Adição de Momento Angular Orbital e Spin

Vamos considerar uma partícula de Spin 1/2 e momento angular orbital $\vec{L}$. Então temos

$$\vec{J} = \vec{L} + \vec{S}$$

Então j pode ter valores

$$l - 1/2 \leq j \leq l + 1/2$$

Mas isto resulta em só 2 possíveis valores

$$j = l \pm 1/2$$

Os estados produto são

$|l, m_l; s, m_s\rangle$ onde $s = 1/2$ e $m_s = \pm\frac{1}{2}$

$\Rightarrow$ Base produto é

$$\left\{ |l, m_l; \tfrac{1}{2}, +\tfrac{1}{2}\rangle , |l, m_l; \tfrac{1}{2}, -\tfrac{1}{2}\rangle \right\}$$

$\forall l$ e $-l \leq m_l \leq l$

A base do momento angular total é

$|j, m\rangle$

$= \{|j = l + \frac{1}{2}, m\rangle, |j = l - \frac{1}{2}, m\rangle\}$

$\forall l$, e tal que

$$-j \leq m \leq j$$

Expandindo cada um deles na base produto, temos

$$|j = l + 1/2, m\rangle = \alpha\,|l, m - \tfrac{1}{2}; \tfrac{1}{2}, +\tfrac{1}{2}\rangle + \beta\,|l, m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

e

$$|j = l - \tfrac{1}{2}, m\rangle = \alpha'\,|l, m - \tfrac{1}{2}; \tfrac{1}{2}, +\tfrac{1}{2}\rangle + \beta'\,|l, m + \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

onde usamos o fato que

$$m = m_l + m_s \Rightarrow m = m_l \pm \tfrac{1}{2}$$

$$\Rightarrow \boxed{m_l = m \mp \tfrac{1}{2}}$$

Para obter os coeficientes α, β, α' e β' impomos que esses estados sejam ortonormais

$$\Rightarrow \quad \alpha^2 + \beta^2 = 1$$
$$\alpha'^2 + \beta'^2 = 1$$

e

$$\alpha\alpha' + \beta\beta' = 0$$

onde assumimos que os coeficientes são reais por convenção. Mas ainda precisamos mais um vínculo para resolver para os 4 coeficientes.

Para isso usamos o fato que a ação de J^2 nos estados da base soma é conhecida. Por exemplo,

$$\left\{ \begin{aligned} J^2 |l+1/2, m\rangle &= \hbar^2 (l+1/2)(l+\tfrac{1}{2}+1)|l+\tfrac{1}{2}, m\rangle \\ &= \hbar^2 (l+\tfrac{1}{2})(l+\tfrac{3}{2})|l+\tfrac{1}{2}, m\rangle \end{aligned} \right\}$$

Mas $J^2 = L^2 + S^2 + 2\vec{L}\cdot\vec{S}$

Mas $\vec{L}\cdot\vec{S} = L_x S_x + L_y S_y + L_z S_z$

Dado que

$$L_\pm = L_x \pm i L_y$$

$$\Rightarrow \begin{cases} L_x = \dfrac{L_+ + L_-}{2} \\ L_y = \dfrac{L_+ - L_-}{2i} \end{cases}$$

E, similarmente, para S_x e S_y temos

$$\begin{cases} S_x = \dfrac{S_+ + S_-}{2} \\ S_y = \dfrac{S_+ - S_-}{2i} \end{cases}$$

$$\Rightarrow L_x S_x + L_y S_y = \frac{(L_+ + L_-)(S_+ + S_-)}{4} - \frac{(L_+ - L_-)(S_+ - S_-)}{4}$$

$$= \frac{L_+ S_- + L_- S_+}{2}$$

$$\Rightarrow J^2 = L^2 + S^2 + L_+ S_- + L_- S_+ + 2 L_z S_z$$

$$\Rightarrow J^2 |l+\tfrac{1}{2}, m\rangle = \left(L^2 + S^2 + 2L_zS_z + L_+S_- + L_-S_+\right)$$

$$\times \left\{ \alpha |l, m-\tfrac{1}{2}; \tfrac{1}{2}, +\tfrac{1}{2}\rangle + \beta |l, m+\tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}\rangle \right\}$$

$$= \hbar^2 \left\{ \left[l(l+1) + \frac{3}{4} + 2\left(m-\tfrac{1}{2}\right)\tfrac{1}{2} \right] \alpha |l, m-\tfrac{1}{2}; \tfrac{1}{2}, +\tfrac{1}{2}\rangle \right.$$

$$+ \left[l(l+1) + \frac{3}{4} + 2\left(m+\tfrac{1}{2}\right)\left(-\tfrac{1}{2}\right) \right] \beta |l, m+\tfrac{1}{2}; \tfrac{1}{2}; -\tfrac{1}{2}\rangle$$

$$\sqrt{\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\left(\tfrac{1}{2}-\tfrac{1}{2}+1\right)} \sqrt{\left(l-m+\tfrac{1}{2}\right)\left(l+m-\tfrac{1}{2}+1\right)} \, \alpha |l, m+\tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

$$+ \sqrt{\left(\tfrac{1}{2}+\tfrac{1}{2}\right)\left(\tfrac{1}{2}-\tfrac{1}{2}+1\right)} \sqrt{\left(l+m+\tfrac{1}{2}\right)\left(l-m-\tfrac{1}{2}+1\right)} \, \beta |l, m-\tfrac{1}{2}; \tfrac{1}{2}, +\tfrac{1}{2}\rangle$$

onde usamos

$$J_\pm |j, m\rangle = \sqrt{(j \mp m)(j \pm m + 1)} \, \hbar \, |j, m \pm 1\rangle$$

para $J_\pm = L_\pm$ ou $S_\pm$

$$\Rightarrow \hbar^2 (l+\tfrac{1}{2})(l+\tfrac{3}{2}) \left\{ \alpha | l, m-\tfrac{1}{2}; \tfrac{1}{2}, +\tfrac{1}{2} \rangle + \beta | l, m+\tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} \rangle \right\}$$

$$= \hbar^2 \left\{ \left(\alpha \left[l(l+1) + \tfrac{3}{4} + m - \tfrac{1}{2} \right] + \beta \sqrt{(l+m+\tfrac{1}{2})(l-m+\tfrac{1}{2})} \right) | l, m-\tfrac{1}{2}; \tfrac{1}{2}, +\tfrac{1}{2} \rangle \right.$$

$$\left. + \left(\beta \left[l(l+1) + \tfrac{3}{4} - m - \tfrac{1}{2} \right] + \alpha \sqrt{(l-m+\tfrac{1}{2})(l+m+\tfrac{1}{2})} \right) | l, m+\tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2} \rangle \right\}$$

$$\Rightarrow \begin{cases} \alpha (l+\tfrac{1}{2})(l+\tfrac{3}{2}) = \alpha \left[l(l+1) + \tfrac{3}{4} + m - \tfrac{1}{2} \right] + \beta \sqrt{(l+m+\tfrac{1}{2})(l-m+\tfrac{1}{2})} \\ \beta (l+\tfrac{1}{2})(l+\tfrac{3}{2}) = \beta \left[l(l+1) + \tfrac{3}{4} - m - \tfrac{1}{2} \right] + \alpha \sqrt{(l-m+\tfrac{1}{2})(l+m+\tfrac{1}{2})} \end{cases}$$

$$\Rightarrow \begin{cases} \alpha (l - m + \tfrac{1}{2}) = \beta \sqrt{(l+m+\tfrac{1}{2})(l-m+\tfrac{1}{2})} \\ \beta (l + m - \tfrac{1}{2}) = \alpha \sqrt{(l-m+\tfrac{1}{2})(l+m+\tfrac{1}{2})} \end{cases}$$

$$\Rightarrow \boxed{\frac{\beta}{\alpha} = \sqrt{\frac{l - m + 1/2}{l + m + 1/2}}}$$

Então, $\alpha^2 + \beta^2 = 1 \Rightarrow$

$$\alpha^2 \left(1 + \frac{l - m + 1/2}{l + m + 1/2} \right) = 1$$

$$\Rightarrow \alpha^2 \frac{2l + 1}{l + m + 1/2} = 1$$

$$\boxed{\alpha = \sqrt{\frac{l + m + 1/2}{2l + 1}}}$$

$$\beta = \sqrt{\frac{l - m + 1/2}{l + m + 1/2}} \cdot \sqrt{\frac{l + m + 1/2}{2l + 1}}$$

$$\Rightarrow \boxed{\beta = \sqrt{\frac{l - m + 1/2}{2l + 1}}}$$

Finalmente, de $\alpha\alpha' + \beta\beta' = 0$

$$\beta'^2 = 1 - \alpha'^2$$

$$\Rightarrow \quad \alpha\alpha' + \beta\sqrt{1-\alpha'^2} = 0 \quad (\dagger)$$

$$\Rightarrow \quad \alpha^2\alpha'^2 = \beta^2(1-\alpha'^2)$$

$$\alpha'^2 = \frac{\beta^2}{\alpha^2}(1-\alpha'^2)$$

$$\alpha'^2\left(1+\frac{\beta^2}{\alpha^2}\right) = \frac{\beta^2}{\alpha^2}$$

$$\alpha'^2\left(1+\frac{l-m+1/2}{l+m+1/2}\right) = \frac{l-m+1/2}{l+m+1/2}$$

$$\alpha'^2\,\frac{2l+1}{l+m+1/2} = \frac{l-m+1/2}{l+m+1/2}$$

$$\Rightarrow \quad \boxed{\alpha' = -\sqrt{\frac{l-m+1/2}{2l+1}}} \quad (-) \text{ pg. } (\dagger)$$

$$\beta' = \sqrt{1-\frac{l-m+1/2}{2l+1}} = \sqrt{\frac{l+m+1/2}{2l+1}}$$

$$\Rightarrow |j=l+1/2, m\rangle = \frac{1}{\sqrt{2l+1}}\left\{\sqrt{l+m+1/2}\,|l, m-\tfrac{1}{2}; \tfrac{1}{2}, +\tfrac{1}{2}\rangle + \sqrt{l-m+1/2}\,|l, m+1/2; \tfrac{1}{2}, -1/2\rangle\right\}$$

$$|j=l-\tfrac{1}{2}, m\rangle = \frac{1}{\sqrt{2l+1}}\left\{-\sqrt{l-m+1/2}\,|l, m-1/2; \tfrac{1}{2}, +1/2\rangle + \sqrt{l+m+1/2}\,|l, m+1/2; \tfrac{1}{2}, -\tfrac{1}{2}\rangle\right\}$$

A ~~base~~ soma é de utilidade em casos nos quais temos, a base soma no Hamiltoniano como por exemplo, um termo no

$$\propto \vec{L}\cdot\vec{S}$$

Dado que $\quad \vec{L}\cdot\vec{S} = \frac{1}{2}\left(J^2 - L^2 - S^2\right)$

vemos que os estados da base soma $|j, m\rangle$ são auto estados de $\vec{L}\cdot\vec{S}$.

Notação Espetroscópica

$$^{2S+1}L_J$$

onde $L = S, P, D$ quer dizer $l = 0, 1, 2$ denota momento angular orbital, J é j - corresponde à soma de $\vec{S}+\vec{L}=\vec{J}$. O $2S+1$ à esquerda indica a multiplicidade do spin.

Ex: $\quad {}^2P_{3/2}$ é $s=1/2$; $j=3/2$, $l=1$

Se temos mais do que 1 elétron $\Rightarrow$ devemos somar os spins e os momentos angulares orbitais de cada um. Por exemplo, o estado fundamental do He tem 2 elétrons com $s=0$, $l=0$, $j=0$

$$\Rightarrow \; {}^1S_0$$