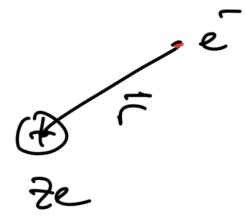
Atome d'hydrogène

structure principale de H : théorie de Schrödinger

$$\mathcal{H} = \frac{\vec{p}^2}{2\mu} - \frac{Ze^2}{4\pi\varepsilon_0 r} \qquad \mu \to m$$



$$E_n = -\frac{R_y}{n^2} \qquad R_y = \frac{\hbar^2}{2ma_0^2} = 13.6\,\mathrm{eV}$$

$n = 1, 2, \ldots, \infty$

$$\psi_{nlm}(r, \vartheta, \phi) = \underbrace{R_{nl}(r)}_{\text{pol. d'ordre } n-1} \; Y_{lm}(\vartheta, \phi)$$

$l = 0, \ldots, n-1 \qquad\qquad m = -l, \ldots, l$

$\hat{\vec{L}}^2 \to \hbar^2 l(l+1) \qquad\qquad \hat{L}^z$

$(\mathcal{H}, \vec{L}^2, L^z \to \text{ECOC})$

électron : m, e, spin

$\hat{\vec{S}}$

$$[\hat{S}^\alpha, \hat{S}^\beta] = i\hbar\, \epsilon_{\alpha\beta\gamma}\, \hat{S}^\gamma$$

moment magnétique :

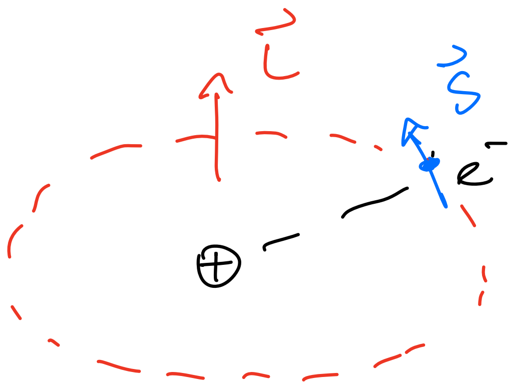
$$\vec{m} = \frac{g\mu_B}{\hbar}\vec{S}$$

$$g \simeq -2 \qquad\qquad \mu_B = \frac{e\hbar}{2m} = 9.27 \times 10^{-24}\ \frac{\mathrm{J}}{\mathrm{T}}$$

magnéton de Bohr

$$|\vec{S}|^2 \to \hbar^2\, s(s+1) \qquad s = \frac{1}{2}$$

Composition des moments cinétiques en MQ



$\vec{S}$ = moment cinétique intrinsèque (de spin)

$\vec{L}$ = " " orbitalaire

$\vec{L}_1$, $\vec{L}_2$ moments cinétiques quelconques

$$\begin{array}{cc} \vec{L}_1 & \vec{L}_2 \\ \downarrow & \downarrow \\ \mathcal{H}_1 & \mathcal{H}_2 \end{array}$$

$$\boxed{\begin{array}{l} \mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2 \\ |\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \end{array}}$$

état intriqué

$$\to \frac{1}{\sqrt{1+|\alpha|^2}} \left(|\psi_1\rangle \otimes |\psi_2\rangle + \alpha |\phi_1\rangle \otimes |\phi_2\rangle \right)$$

$$\langle \psi_1 | \phi_1 \rangle = 0$$

$$\langle \psi_2 | \phi_2 \rangle = 0$$

$\hat{L}_1^\alpha$ opérateur qui agit sur $|\psi_1\rangle \in \mathcal{H}_1$

$\alpha = x, y, z$

" " " " $|\psi_{12}\rangle \in \mathcal{H}_{12}$

$$(\hat{L}_1^\alpha \otimes \hat{\mathbb{1}}) \, |\psi_1\rangle \otimes |\psi_2\rangle$$

$$= \left(\hat{L}_1^\alpha |\psi_1\rangle\right) \otimes |\psi_2\rangle$$

$$\hat{L}_2^\alpha \to (\mathbb{1} \otimes \hat{L}_2^\alpha)$$

$$\left[\hat{L}_1^\alpha \otimes \mathbb{1}, \mathbb{1} \otimes \hat{L}_2^\beta\right] = 0$$

$\alpha, \beta = x, y, z$

$|\psi_1\rangle \otimes |\psi_2\rangle$

"étiquettes" quantiques $\to$ nombres quantiques

$$\hat{L}_1^2, \hat{L}_1^z \qquad \hat{L}_2^2, \hat{L}_2^z$$

$$l_1 \quad m_1 \qquad l_2 \quad m_2$$

ECOC : ensemble complet d'observables compatibles

$$\underbrace{|l_1 m_1\rangle}_{\mathcal{H}_1} \otimes \underbrace{|l_2 m_2\rangle}_{\mathcal{H}_2} \to |l_1 m_1\rangle |l_2 m_2\rangle$$

$$\vec{L} = \vec{L}_1 + \vec{L}_2$$

$$[\hat{L}^\alpha, \hat{L}^\beta] = i\hbar\, \epsilon_{\alpha\beta\gamma}\, \hat{L}^\gamma$$

$$[\hat{\vec{L}}^2, \hat{L}^z] = 0 \qquad (\hat{A}+\hat{B})^2 = \hat{A}^2 + \hat{B}^2 + \hat{A}\hat{B} + \hat{B}\hat{A}$$

$$\downarrow$$

$$\hat{L}^z = \hat{L}_1^z + \hat{L}_2^z$$

commutent avec $\vec{L}_1^2$, $\vec{L}_2^2$

$$[\vec{L}^2_{1(2)}, \vec{L}^2] = [\vec{L}_{1(2)}, \hat{\vec{L}}_1^2 + \hat{\vec{L}}_2^2 + 2\hat{\vec{L}}_1\cdot\hat{\vec{L}}_2 + \cancel{\hat{\vec{L}}_2\cdot\hat{\vec{L}}_1}]$$

$\vec{L}_1^2$ commute avec toutes les composantes de $\vec{L}_1$

$$= 0$$

$$\vec{L}_1^2,\ \vec{L}_2^2,\ \vec{L}^2,\ L^z$$

$$|l_1\ l_2 ; L\ M\rangle \in \mathcal{H}_1$$

$$\begin{cases} \vec{L}^2 \to \hbar^2 L(L+1) \\ L^z \to \hbar M \end{cases}$$

coefficients de Clebsch-Gordan

$$C^{l_1 l_2}_{m_1 m_2 ; LM} \in \mathbb{R}$$

Changer de base

1) 2)

$$|l_1 m_1\rangle \otimes |l_2 m_2\rangle = \sum_{L=0}^{\infty} \sum_{M=-L}^{L} \langle l_1 l_2 ; LM | l_1 m_1\rangle |l_2 m_2\rangle \; |l_1 l_2 ; LM\rangle$$

$$\left(\mathbb{1}_{H_{12}} = \sum_{L=0}^{\infty} \sum_{M=-L}^{L} |\ell_1 \ell_2 ; LM\rangle \langle \ell_1 \ell_2 ; LM| \right)$$

valeurs possibles pour L étant donné ℓ_1, ℓ_2

$$L^z = L_1^z + L_2^z$$

$$\hat{L}^z \left(|\ell_1 m_1\rangle \cdot |\ell_2 m_2\rangle \right) = \left(\hat{L}_1^z \otimes \hat{\mathbb{1}} + \hat{\mathbb{1}} \otimes \hat{L}_2^z \right) |\ell_1 m_1\rangle \otimes |\ell_2 m_2\rangle$$

$$= (\hbar m_1 + \hbar m_2) |\ell_1 m_1\rangle |\ell_2 m_2\rangle$$

$$= \hbar (m_1 + m_2) |\ell_1 m_1\rangle |\ell_2 m_2\rangle$$

$$M = m_1 + m_2$$

$$C^{\ell_1 \ell_2}_{m_1 m_2, LM} \sim \delta_{M, m_1+m_2}$$

$$\hat{L}^{\pm}_{1(2)} = \hat{L}^x_{1(2)} \pm i \hat{L}^y_{1(2)}$$

$$\hat{L}^{\pm}_{1(2)} |\ell_{1(2)} m_{1(2)}\rangle = \hbar \sqrt{\ell(\ell+1) - m(m \pm 1)}\, |\ell, m \pm 1\rangle$$

$$\hat{L}^{\pm} = L_1^{\pm} + L_2^{\pm}$$

$|\ell_1 m_1\rangle |\ell_2 m_2\rangle$ $\quad$ ℓ_1, ℓ_2 sont fixés

$m_1 = -\ell_1, \dots, \ell_1$ $\quad$ $m_2 = -\ell_2, \dots, \ell_2$

M : valeur maximale

$$M_{max} = \ell_1 + \ell_2$$

$$|\ell_1 \ell_2 ; LM\rangle \underset{M=M_{max}}{\rightarrow} |\ell_1 \ell_2 ; \overset{\ell_1+\ell_2}{L}, \ell_1+\ell_2\rangle$$

$$= |\ell_1, \ell_1\rangle |\ell_2, \ell_2\rangle$$

$$\rightarrow \hat{L}^+ |\ell_1 \ell_2 ; L_{max}, \overset{M}{\ell_1+\ell_2}\rangle = 0$$

$$L_{max} = \ell_1+\ell_2$$

$$\rightarrow L_{max} = \ell_1+\ell_2$$

$$\hat{L}^- |\ell_1 \ell_2 ; \ell_1+\ell_2, \ell_1+\ell_2\rangle$$

$|\ell_1 \ell_2 ; LM\rangle$

$$= \hbar \sqrt{L(L+1) - M(M-1)}\ |\ell_1 \ell_2 ; \ell_1+\ell_2, \ell_1+\ell_2-1\rangle$$

$$L = \ell_1+\ell_2 = M$$

$$= (\hat{L}_1^- + \hat{L}_2^-) |\ell_1 \ell_1\rangle |\ell_2 \ell_2\rangle$$

$|\ell_1 m_1\rangle |\ell_2 m_2\rangle$

$$= \hbar \sqrt{\ell_1(\ell_1+1) - \ell_1(\ell_1-1)}\ |\ell_1 \ell_1 - 1\rangle |\ell_2, \ell_2\rangle \qquad \sqrt{2\ell_1}$$

$$+ \hbar \sqrt{\ell_2(\ell_2+1) - \ell_2(\ell_2-1)}\ |\ell_1, \ell_1\rangle |\ell_2, \ell_2 - 1\rangle \qquad \sqrt{2\ell_2}$$

construire un autre état avec $M = \ell_1+\ell_2-1$

$$\sqrt{2\ell_2}\ |\ell_1 \ell_1-1\rangle |\ell_2 \ell_2\rangle - \sqrt{2\ell_1}\ |\ell_1 \ell_1\rangle |\ell_2, \ell_2-1\rangle$$

$$\rightarrow M = \ell_1+\ell_2-1 \leftarrow$$

$L = L_{max}$

$|l_1, l_2; \underbrace{l_1+l_2}_{L}, l_1+l_2\rangle$

L^-

$L = L_{max} - 1$

$|l_1, l_2; \underbrace{l_1+l_2}_{L}, l_1+l_2-1\rangle \xrightarrow{\text{orth.}} |l_1, l_2; \underbrace{l_1+l_2-1}_{L}, \underbrace{l_1+l_2-1}_{M}\rangle$

L^-

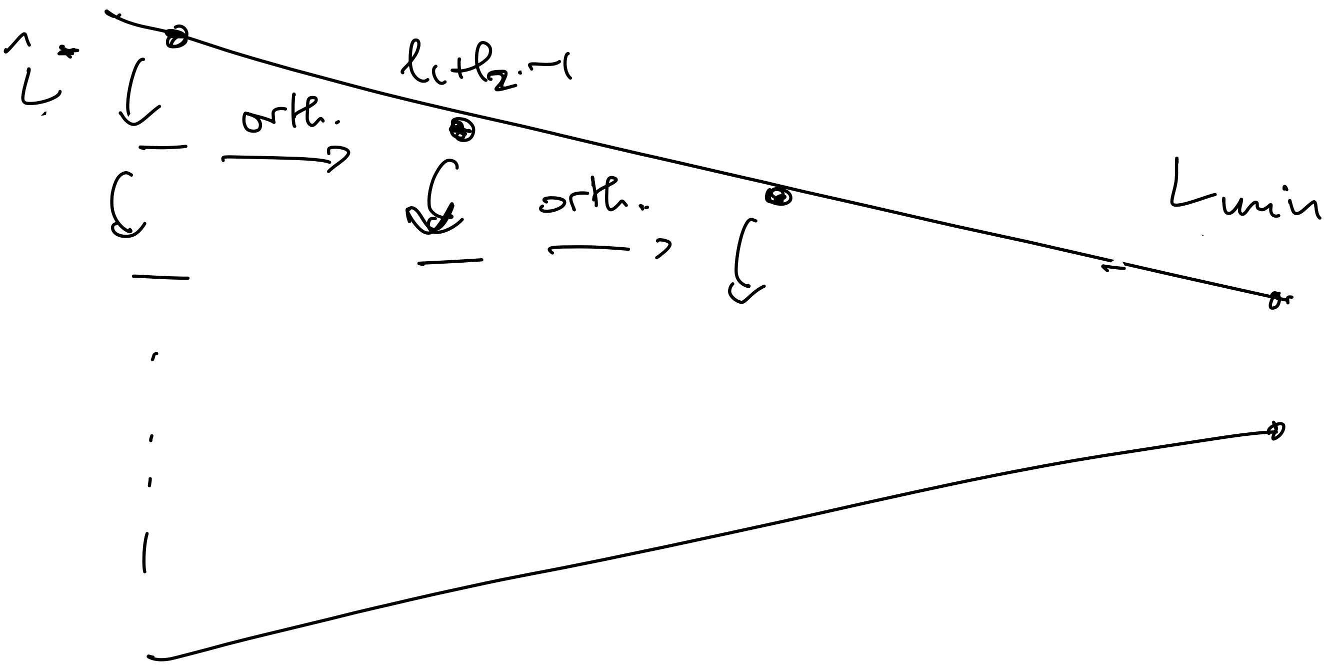
L^-

$-2\rangle$

$\vdots$

$|l_1, l_2; \underbrace{l_1+l_2}_{L}, -l_1-l_2\rangle$

$L = l_1+l_2 = L_{max}$



L_{min} ?

$$\begin{cases} \vec{L}_1^2 \rightarrow \hbar^2 \ell_1(\ell_1+1) \\ \vec{L}_2^2 \rightarrow \hbar^2 \ell_2(\ell_2+1) \end{cases}$$

$$\vec{L}^2 = (\vec{L}_1 + \vec{L}_2)^2$$

si $\ell_2 = 0$ $\qquad \vec{L} = \vec{L}_1$

$\ell_1 \neq 0$ $\qquad L = \ell_1$

$$L_{min} = |\ell_1 - \ell_2| \leftarrow$$

$$\geq 0$$

$$\boxed{L = |\ell_1 - \ell_2|,\ |\ell_1 - \ell_2| + 1,\ \ldots,\ \ell_1 + \ell_2}$$

$$C^{\ell_1 \ell_2}_{m_1 m_2, LM} \neq 0$$

$$H_{12} = H_1 \otimes H_2 \qquad \dim(H_{12}) = (2\ell_1+1)(2\ell_2+1)$$

$|\ell_1, m_1\rangle \quad |\ell_2, m_2\rangle$

$\dim(H_1) = 2\ell_1+1 \qquad \dim(H_2) = 2\ell_2+1$

$$|\overbrace{\underbrace{\ell_1, \ell_2}}\, ; \, L M\rangle$$

$$= \underset{\substack{\downarrow \\ (2L_{max}+1)}}{\mathcal{H}_{L_{max}}} \oplus \underset{\substack{\downarrow \\ (2(L_{max}-1)+1)}}{\mathcal{H}_{L_{max}-1}} \oplus \cdots \oplus \mathcal{H}_{L_{min}}$$

$$\sum_{L = L_{min} (= |\ell_1 - \ell_2|)}^{L_{max} (= \ell_1 + \ell_2)} (2L+1) = (2\ell_1+1)(2\ell_2+1)$$

$$\sum_{M=-L}^{L} = \dim (\mathcal{H}_{12})$$

Composition de deux moments cinétiques de spin $s = \frac{1}{2}$

$$(\vec{L}_1) \qquad (\vec{L}_2)$$

$$\nearrow \qquad \nearrow$$

$$\vec{S}_1 \,, \quad \vec{S}_2 \qquad \ell_1 = \ell_2 = \frac{1}{2}$$

$\langle\uparrow|\sigma^x|\uparrow\rangle$

$$\hat{S}^x_{1(2)} \to \frac{\hbar}{2}\sigma^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2} \begin{array}{c} \\ \langle\uparrow| \\ \langle\downarrow| \end{array} \begin{array}{c} \begin{array}{cc} |\uparrow\rangle & |\downarrow\rangle \end{array} \\ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{array}$$

$$\hat{S}^y_{1(2)} \to \frac{\hbar}{2}\sigma^y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\hat{S}^z_{1(2)} \to \frac{\hbar}{2}\sigma^z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$\mathcal{H}_{12} \to$ base $\quad |\uparrow\uparrow\rangle, \; |\uparrow\downarrow\rangle, \; |\downarrow\uparrow\rangle, \; |\downarrow\downarrow\rangle$

$$\left(\hat{S}^z |\uparrow\rangle = \hbar \frac{1}{2} |\uparrow\rangle \qquad \hat{S}^z |\downarrow\rangle = -\frac{1}{2}\hbar |\downarrow\rangle \right)$$

$$|\tfrac{1}{2}, \tfrac{1}{2}\rangle \qquad\qquad = -\frac{1}{2}\hbar \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle$$

$$|\uparrow\uparrow\rangle \to |l_1 m_1\rangle |l_2 m_2\rangle = |\tfrac{1}{2}, \tfrac{1}{2}\rangle |\tfrac{1}{2}, \tfrac{1}{2}\rangle$$

$$S_1^z = \frac{\hbar}{2} \begin{array}{c|cccc} & |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \\ \hline \langle\uparrow\uparrow| & 1 & & & \\ \langle\uparrow\downarrow| & & 1 & & 0 \\ \langle\downarrow\uparrow| & & 0 & -1 & \\ \langle\downarrow\downarrow| & & & & -1 \end{array}$$

$\perp$

H_{12}

$$\hat{S}_1^x = \frac{\hbar}{2} \begin{array}{c|cccc} & |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \\ \hline \langle\uparrow\uparrow| & 0 & 0 & 1 & 0 \\ \langle\uparrow\downarrow| & 0 & 0 & 0 & 1 \\ \langle\downarrow\uparrow| & 1 & 0 & 0 & 0 \\ \langle\downarrow\downarrow| & 0 & 1 & 0 & 0 \end{array}$$

$=$ $\rightarrow$

$$\hat{S}_1^y = \frac{\hbar}{2} \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}$$

$\uparrow$

$$\hat{S}_2^z = \frac{\hbar}{2} \begin{pmatrix} 1 & & & \\ & -1 & & 0 \\ & & 1 & \\ & 0 & & -1 \end{pmatrix}$$

$$\hat{S}_2^x = \frac{\hbar}{2}\begin{pmatrix} \begin{matrix} 0 & 1 \\ 1 & 0 \end{matrix} & 0 \\ 0 & \begin{matrix} 0 & 1 \\ 1 & 0 \end{matrix} \end{pmatrix}$$

$$\hat{S}_2^y = \frac{\hbar}{2}\begin{pmatrix} \begin{matrix} 0 & -i \\ i & 0 \end{matrix} & 0 \\ 0 & \begin{matrix} 0 & -i \\ i & 0 \end{matrix} \end{pmatrix}$$

$$S^z = S_1^z + S_2^z = \hbar\begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & -1 \end{pmatrix}$$

$$S^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

$$S^y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix}$$

$$\vec{S}^2 = \hbar^2 \begin{array}{c|c} & \begin{array}{cccc} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \begin{array}{c} \langle\uparrow\uparrow| \\ \langle\uparrow\downarrow| \\ \langle\downarrow\uparrow| \\ \langle\downarrow\downarrow| \end{array} & \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \end{array}$$

$$\underbrace{\vec{S}^2}_{\hbar^2 s(s+1)} |\uparrow\uparrow\rangle = \hbar^2 \underbrace{2}_{(1+1)\,1} |\uparrow\uparrow\rangle$$

$$s = 1 = \frac{1}{2} + \frac{1}{2} = l_1 + l_2$$

$$\begin{vmatrix} 1-\lambda & 1 \\ 1 & 1-\lambda \end{vmatrix} = (1-\lambda)^2 - 1 = 0$$

$$\cancel{1} - 2\lambda + \lambda^2 - \cancel{1} = 0$$

$$\lambda(\lambda - 2) = 0$$

$$\lambda = 0, 2$$

$$\hbar^2 s(s+1) = \hbar^2 0$$

$$s = 0 = \left|\frac{1}{2} - \frac{1}{2}\right| = |l_1 - l_2|$$

états propres pour la somme

$l_1 \quad l_2 \quad L \quad M$

$\underline{\underline{S=0}}$ $\qquad |\tfrac{1}{2}\,\tfrac{1}{2};\,0,0\rangle = \dfrac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$

singulet

intriqués

(états de Bell)

$S=1 \qquad |\tfrac{1}{2}\,\tfrac{1}{2};\,1\,1\rangle = |\uparrow\uparrow\rangle$

$|\tfrac{1}{2}\,\tfrac{1}{2};\,1\,0\rangle = \dfrac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}$

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