Aula 9

Função de onda de duas partículas

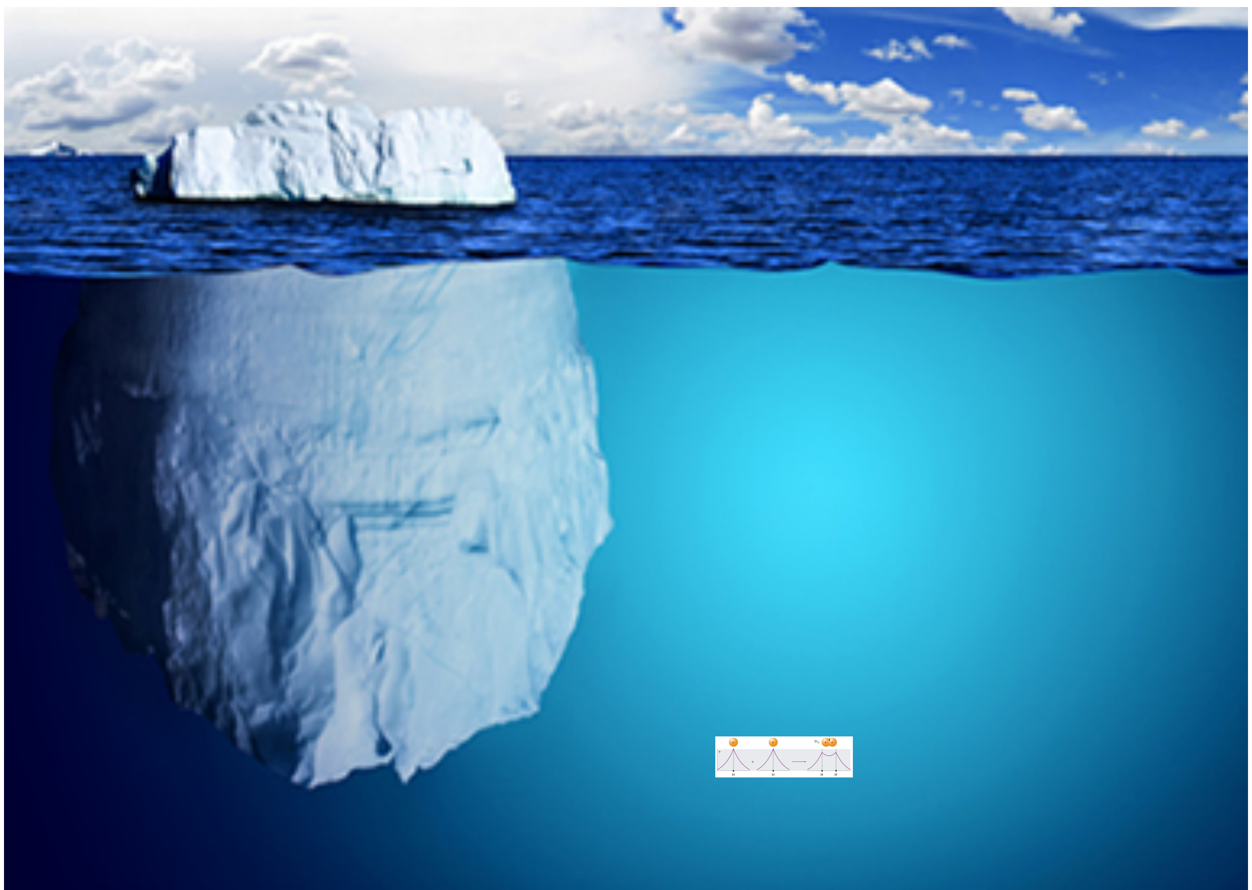
Adição de spins

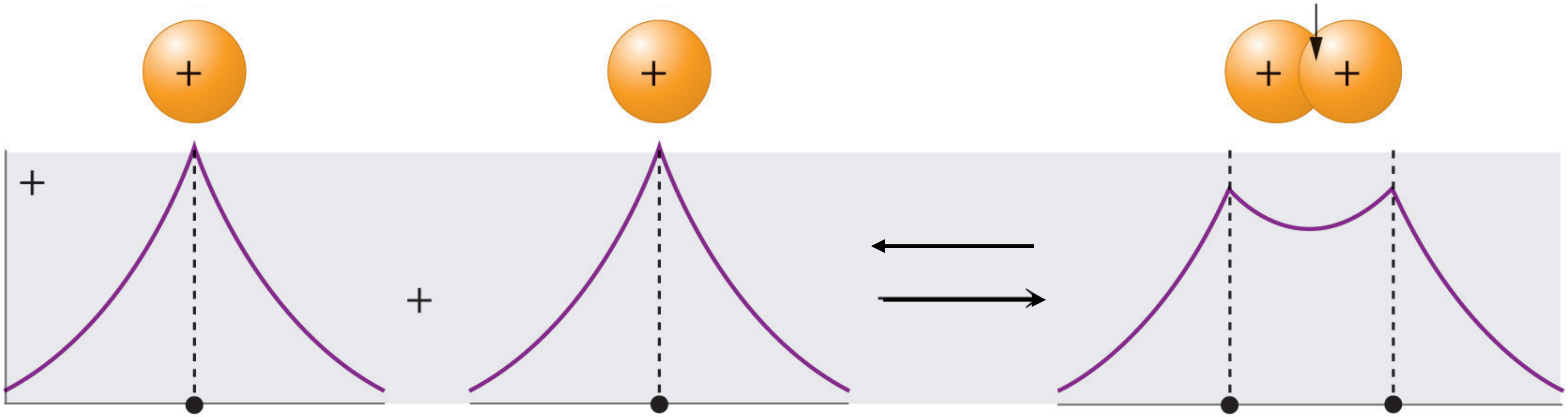
Exemplos

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

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

Porque a função de onda é o produto ?

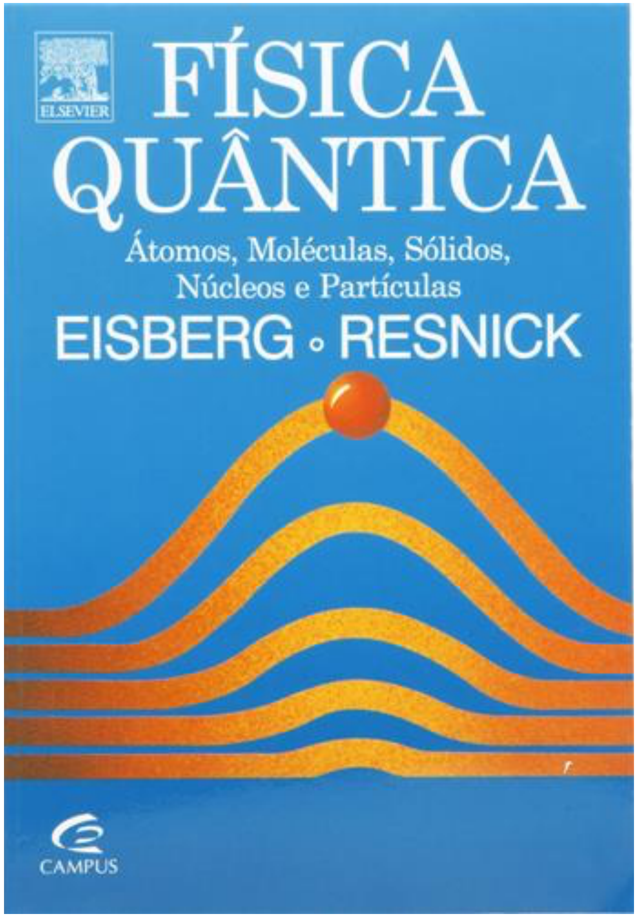




Cada partícula tem uma onda (extensa) associada

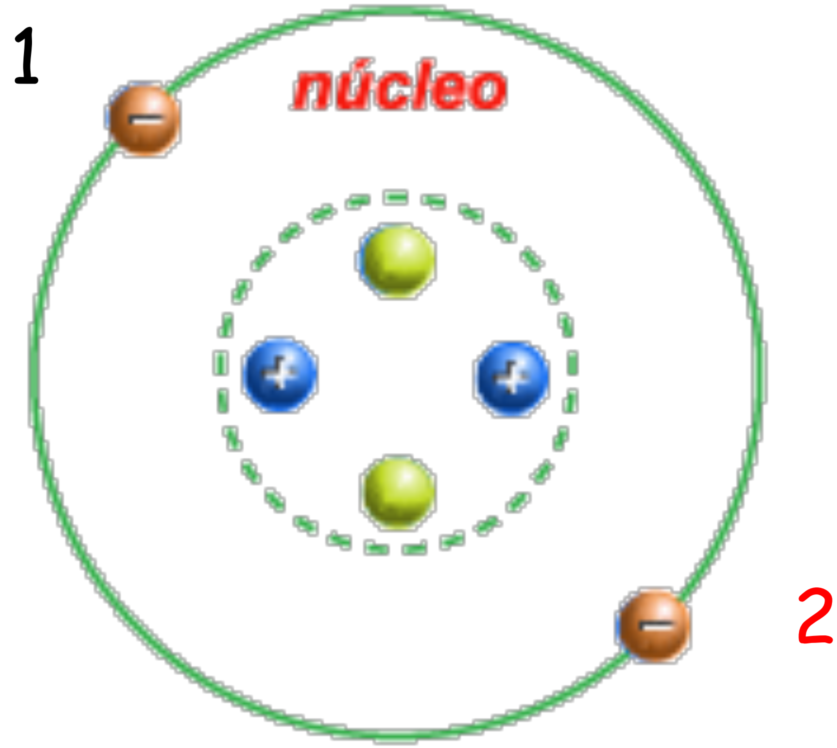
Quando dizer que dois corpos estão realmente separados ?

Sistemas de duas partículas



Capítulo 9

Sistemas de duas partículas



átomo de hélio

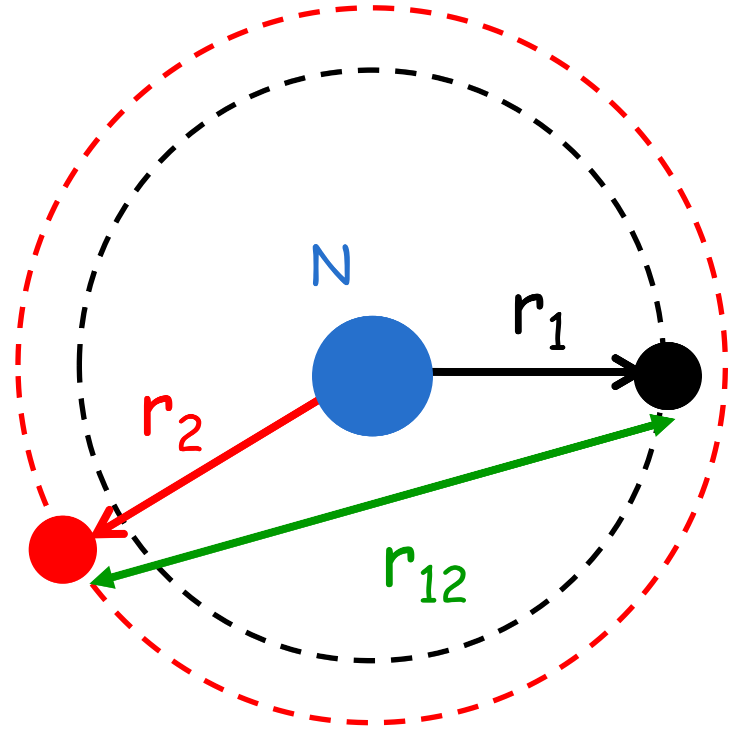
T_1 = energia cinética de 1

V_1 = energia potencial entre 1 e N

T_2 = energia cinética de 2

V_2 = energia potencial entre 2 e N

V_{12} = energia potencial entre 1 e 2



$$H_1 = T_1 + V_1$$

$$H_2 = T_2 + V_2$$

$$H_{12} = V_{12}$$

$$H = H_1 + H_2 + H_{12}$$

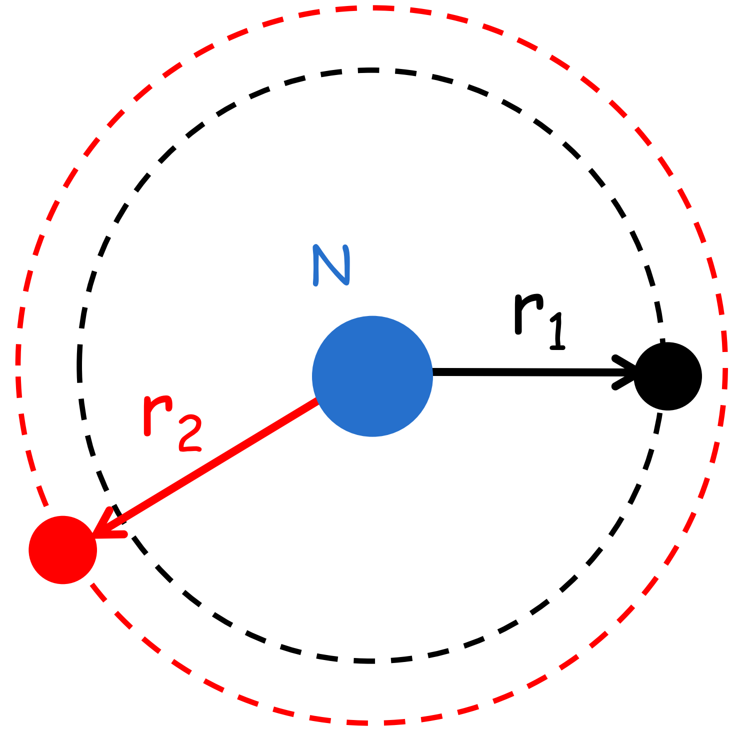
T_1 = energia cinética de 1

V_1 = energia potencial entre 1 e N

T_2 = energia cinética de 2

V_2 = energia potencial entre 2 e N

V_{12} = energia potencial entre 1 e 2



$$H_1 = T_1 + V_1$$

$$H_2 = T_2 + V_2$$

$$H_{12} = 0$$

$$H = H_1 + H_2$$

Desprezamos a interação entre os dois eletrons !!!

Função Hamiltoniana $\longrightarrow$ Operador Hamiltoniano

$$H = H_1 + H_2 \longrightarrow \begin{cases} \hat{H}_1 = -\dfrac{\hbar^2}{2\,m}\dfrac{\partial^2}{\partial x_1^2} + V_1 \\[2ex] \hat{H}_2 = -\dfrac{\hbar^2}{2\,m}\dfrac{\partial^2}{\partial x_2^2} + V_2 \end{cases}$$

$$\hat{H}\,\psi = E\,\psi$$

$$-\frac{\hbar^2}{2\,m}\frac{\partial^2\,\psi(x_1,x_2)}{\partial x_1^2} - \frac{\hbar^2}{2\,m}\frac{\partial^2\,\psi(x_1,x_2)}{\partial x_2^2} +$$

$$+\,V_1\,\psi(x_1,x_2) + V_2\,\psi(x_1,x_2) = E\,\psi(x_1,x_2)$$

$$-\frac{\hbar^2}{2\,m}\,\frac{\partial^2\,\psi(x_1,x_2)}{\partial x_1^2}\;-\;\frac{\hbar^2}{2\,m}\,\frac{\partial^2\,\psi(x_1,x_2)}{\partial x_2^2}+V_1\,\psi(x_1,x_2)\;+\;V_2\,\psi(x_1,x_2)\;=\;E\,\psi(x_1,x_2)$$

Ansatz : $\psi(x_1,x_2)\;=\;\psi_1(x_1)\,\psi_2(x_2)$

Substituimos $\psi(x_1,x_2)\;=\;\psi_1(x_1)\,\psi_2(x_2)$ e dividimos por $\psi_1(x_1)\,\psi_2(x_2)$

$$-\frac{\hbar^2}{2\,m}\,\frac{1}{\psi_1(x_1)}\,\frac{\partial^2\,\psi_1(x_1)}{\partial x_1^2}\;+\;V_1\;-\;\frac{\hbar^2}{2\,m}\,\frac{1}{\psi_2(x_2)}\,\frac{\partial^2\,\psi_2(x_2)}{\partial x_2^2}\;+\;V_2\;=\;E$$

Passamos as funções de x_2 para o lado direito :

$$-\frac{\hbar^2}{2\,m}\,\frac{1}{\psi_1(x_1)}\,\frac{\partial^2\,\psi_1(x_1)}{\partial x_1^2}\;+\;V_1(x_1)\;=\;E\;+\;\frac{\hbar^2}{2\,m}\,\frac{1}{\psi_2(x_2)}\,\frac{\partial^2\,\psi_2(x_2)}{\partial x_2^2}\;-\;V_2(x_2)$$

$$-\frac{\hbar^2}{2\,m}\,\frac{1}{\psi_1(x_1)}\,\frac{\partial^2\,\psi_1(x_1)}{\partial x_1^2}\;+\;V_1(x_1)\;=\;E\;+\;\frac{\hbar^2}{2\,m}\,\frac{1}{\psi_2(x_2)}\,\frac{\partial^2\,\psi_2(x_2)}{\partial x_2^2}\;-\;V_2(x_2)$$

$f(x_1) = g(x_2)$ verdade para qualquer x_1 e x_2 se $f(x_1) = g(x_2) = cte$

$$-\frac{\hbar^2}{2\,m}\,\frac{1}{\psi_1(x_1)}\,\frac{\partial^2\,\psi_1(x_1)}{\partial x_1^2}\;+\;V_1(x_1)\;=\;E\;+\;\frac{\hbar^2}{2\,m}\,\frac{1}{\psi_2(x_2)}\,\frac{\partial^2\,\psi_2(x_2)}{\partial x_2^2}\;-\;V_2(x_2)\;=\;E_1$$

$$\begin{cases}-\dfrac{\hbar^2}{2\,m}\,\dfrac{1}{\psi_1(x_1)}\,\dfrac{\partial^2\,\psi_1(x_1)}{\partial x_1^2}\;+\;V_1(x_1)\;=\;E_1\\[2ex]-\dfrac{\hbar^2}{2\,m}\,\dfrac{1}{\psi_2(x_2)}\,\dfrac{\partial^2\,\psi_2(x_2)}{\partial x_2^2}\;+\;V_2(x_2)\;=\;E\;-\;E_1\;=\;E_2\end{cases}$$

estas equações têm solução conhecida !!!

Encontramos $\psi(x_1, x_2) = \psi_1(x_1)\,\psi_2(x_2)$ e $E = E_1 + E_2$

Partículas independentes:

$$\psi(x_1, x_2) \;=\; \psi_1(x_1)\,\psi_2(x_2)$$

Produto é solução da ESIT !

E se forem matrizes ?

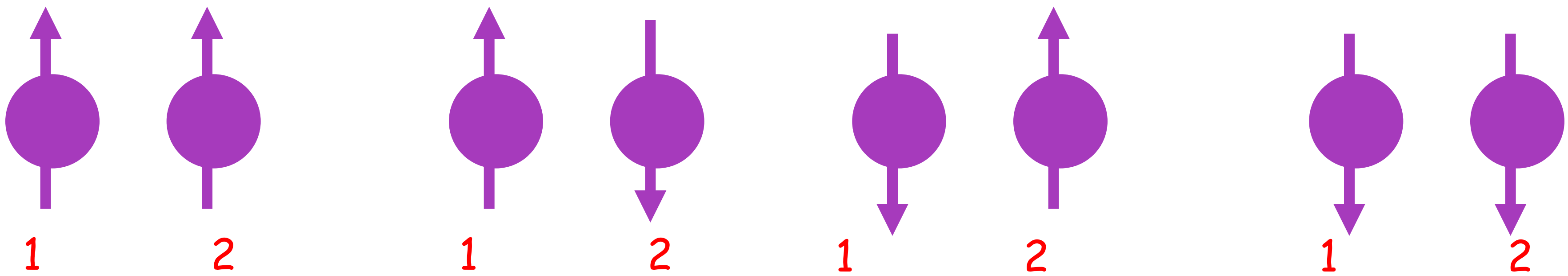
$$\psi(1,2) = \psi_s(1,2) = |\uparrow\uparrow\rangle = |\uparrow\rangle\,|\uparrow\rangle = \chi_+^{(1)}\,\chi_+^{(2)}$$

E a comutação ?

Tudo bem... elas estão em espaços diferentes

(espaço 1 da partícula 1 ; espaço 2 da partícula 2)

Projeção do spin total na direção z



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

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

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

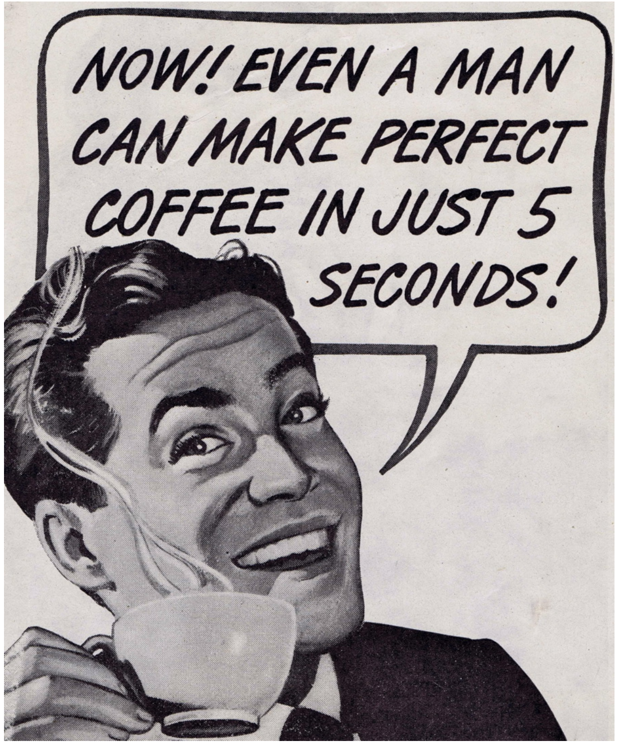
$$= (m_1 + m_2)\,\hbar\,\chi_1\,\chi_2$$

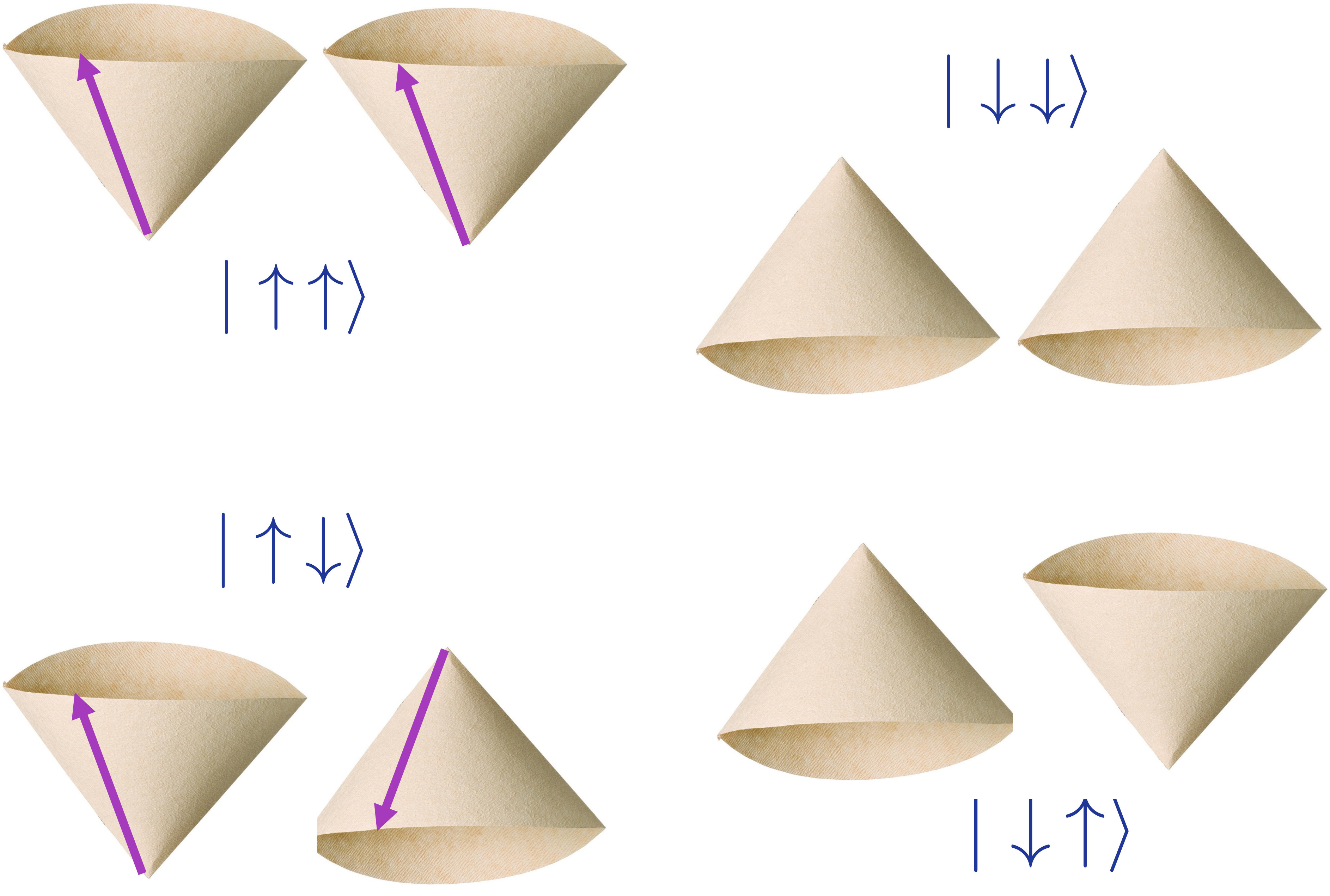
$$\boxed{S_z\,\chi_1\,\chi_2 = m\,\hbar\,\chi_1\,\chi_2} \qquad m = (m_1 + m_2)$$

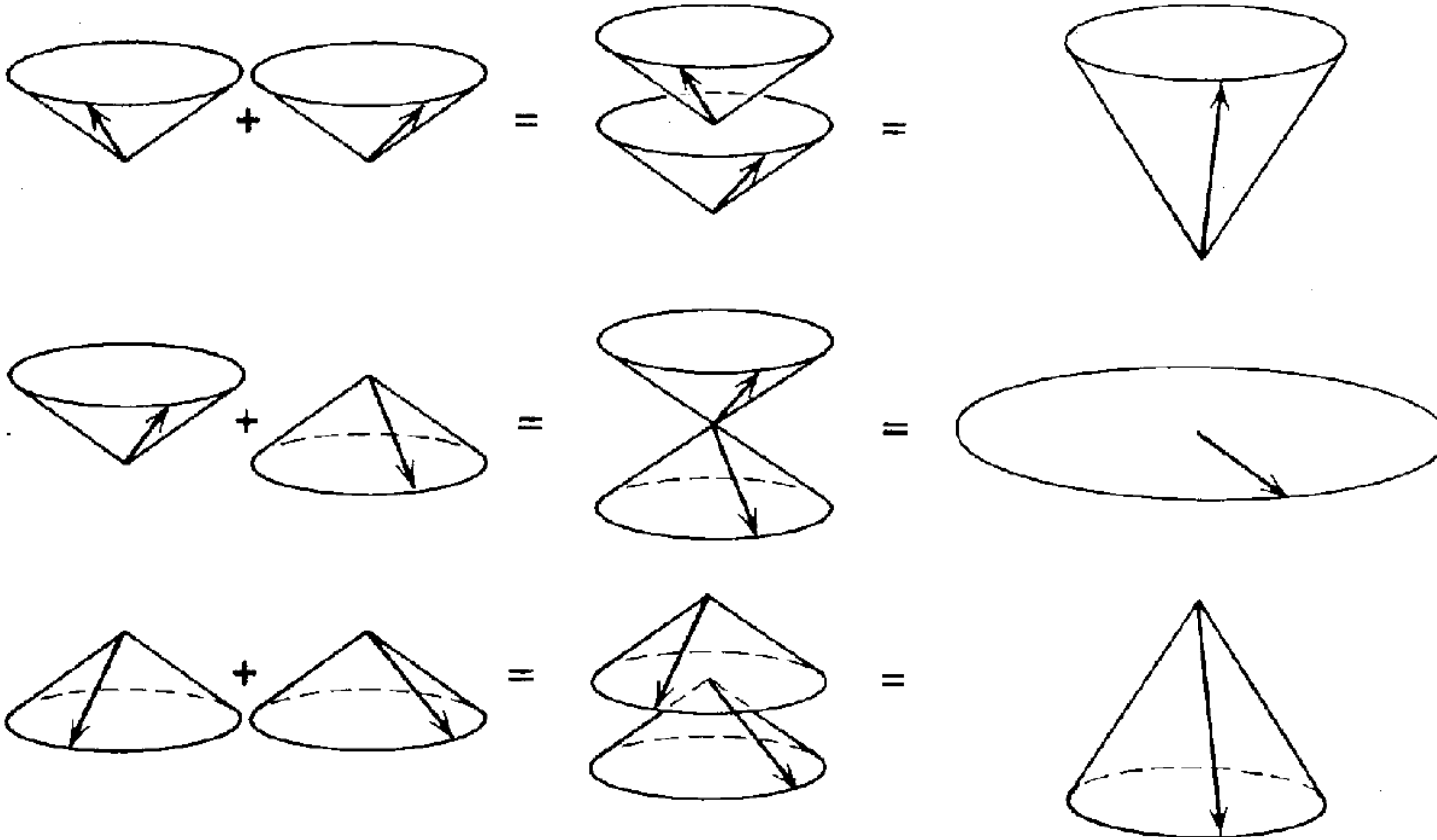
m = 1 m = -1 m = 0 m = 0

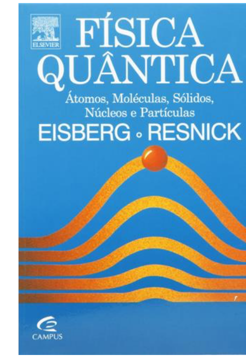
Vamos "ver" os spins das duas partículas

Faça você mesmo em casa !




$|\uparrow\uparrow\rangle$
$|\downarrow\downarrow\rangle$
$|\uparrow\downarrow\rangle$
$|\downarrow\uparrow\rangle$

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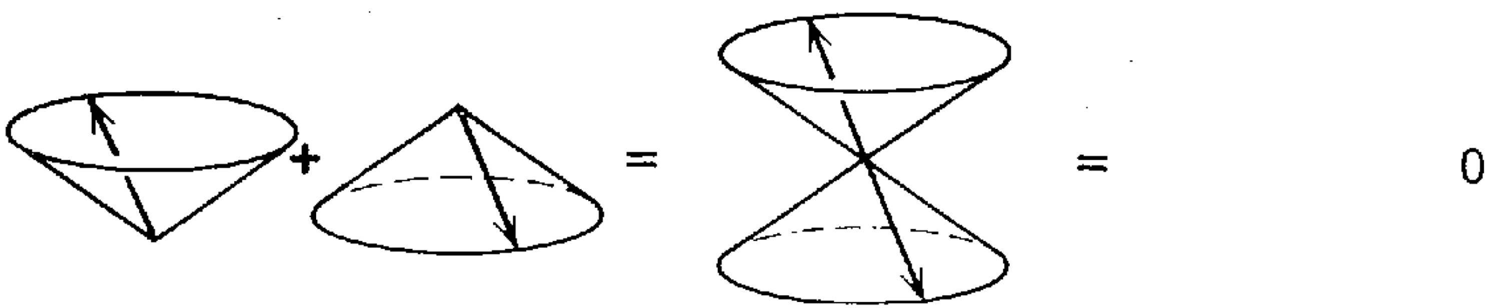
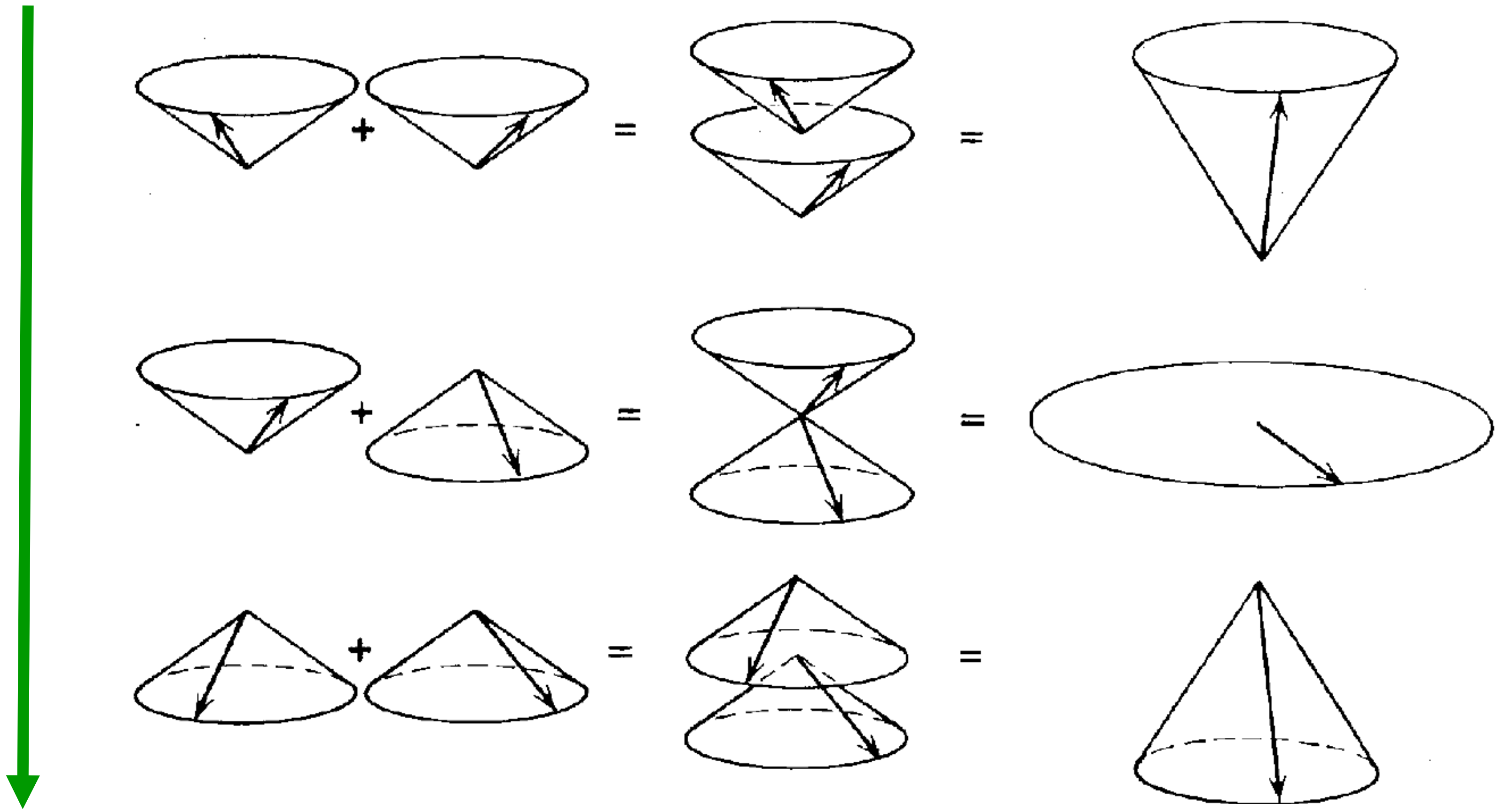

0



As três combinações estão conectadas pelo operador escada !

O conjunto é chamado tripleto !

Vamos "abaixar" o spin do estado

$$|\uparrow\uparrow\rangle \;=\; \chi_{+}^{(1)}\,\chi_{+}^{(2)}$$

Lembramos que :

$$\hat{S}_+ \,|\downarrow\rangle = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\boxed{\hat{S}_+ \,|\downarrow\rangle = \hbar |\uparrow\rangle}$$

$$\hat{S}_+ \,|\uparrow\rangle = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\boxed{\hat{S}_+ \,|\uparrow\rangle = 0}$$

$$\hat{S}_- \,|\uparrow\rangle = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\boxed{\hat{S}_- \,|\uparrow\rangle = \hbar |\downarrow\rangle}$$

$$\hat{S}_- \,|\downarrow\rangle = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\boxed{\hat{S}_- \,|\downarrow\rangle = 0}$$

$$S_- = S_-^{(1)} + S_-^{(2)}$$

$$S_- \, \chi_+^{(1)} \, \chi_+^{(2)} = (S_-^{(1)} + S_-^{(2)}) \chi_+^{(1)} \, \chi_+^{(2)}$$

$$= S_-^{(1)} \, \chi_+^{(1)} \, \chi_+^{(2)} + S_-^{(2)} \, \chi_+^{(1)} \, \chi_+^{(2)}$$

$$= \hbar \, \chi_-^{(1)} \, \chi_+^{(2)} + \hbar \, \chi_+^{(1)} \, \chi_-^{(2)}$$

$$\boxed{S_- \, |\uparrow\uparrow\rangle = \hbar \, (|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle)}$$

Vamos "abaixar" o spin do estado

$$|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle$$

$$S_- \left[\hbar\,\chi_-^{(1)}\,\chi_+^{(2)} + \hbar\,\chi_+^{(1)}\,\chi_-^{(2)}\right] =$$

$$= S_-^{(1)} \left[\underset{0}{\hbar\,\chi_-^{(1)}\,\chi_+^{(2)}} + \hbar\,\chi_+^{(1)}\,\chi_-^{(2)}\right] +$$

$$+ S_-^{(2)} \left[\hbar\,\chi_-^{(1)}\,\chi_+^{(2)} + \underset{0}{\hbar\,\chi_+^{(1)}\,\chi_-^{(2)}}\right]$$

$$S_- \left[\hbar\,\chi_-^{(1)}\,\chi_+^{(2)} + \hbar\,\chi_+^{(1)}\,\chi_-^{(2)}\right] =$$

$$= \hbar^2\,\chi_-^{(1)}\,\chi_-^{(2)} + \hbar^2\,\chi_-^{(1)}\,\chi_-^{(2)} = 2\,\hbar^2\,\chi_-^{(1)}\,\chi_-^{(2)}$$

$$\boxed{S_-\,\hbar\,(\,|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\,) = 2\,\hbar^2\,|\downarrow\downarrow\rangle}$$

Três estados $|s, m_s\rangle$ conectados por S_- :

$$|1,1\rangle \rightarrow |1,0\rangle \rightarrow |1,-1\rangle$$

Este é o tripleto de spin 1

Vamos mostrar que o tripleto tem spin 1

Vamos verificar que todos eles têm spin 1

$$S^2 = \vec{S} \, . \, \vec{S} = \left(\vec{S}^{(1)} + \vec{S}^{(2)} \right) . \left(\vec{S}^{(1)} + \vec{S}^{(2)} \right)$$

$$S^2 = \left(S^{(1)} \right)^2 + \left(S^{(2)} \right)^2 + 2 \, \vec{S}^{(1)} \, . \, \vec{S}^{(2)}$$

$$= \left(S^{(1)} \right)^2 + \left(S^{(2)} \right)^2 + 2 \left(S_x^{(1)} \, . \, S_x^{(2)} + S_y^{(1)} \, . \, S_y^{(2)} + S_z^{(1)} \, . \, S_z^{(2)} \right)$$

$$S^2 \, |1\,1\rangle = S^2 \, \chi_+^{(1)} \, \chi_+^{(2)}$$

$$= \left(S^{(1)} \right)^2 \chi_+^{(1)} \, \chi_+^{(2)} + \left(S^{(2)} \right)^2 \chi_+^{(1)} \, \chi_+^{(2)} +$$

$$+ 2 \left(S_x^{(1)} \, . \, S_x^{(2)} + S_y^{(1)} \, . \, S_y^{(2)} + S_z^{(1)} \, . \, S_z^{(2)} \right) \chi_+^{(1)} \, \chi_+^{(2)}$$

Vamos usar :

$$S_z\,\chi_+ = \frac{\hbar}{2}\,\chi_+ \qquad S_x\,\chi_- = \frac{\hbar}{2}\,\chi_+ \qquad S_y\,\chi_+ = -\frac{\hbar}{2i}\,\chi_-$$

$$S_z\,\chi_- = -\frac{\hbar}{2}\,\chi_- \qquad S_x\,\chi_+ = \frac{\hbar}{2}\,\chi_- \qquad S_y\,\chi_- = \frac{\hbar}{2i}\,\chi_+$$

$$S^2\,\chi_+ = \frac{3}{4}\,\hbar^2\,\chi_+ \qquad S^2\,\chi_- = \frac{3}{4}\,\hbar^2\,\chi_-$$

Exercício

$$= \left(S^{(1)}\right)^2 \chi_+^{(1)}\,\chi_+^{(2)} + \left(S^{(2)}\right)^2 \chi_+^{(1)}\,\chi_+^{(2)} +$$

$$+\,2\left(S_x^{(1)}\,.\,S_x^{(2)} + S_y^{(1)}\,.\,S_y^{(2)} + S_z^{(1)}\,.\,S_z^{(2)}\right)\chi_+^{(1)}\,\chi_+^{(2)}$$

$$= \left(S^{(1)}\right)^2 \chi_+^{(1)} \chi_+^{(2)} + \left(S^{(2)}\right)^2 \chi_+^{(1)} \chi_+^{(2)} +$$

$$+\, 2 \left(S_x^{(1)} . S_x^{(2)} + S_y^{(1)} . S_y^{(2)} + S_z^{(1)} . S_z^{(2)}\right) \chi_+^{(1)} \chi_+^{(2)}$$

$$= \frac{3}{4} \hbar^2 \chi_+^{(1)} \chi_+^{(2)} + \frac{3}{4} \hbar^2 \chi_+^{(1)} \chi_+^{(2)} +$$

$$+\, 2\, \cancel{\frac{\hbar}{2} \chi_-^{(1)} \frac{\hbar}{2} \chi_-^{(2)} + 2\,(-1)\, \frac{\hbar}{2i} \chi_-^{(1)}\, (-1) \frac{\hbar}{2i} \chi_-^{(2)}} + 2\, \frac{\hbar}{2} \chi_+^{(1)} \frac{\hbar}{2} \chi_+^{(2)}$$

$$= \frac{3}{2} \hbar^2 \chi_+^{(1)} \chi_+^{(2)} + \frac{\hbar^2}{2} \chi_+^{(1)} \chi_+^{(2)} = 2\hbar^2 \chi_+^{(1)} \chi_+^{(2)}$$

$$\boxed{S^2 \chi_+^{(1)} \chi_+^{(2)} = 2\hbar^2 \chi_+^{(1)} \chi_+^{(2)}}$$

$$\boxed{S^2\,\chi_+^{(1)}\,\chi_+^{(2)} \;=\; 2\hbar^2\,\chi_+^{(1)}\,\chi_+^{(2)}}$$

Lembrando que
$$\left\{\begin{aligned} \hat{S}^2\,\psi &= s\,(s+1)\,\hbar^2\,\psi \\ \hat{S}_z\,\psi &= m_s\,\hbar\,\psi \end{aligned}\right.$$

$$S^2\,\chi_+^{(1)}\,\chi_+^{(2)} \;=\; s\,(s+1)\,\hbar^2\,\chi_+^{(1)}\,\chi_+^{(2)}$$

$$s\,(s+1)\;=2$$

$$\boxed{s \;=\; 1}$$

Exercício: verifique que os estados abaixo tem spin 1

$$|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle = \chi_-^{(1)}\,\chi_+^{(2)} + \chi_+^{(1)}\,\chi_-^{(2)}$$

$$|\downarrow\downarrow\rangle = \chi_-^{(1)}\,\chi_-^{(2)}$$

Exercício: verifique que o estado abaixo tem spin 0

$$|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle = \chi_-^{(1)}\,\chi_+^{(2)} - \chi_+^{(1)}\,\chi_-^{(2)}$$

Não são 4 combinações ! São 3 + 1 !

$$\left\{ \begin{array}{l} |\uparrow\uparrow\rangle \\ \\ |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle \\ \\ |\downarrow\downarrow\rangle \end{array} \right.$$

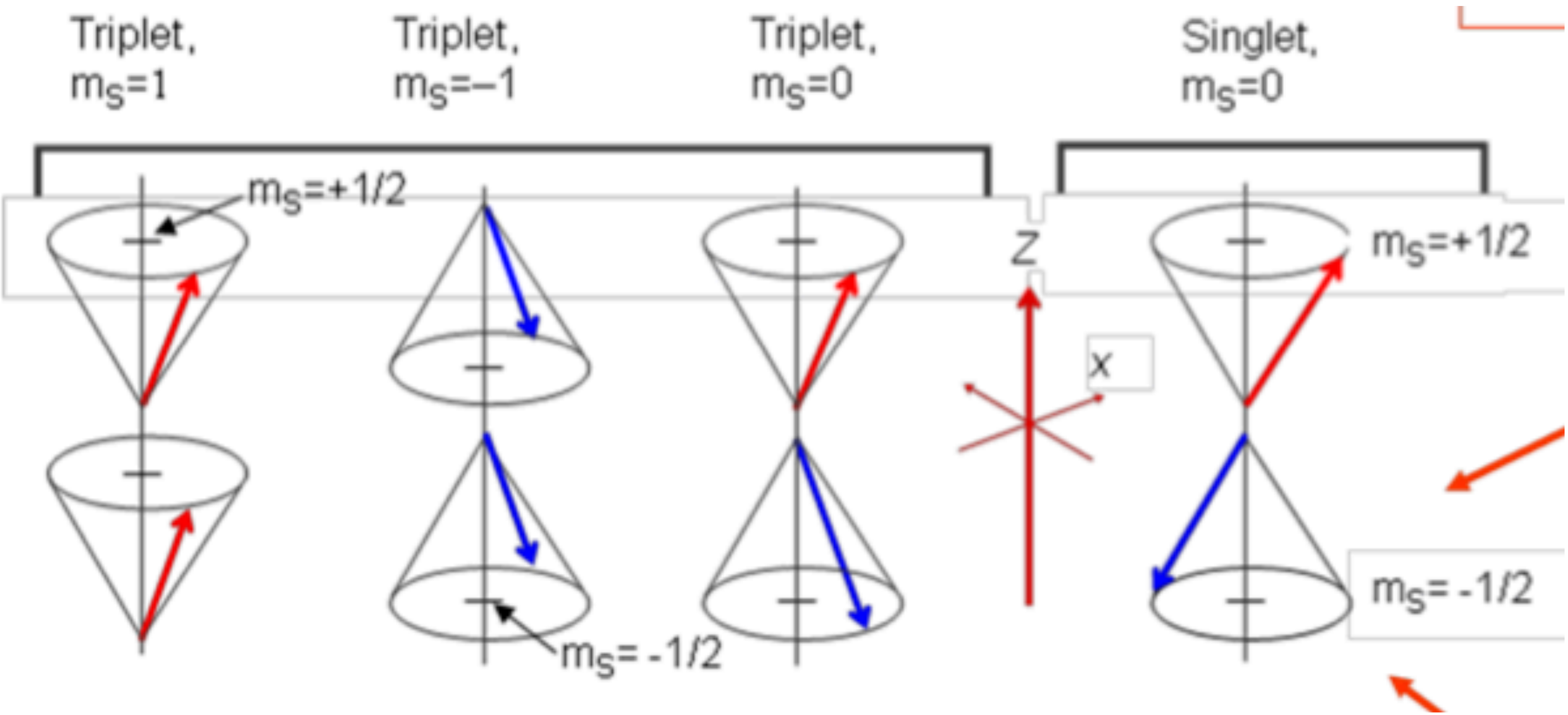
Tripleto de spin 1

Conectados pelos operadores escada

$$|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle$$

Singleto de spin 0

"aniquilado" pela escada



Triplet,
m_S=1
Triplet,
m_S=–1
Triplet,
m_S=0
Singlet,
m_S=0
m_S=+1/2
Z
X
m_S=+1/2
m_S= -1/2
m_S= -1/2

Simetria de troca da função de onda

$$1 \rightarrow 2 \qquad\qquad 2 \rightarrow 1$$

$$\left\{ \begin{array}{l} |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle \;\rightarrow\; |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \\ \\ |\downarrow\downarrow\rangle \;\rightarrow\; |\downarrow\downarrow\rangle \\ \\ |\uparrow\uparrow\rangle \;\rightarrow\; |\uparrow\uparrow\rangle \end{array} \right.$$

Tripleto é simétrico !!!

$$|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \;\rightarrow\; |\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle = -\left[\, |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \,\right]$$

Singleto é antissimétrico !!!