = (x-a)|x\rangle$

→ $H|\phi_n\rangle = E_n|\phi_n\rangle$
$T(a)|\phi_n\rangle = c|\phi_n\rangle \rightarrow c = e^{i\theta}$ pois $T$ é unitário
$\langle x|T(a)|\phi_n\rangle = e^{i\theta}\langle x|\phi_n\rangle$
$(T^\dagger(a)|x\rangle)^\dagger|\phi_n\rangle = e^{i\theta}\phi_n(x)$
$(x-a)\,\phi_n(x) = e^{i\theta}\phi_n(x)$

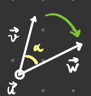
⋮

## ✲ Translação temporal $U(t)$:

## ✲ Rotações espaciais

→ $R_{\hat{u}}(\alpha)\,\vec{v} = \vec{w}, \quad |\vec{v}| = |\vec{w}|$

→ Rotação ativa: base fixa




Rotações infinitesimais:

$$R_{\hat{z}}(\varepsilon) = \begin{pmatrix} 1-\frac{\varepsilon^2}{2} & -\varepsilon & 0 \\ \varepsilon & 1-\frac{\varepsilon^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R_{\hat{x}}(\varepsilon) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\frac{\varepsilon^2}{2} & -\varepsilon \\ 0 & \varepsilon & 1-\frac{\varepsilon^2}{2} \end{pmatrix}$$

$$R_{\hat{y}}(\varepsilon) = \begin{pmatrix} 1-\frac{\varepsilon^2}{2} & 0 & \varepsilon \\ 0 & 1 & 0 \\ -\varepsilon & 0 & 1-\frac{\varepsilon^2}{2} \end{pmatrix}$$

$$R_{\hat{x}}(\varepsilon)R_{\hat{y}}(\varepsilon) - R_{\hat{y}}(\varepsilon)R_{\hat{x}}(\varepsilon) = \begin{pmatrix} 0 & -\varepsilon^2 & 0 \\ \varepsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = O(\varepsilon^2)$$

$$\boxed{R_{\hat{x}}(\varepsilon)R_{\hat{y}}(\varepsilon) - R_{\hat{y}}(\varepsilon)R_{\hat{x}}(\varepsilon) = R_{\hat{z}}(\varepsilon^2) - 1}$$

Álgebra do grupo de rotação

✲ $\mathcal{R}$: matrizes ortogonais → representação do grupo de rotação em $\mathbb{R}^3$

✲ $R$: Operador unitário → representação do grupo de rotação em $\mathcal{E}$ → $R|\psi\rangle = |\psi'\rangle$, $RR^\dagger = R^\dagger R = 1$

Definição: $\boxed{\begin{aligned} R|\vec{r}\rangle &= |\mathcal{R}\vec{r}\rangle \\ R^\dagger|\vec{r}\rangle &= |\mathcal{R}^{-1}\vec{r}\rangle \end{aligned}}$

$\langle\vec{r}|R|\psi\rangle = \langle\vec{r}|\psi'\rangle = \psi'(\vec{r})$

$\boxed{\psi'(\vec{r}) = \psi(\mathcal{R}^{-1}\vec{r})}$

$$\rightarrow R_z^{-1}\vec{r} = \begin{pmatrix}1 & \varepsilon & 0\\ -\varepsilon & 1 & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} = \begin{pmatrix}x+\varepsilon y\\ -\varepsilon x + y\\ z\end{pmatrix} \rightarrow \psi'(x,y,z) = \psi(x+\varepsilon y,\ y-\varepsilon x,\ z)$$

$$= \psi(x,y,z) + \overbrace{\varepsilon y}^{\Delta x}\frac{\partial \psi}{\partial x} \overbrace{-\varepsilon x}^{\Delta y}\frac{\partial \psi}{\partial y}$$

$$= \psi(x,y,z) + \left(-\frac{i}{\hbar}\varepsilon\right) L_z \psi$$

$$= \left(1 - \frac{i}{\hbar}\varepsilon L_z\right)\psi$$

$L_z = xP_y - yP_x$

$\therefore \boxed{R_z(\varepsilon) = \left(1 - \frac{i}{\hbar}\varepsilon L_z\right)}$ → $L_z$ é o gerador da rotação em torno de z

$$\rightarrow R_x(\varepsilon)R_y(\varepsilon) - R_y(\varepsilon)R_x(\varepsilon) = R_z(\varepsilon^2) - 1$$

$$\left(\cancel{1} - \frac{i\varepsilon}{\hbar}L_x\right)\left(\cancel{1} - \frac{i\varepsilon}{\hbar}L_y\right) - \left(\cancel{1} - \frac{i\varepsilon}{\hbar}L_y\right)\left(1 - \frac{i\varepsilon}{\hbar}L_x\right) = \left(\cancel{1} - \frac{i\varepsilon^2}{\hbar}L_z\right) - \cancel{1}$$

$$-\frac{\varepsilon^2}{\hbar^2}L_xL_y + \frac{\varepsilon^2}{\hbar^2}L_yL_x = -\frac{i}{\hbar}\varepsilon^2 L_z \Rightarrow \boxed{[L_x, L_y] = i\hbar L_z}$$

↳ Rotação finita:

$$R_{\vec{u}}(\alpha + \overbrace{d\alpha}^{\varepsilon}) = R_{\vec{u}}(\alpha)\, R_{\vec{u}}(d\alpha)$$

$$= R_{\vec{u}}(\alpha)\left(1 - \frac{i}{\hbar}d\alpha\, \vec{u}\cdot\vec{L}\right)$$

$$\frac{R_{\vec{u}}(\alpha + d\alpha) - R_{\vec{u}}(\alpha)}{d\alpha} = -\frac{i}{\hbar}\vec{u}\cdot\vec{L}\, R_{\vec{u}}(\alpha)$$

$$\frac{dR_{\vec{u}}(\alpha)}{d\alpha} = -\frac{i}{\hbar}\vec{u}\cdot\vec{L}\, R_{\vec{u}}(\alpha)$$

$$\boxed{R_{\vec{u}}(\alpha) = e^{-\frac{i}{\hbar}\alpha\, \vec{u}\cdot\vec{L}}}$$