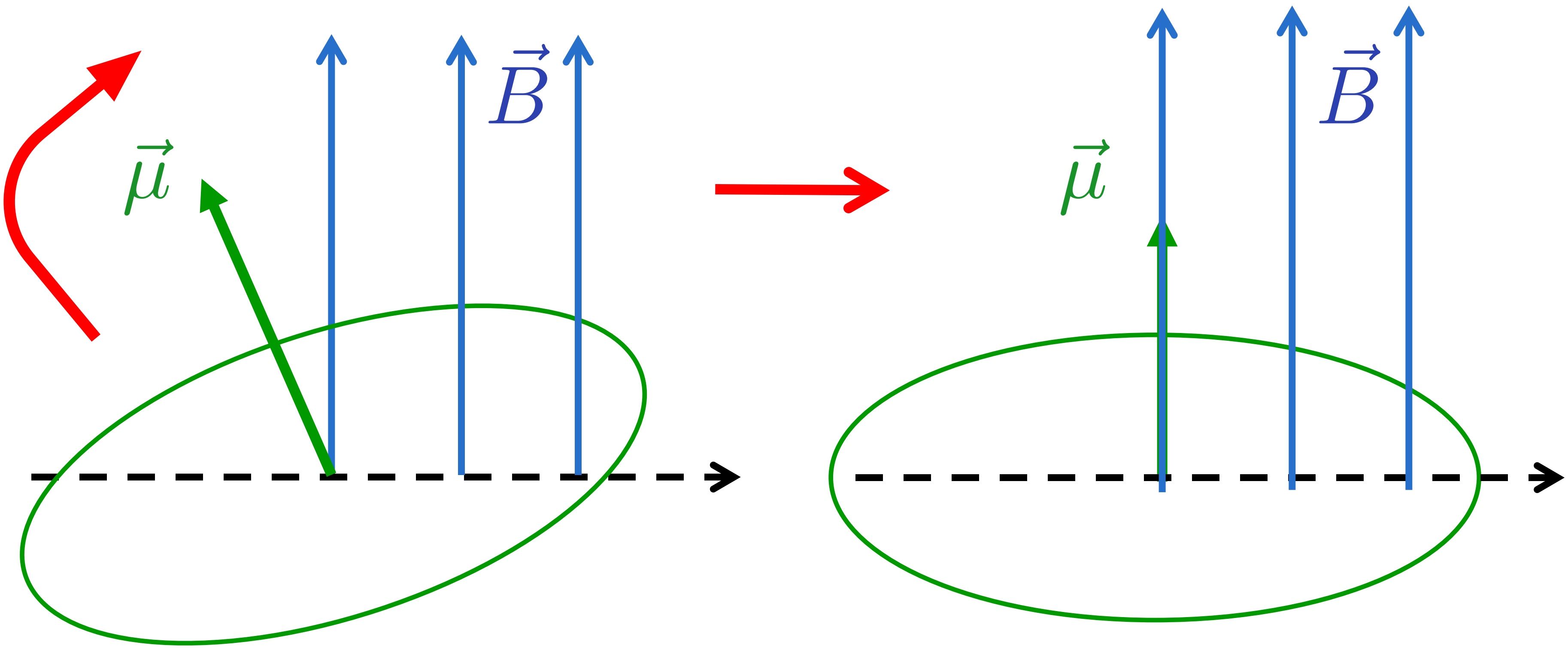
# Aula 8

Valor médio: precessão de Larmor

Adição de spins

Exemplos

# Espira tenta se alinhar como uma bússola !



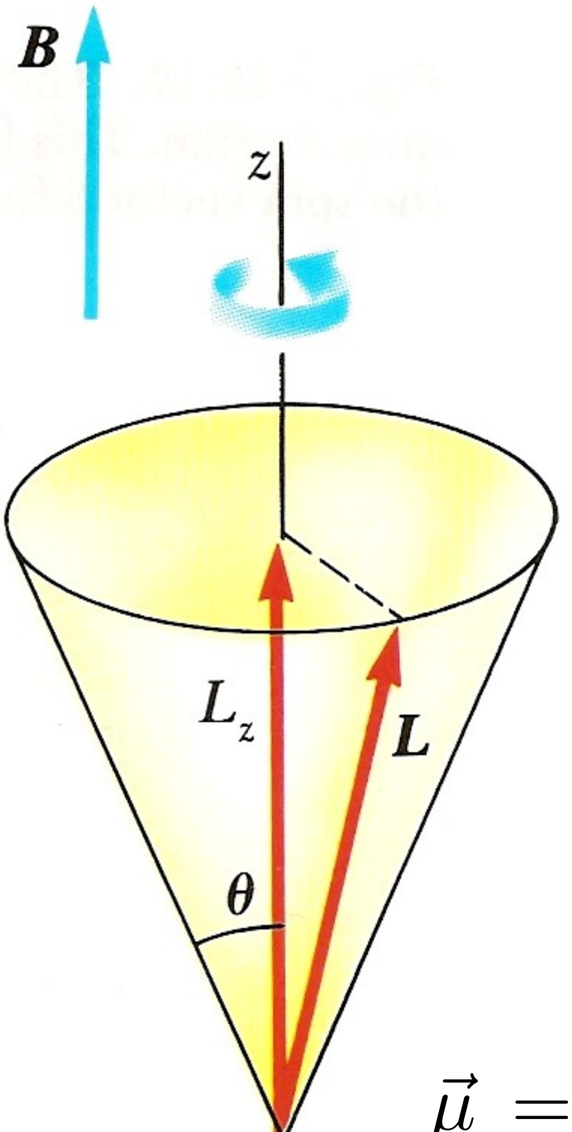

mais energia !

menos energia !

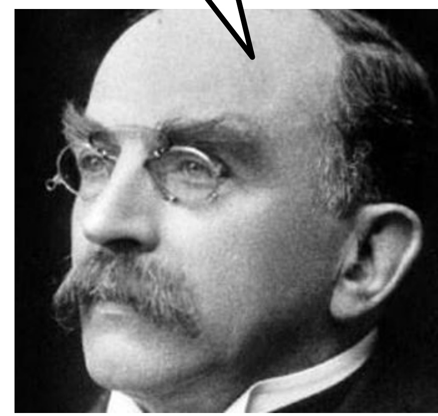
Energia potencial de orientação

$$\boxed{U = -\vec{\mu} \cdot \vec{B}}$$

# Mas nunca se alinha ! Precessiona !



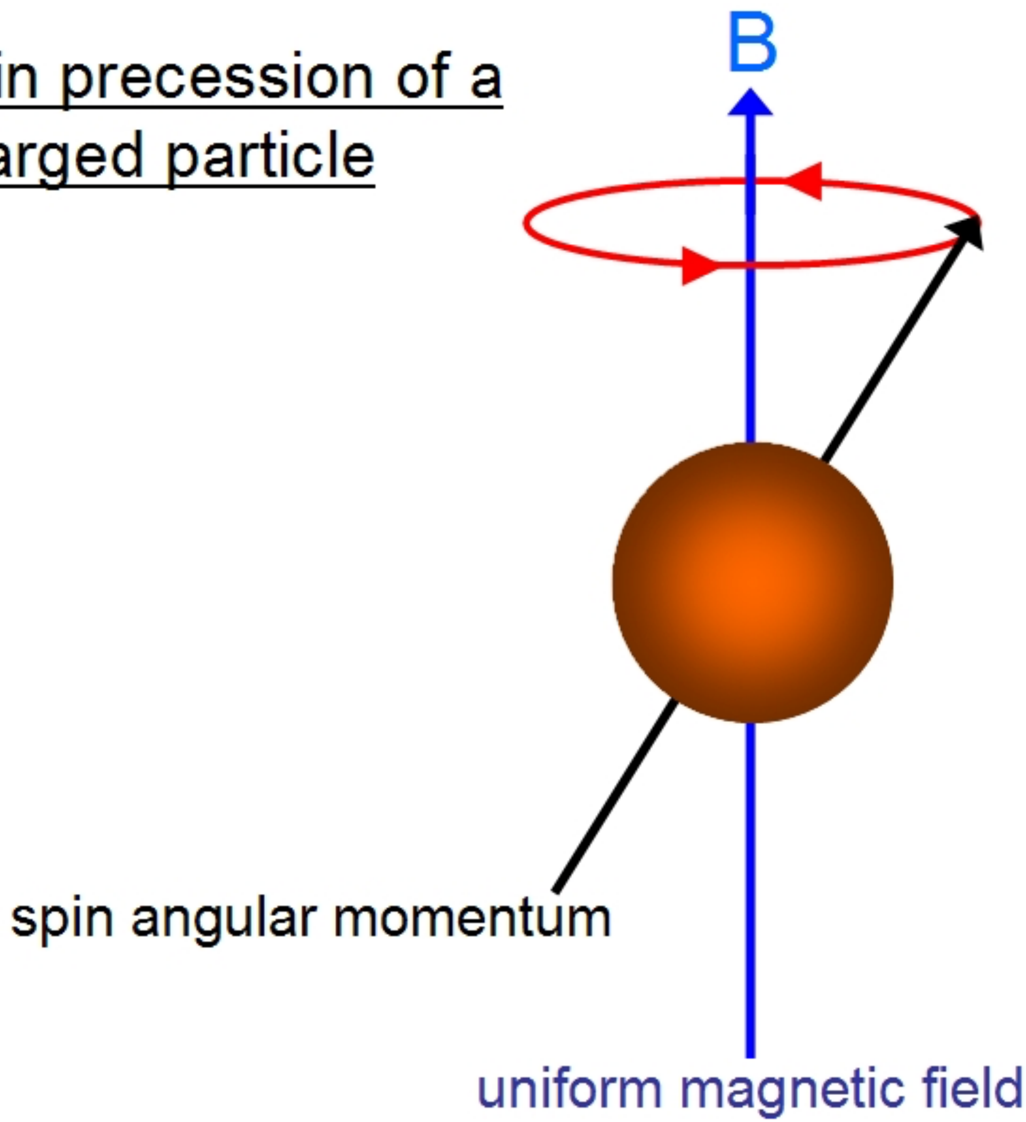

Precessão de Larmor

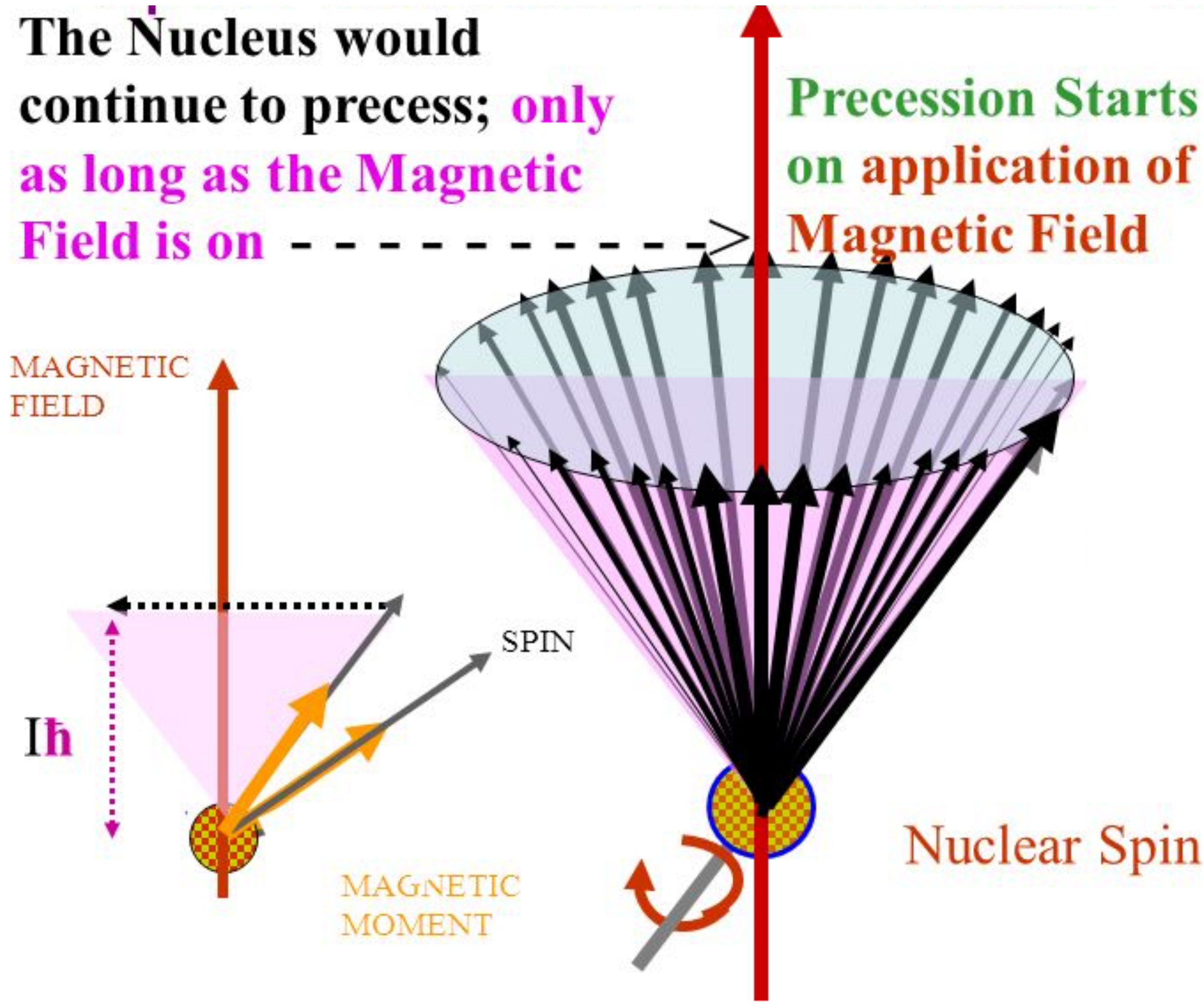


Joseph Larmor

$$\vec{\mu} = \frac{g_l \, \mu_b}{\hbar} \vec{L}$$

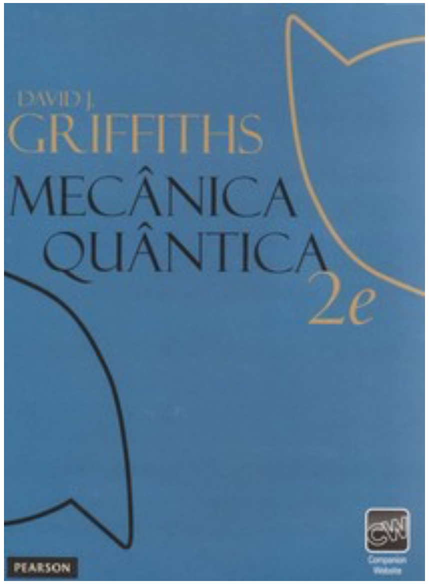
# Spin precession of a charged particle




The Nucleus would continue to precess; only as long as the Magnetic Field is on
Precession Starts on application of Magnetic Field
MAGNETIC FIELD
SPIN
Iħ
MAGNETIC MOMENT
Nuclear Spin

Isto é uma descrição clássica !
...poderia ser um pião...

Como fazer um estudo quântico da precessão do spin ?



$$U = -\vec{\mu}_s \,.\, \vec{B}$$

$$\begin{cases} \vec{B} = B_0\, \hat{k} \\ \vec{\mu}_s = \dfrac{g_s\, \mu_b}{\hbar}\, \vec{S} = \gamma\, \vec{S} \end{cases}$$

$$U = -\gamma\, \vec{S} \,.\, \vec{B}$$

$\gamma$ é a razão giromagnética

Função Hamiltoniana :

$$H = T + U = \text{e. cinética} + \text{e. potencial}$$

$$H = -\gamma\, \vec{S} \,.\, \vec{B} = -\gamma\, B_0\, S_z$$

# Quantização : funções viram operadores

$$H = -\gamma\,\vec{S}\,.\,\vec{B} = -\gamma\,B_0\,S_z$$

$$H \rightarrow \hat{H}$$ Operador Hamiltoniano

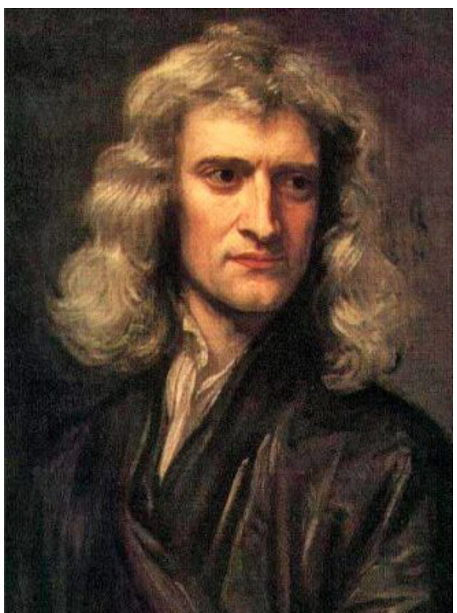
$$S_z \rightarrow \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\hat{H} = -\gamma\,B_0\,\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

## Mecânica clássica

2ª lei de Newton

$$\frac{d^2 x}{dt^2} = - \frac{1}{m} \frac{\partial V}{\partial x}$$



## Mecânica quântica

Equação de Schrödinger

$$i \hbar \frac{\partial \Psi}{\partial t} = - \frac{\hbar^2}{2\, m} \frac{\partial^2 \Psi}{\partial x^2} + V \Psi$$

$$\hat{H} = - \frac{\hbar^2}{2\, m} \frac{\partial^2}{\partial x^2} + V$$

( Hamiltoniano )

$$\boxed{i \hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi}$$

$$i\,\hbar\,\frac{\partial \Psi}{\partial t} = \hat{H}\,\Psi$$

Ansatz :

$$\Psi(t) = \psi_s\, e^{-i\,(E\,t)/\hbar} = |\chi\rangle\, e^{-i\,(E\,t)/\hbar}$$

$$\hat{H}\,|\chi\rangle = E\,|\chi\rangle$$

Já sabemos que só existem dois autoestados de spin:

$$|\chi\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\chi\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Aplicando ao estado com spin pracima

$$\hat{H} = -\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad |\chi\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\hat{H}\,|\uparrow\rangle = -\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\hat{H}\,|\uparrow\rangle = -\gamma B_0 \frac{\hbar}{2}\,|\uparrow\rangle$$

$$\hat{H}\,|\uparrow\rangle = E_+\,|\uparrow\rangle$$

$$\boxed{E_+ = -\gamma B_0 \frac{\hbar}{2}}$$

Aplicando ao  estado com spin prabaixo

$$\hat{H} = -\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad |\chi\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\hat{H}\,|\downarrow\rangle = -\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = +\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\hat{H}\,|\downarrow\rangle = +\gamma B_0 \frac{\hbar}{2}\,|\downarrow\rangle$$

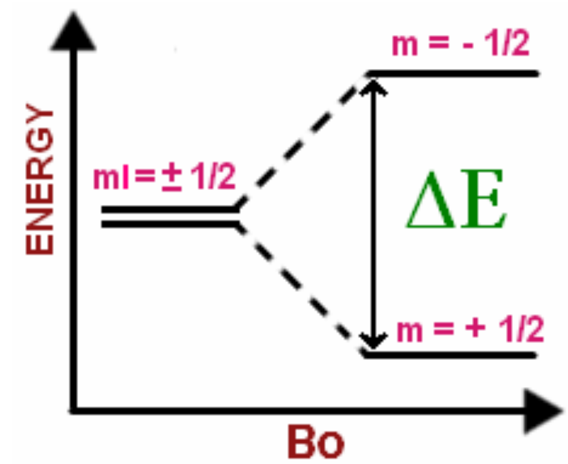
$$\hat{H}\,|\downarrow\rangle = E_-\,|\downarrow\rangle$$

$$\boxed{E_- = +\gamma B_0 \frac{\hbar}{2}}$$

$$\Psi(t) \;=\; |\chi\rangle\, e^{-i\,(E\,t)/\hbar}$$

Encontramos dois estados :

$$\begin{cases} \Psi_+(t) \;=\; |\uparrow\rangle\, e^{-i\,(E_+\,t)/\hbar} \\ \Psi_-(t) \;=\; |\downarrow\rangle\, e^{-i\,(E_-\,t)/\hbar} \end{cases}$$




Solução geral :

$$\Psi(t) \;=\; a\,\Psi_+ \;+\; b\,\Psi_- \;=\; a\,|\uparrow\rangle\, e^{-i\,(E_+\,t)/\hbar} \;+\; b\,|\downarrow\rangle\, e^{-i\,(E_-\,t)/\hbar}$$

$$|a|^2 \;+\; |b|^2 \;=\; 1 \quad \longrightarrow \quad a \;=\; cos\,(\frac{\alpha}{2}) \qquad b \;=\; sen\,(\frac{\alpha}{2})$$

$$\Psi(t) \;=\; cos\,(\frac{\alpha}{2})\,\begin{pmatrix} 1 \\ 0 \end{pmatrix}\, e^{-i\,(E_+\,t)/\hbar} \,+\, sen\,(\frac{\alpha}{2})\,\begin{pmatrix} 0 \\ 1 \end{pmatrix}\, e^{-i\,(E_-\,t)/\hbar}$$

$$\Psi(t) \;=\; \begin{pmatrix} cos\,(\frac{\alpha}{2})\; e^{-i\,(E_+\,t)/\hbar} \\ \\ sen\,(\frac{\alpha}{2})\, e^{-i\,(E_-\,t)/\hbar} \end{pmatrix}$$

$$E_+ \;=\; -\,\gamma\,B_0\,\frac{\hbar}{2}$$

$$E_- \;=\; +\,\gamma\,B_0\,\frac{\hbar}{2}$$

$$\Psi(t) \;=\; \begin{pmatrix} cos\,(\frac{\alpha}{2})\; e^{+i\,(\gamma\,B_0\,t)/2} \\ \\ sen\,(\frac{\alpha}{2})\, e^{-i\,(\gamma\,B_0\,t)/2} \end{pmatrix}$$

$$\Psi^\dagger(t) \;=\; \begin{pmatrix} cos\,(\frac{\alpha}{2})\; e^{-i\,(\gamma\,B_0\,t)/2} & \quad sen\,(\frac{\alpha}{2})\, e^{+i\,(\gamma\,B_0\,t)/2} \end{pmatrix}$$

# Valor esperado de $S_x$

$$\langle \hat{S}_x \rangle \;=\; \langle \Psi \,|\, \hat{S}_x \,|\, \Psi \rangle \;=\; \Psi^{\dagger}\, \hat{S}_x\, \Psi$$

$$= \begin{pmatrix} cos\,(\frac{\alpha}{2})\; e^{-i\,(\gamma\, B_0\, t)/2} & sen\,(\frac{\alpha}{2})\, e^{+i\,(\gamma\, B_0\, t)/2} \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} cos\,(\frac{\alpha}{2})\; e^{+i\,(\gamma\, B_0\, t)/2} \\ sen\,(\frac{\alpha}{2})\, e^{-i\,(\gamma\, B_0\, t)/2} \end{pmatrix}$$

$$= \frac{\hbar}{2} \begin{pmatrix} cos\,(\frac{\alpha}{2})\; e^{-i\,(\gamma\, B_0\, t)/2} & sen\,(\frac{\alpha}{2})\, e^{+i\,(\gamma\, B_0\, t)/2} \end{pmatrix} \begin{pmatrix} sen\,(\frac{\alpha}{2})\, e^{-i\,(\gamma\, B_0\, t)/2} \\ cos\,(\frac{\alpha}{2})\; e^{+i\,(\gamma\, B_0\, t)/2} \end{pmatrix}$$

$$= \frac{\hbar}{2} \left( cos\,\frac{\alpha}{2}\, sen\frac{\alpha}{2}\;\; e^{-i\,\gamma\, B_0\, t} \;+\; sen\,\frac{\alpha}{2}\, cos\,\frac{\alpha}{2}\;\; e^{+i\,\gamma\, B_0\, t} \right)$$

$$= \frac{\hbar}{2}\, cos\,\frac{\alpha}{2}\, sen\frac{\alpha}{2}\;\left( e^{-i\,\gamma\, B_0\, t} \;+\; e^{+i\,\gamma\, B_0\, t} \right)$$

$$= \frac{\hbar}{2} \, cos \, \frac{\alpha}{2} \, sen \frac{\alpha}{2} \, \left( e^{-i\,\gamma\, B_0\, t} + e^{+i\,\gamma\, B_0\, t} \right)$$

$$= \frac{\hbar}{2} \, \frac{1}{2} \, sen \, \alpha \quad 2 \, cos \, (\gamma \, B_0 \, t)$$

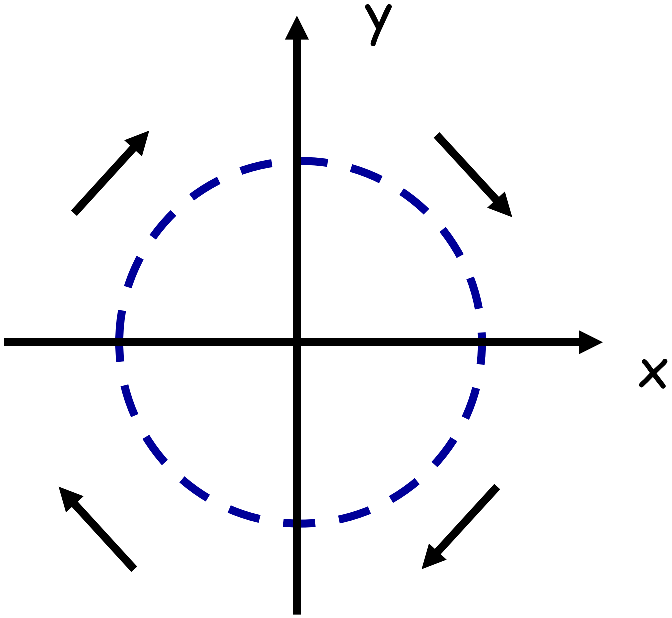
$$\begin{cases} \langle \hat{S}_x \rangle = \dfrac{\hbar}{2} \, \dfrac{1}{2} \, sen \, \alpha \quad 2 \, cos \, (\gamma \, B_0 \, t) \\[2ex] \langle \hat{S}_y \rangle = -\dfrac{\hbar}{2} \, \dfrac{1}{2} \, sen \, \alpha \quad 2 \, sen \, (\gamma \, B_0 \, t) \end{cases}$$

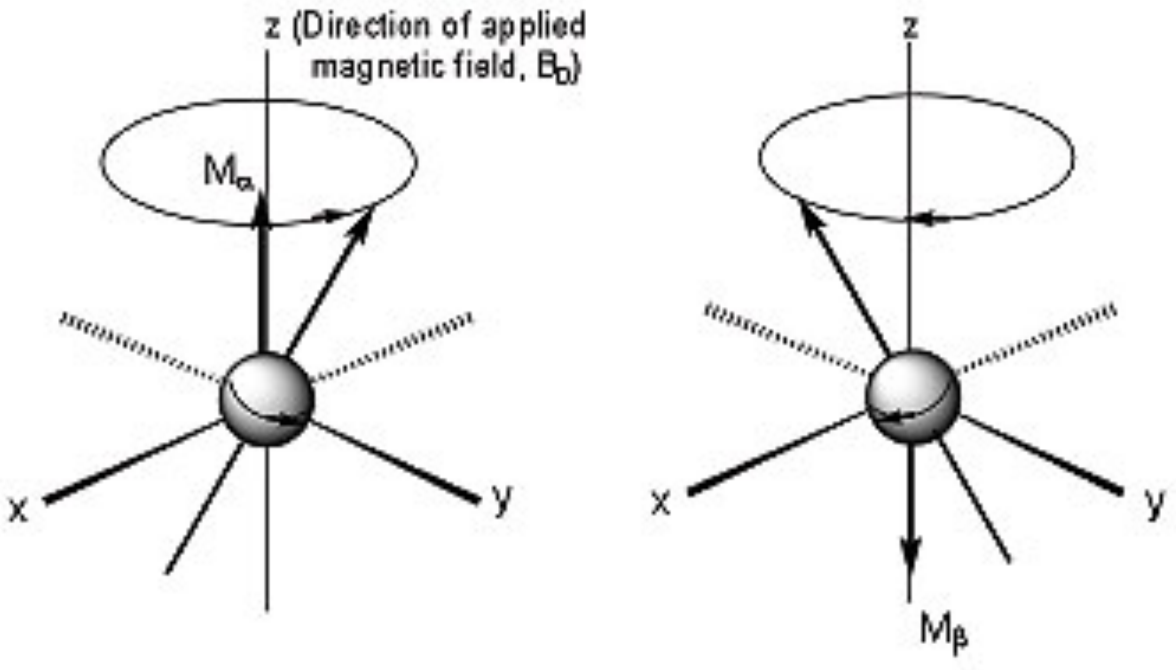
(Exercício)

$$\boxed{\omega = \gamma \, B_0 = \frac{g_s \, \mu_b B_0}{\hbar}}$$

frequência de Larmor

$$\begin{cases} \langle \hat{S}_x \rangle = \dfrac{\hbar}{2} \; \dfrac{1}{2} \, sen\, \alpha \quad 2 \, cos\, (\gamma \, B_0 \, t) \\[2ex] \langle \hat{S}_y \rangle = -\dfrac{\hbar}{2} \; \dfrac{1}{2} \, sen\, \alpha \quad 2 \, sen\, (\gamma \, B_0 \, t) \end{cases}$$



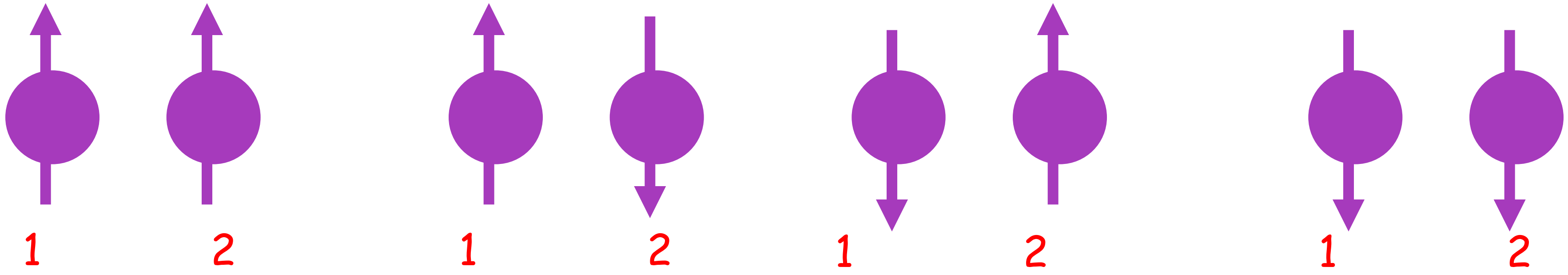



# Adição de spins

Vamos somar os spins de duas partículas de spin 1/2

Por exemplo: spin total do átomo de hidrogênio

Projeções na direção z




Classicamente somamos os dois vetores de spin:

$$\vec{S} = \vec{S}^{(1)} + \vec{S}^{(2)}$$

Função de onda (autoestado) de spin de duas partículas :

$$|\chi\rangle = |\chi_1\rangle\,|\chi_2\rangle = \chi_1\,\chi_2$$

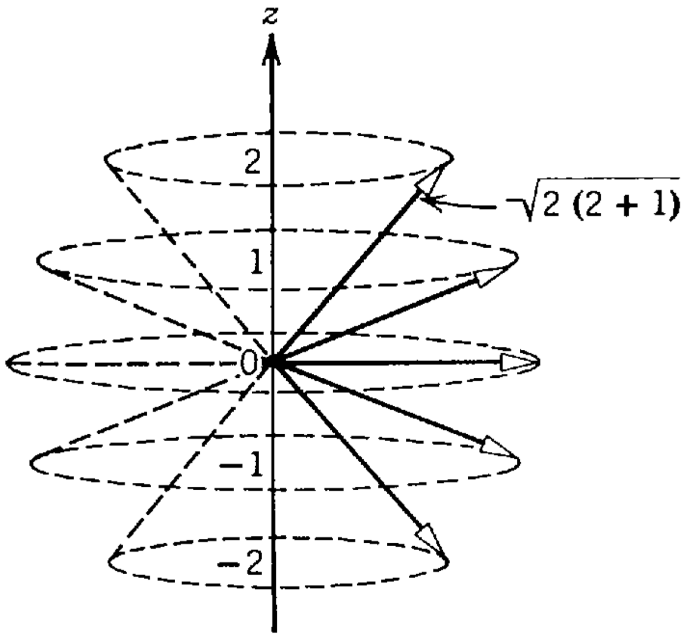
Autovalor de $S_z$ no estado composto :

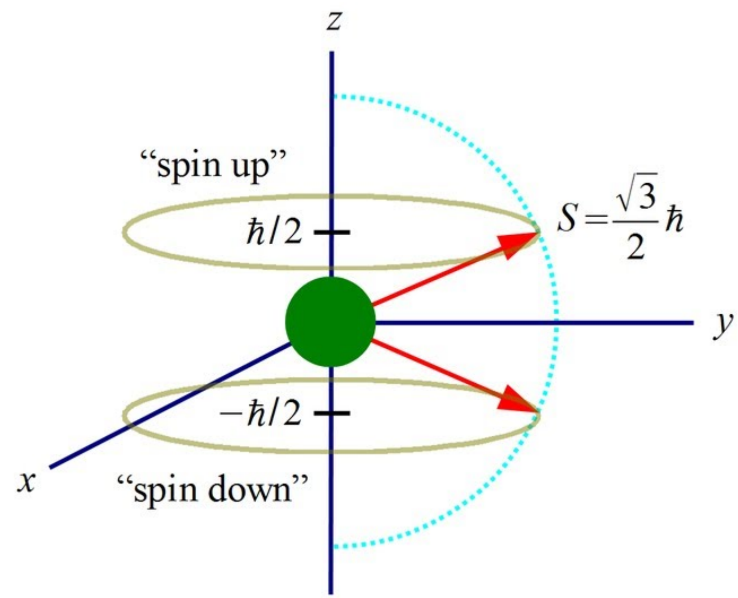
$$\vec{S} = \vec{S}^{(1)} + \vec{S}^{(2)} \longrightarrow \hat{S} = \hat{S}^{(1)} + \hat{S}^{(2)}$$

(operadores)

$$\hat{S}_z = \hat{S}_z^{(1)} + \hat{S}_z^{(2)} \longrightarrow S_z = S_z^{(1)} + S_z^{(2)}$$

$$S_z\,\chi_1\,\chi_2 = (S_z^{(1)} + S_z^{(2)})\chi_1\,\chi_2$$




$$L = \sqrt{l\,(l+1)}\,\hbar$$

$$L_z = m_l\,\hbar$$

$$-l \le m_l \le l$$

$$l = 0\,,\,1\,,\,2\,,\,\dots$$

$$S = \sqrt{s\,(s+1)}\,\hbar$$

$$\boxed{S_z = m_s\,\hbar}$$

$$s = \frac{1}{2} \qquad m_s = -\frac{1}{2}\,,\,+\frac{1}{2}$$

$$\boxed{\hat{S}_z\,\psi = m_s\,\hbar\,\psi}$$

$$S_z \chi_1 \chi_2 = (S_z^{(1)} + S_z^{(2)}) \chi_1 \chi_2$$

$$S_z \chi_1 \chi_2 = S_z^{(1)} \chi_1 \chi_2 + S_z^{(2)} \chi_1 \chi_2$$

$$S_z \chi_1 \chi_2 = m_1 \hbar \chi_1 \chi_2 + m_2 \hbar \chi_1 \chi_2$$

$$S_z \chi_1 \chi_2 = (m_1 + m_2) \hbar \chi_1 \chi_2$$

$$S_z \chi_1 \chi_2 = m \hbar \chi_1 \chi_2$$

| | | | |
|---|---|---|---|
| $\uparrow\uparrow$ | m = 1 | $\downarrow\uparrow$ | m = 0 |
| $\uparrow\downarrow$ | m = 0 | $\downarrow\downarrow$ | m = -1 |