VALEURS PROPRES et VECTEURS PROPRES DU MOMENT ANGULAIRE

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$$[\hat{L}^\alpha, \hat{L}^\beta] = i\hbar \sum_\gamma \epsilon_{\alpha\beta\gamma} \hat{L}^\gamma \qquad \epsilon_{\alpha\beta\gamma} = \begin{cases} 1 & (\alpha\beta\gamma) \text{ permutation paire de } (xyz) \\ -1 & \text{" " impaire " "} \\ 0 & \text{autrement} \end{cases}$$

$\hat{\vec{L}}$

$$\hat{R}_{\vec{n}}(\vartheta) = e^{-\frac{i}{\hbar}\hat{\vec{L}}\cdot\vec{n}\,\vartheta}$$

$$[\hat{\vec{L}}^2, \hat{R}_{\vec{n}}(\vartheta)] = 0 \quad \underset{\vartheta \to 0}{\Longrightarrow} \quad \boxed{[\hat{\vec{L}}^2, \hat{L}^\alpha] = 0}$$

base simultanée de vecteurs propres de $\hat{\vec{L}}^2, \hat{L}^z$: $|l\,m\rangle$

ECOC
ensemble complet d'observables compatibles → spécifier les propriétés angulaires de la fonction d'onde

$l > 0 \quad l \in \mathbb{R}, \ m \in \mathbb{R}$

$$\begin{cases} \hat{\vec{L}}^2 |lm\rangle = \hbar^2 l(l+1) |lm\rangle \\ \hat{L}^z |lm\rangle = \hbar m |lm\rangle \end{cases}$$

$|lm\rangle$ non dégénérés

l, m $\boxed{\text{nombres quantiques}}$

l ↓ nombre quantique du module de L

m → nombre quantique de la projection suivant z

opérateurs montée / descente

$$\begin{cases} \hat{L}^+ = \hat{L}^x + i\hat{L}^y \\ \hat{L}^- = \hat{L}^x - i\hat{L}^y \end{cases}$$

$$[\hat{L}^z, \hat{L}^\pm] = [\hat{L}^z, \hat{L}^x \pm i\hat{L}^y] = i\hbar(\hat{L}^y \mp i\hat{L}^x) = \pm\hbar(\hat{L}^x \pm i\hat{L}^y) = \pm\hbar\hat{L}^\pm$$

$$\boxed{[\hat{L}^z, \hat{L}^\pm] = \pm\hbar\hat{L}^\pm}$$

$$\hat{L}^z\hat{L}^\pm = \hat{L}^\pm(\hat{L}^z \pm \hbar)$$

$|lm\rangle \to$ $\boxed{\hat{L}^{\pm}|lm\rangle}$ état propre de $\hat{L}^z$ avec valeur propre $\hbar(m\pm 1)$ ②

$$\hat{L}^z\left(\hat{L}^{\pm}|lm\rangle\right) = \hat{L}^{\pm}(\hbar m \pm \hbar)|lm\rangle = \hbar(m\pm 1)\hat{L}^{\pm}|lm\rangle$$

$$\boxed{\hat{L}^{\pm}|lm\rangle \sim |l, m\pm 1\rangle}$$

$$\langle lm|l'm'\rangle = \delta_{ll'}\delta_{mm'}$$

$$\hat{L}^{\pm}|lm\rangle = \underbrace{\|\hat{L}^{\pm}|lm\rangle\|}\ |l, m\pm 1\rangle$$

$$\boxed{\hat{L}^2 = (\hat{L}^x)^2 + (\hat{L}^y)^2 + (\hat{L}^z)^2}$$

$$\|\hat{L}^{\pm}|lm\rangle\|^2 = \langle lm|\hat{L}^{\mp}\hat{L}^{\pm}|lm\rangle$$

$$\hat{L}^+\hat{L}^- = (\hat{L}^x + i\hat{L}^y)(\hat{L}^x - i\hat{L}^y) = (\hat{L}^x)^2 + (\hat{L}^y)^2 - i\underbrace{[\hat{L}^x, \hat{L}^y]}_{\sim i\hbar \hat{L}^z}$$

$$= \hat{L}^2 - (\hat{L}^z)^2 + \hbar\hat{L}^z = \hat{L}^2 - \hat{L}^z(\hat{L}^z - \hbar)$$

$$\hat{L}^-\hat{L}^+ = \hat{L}^2 - \hat{L}^z(\hat{L}^z + \hbar)$$

$$\boxed{\hat{L}^{\pm}\hat{L}^{\mp} = \hat{L}^2 - \hat{L}^z(\hat{L}^z \mp \hbar)}$$

$$= \hbar^2\left[l(l+1) - m(m\pm 1)\right]$$

$$\boxed{\hat{L}^{\pm}|lm\rangle = \hbar\sqrt{l(l+1) - m(m\pm 1)}\ |l, m\pm 1\rangle}$$

$$\hat{L}^2\hat{L}^{\pm}|lm\rangle = \hat{L}^{\pm}\hbar^2 l(l+1)|lm\rangle = \hbar^2 l(l+1)\hat{L}^{\pm}|lm\rangle$$

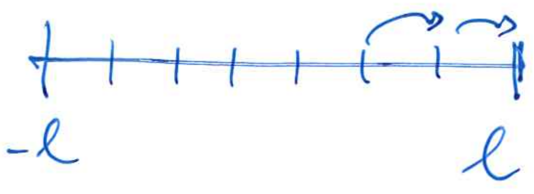
$$\|\hat{L}^{\pm}|lm\rangle\|^2 = \hbar^2\left[l(l+1) - m(m\pm 1)\right] \geq 0$$

(+) $l(l+1) - m(m+1) = (l-m)(l+m+1) \geq 0$

$$\begin{cases} \boxed{m \leq l} & \checkmark \\ m \geq -l-1 & \end{cases} \qquad \begin{matrix} m \geq l \\ m \leq -l-1 \end{matrix} \quad \times$$

(−) $\ell(\ell+1) - m(m-1) = (\ell+m)(\ell-m+1) \geq 0$ $\quad \begin{cases} \boxed{m \geq -\ell} \\ m \leq \ell+1 \end{cases}$ ✓

$$\boxed{-\ell \leq m \leq \ell} \longleftarrow -|\vec{L}| \leq L^z \leq |\vec{L}|$$



$$\hat{L}^z (\hat{L}^\pm)^2 |\ell m\rangle = \hbar(m \pm 2)(\hat{L}^\pm)^2 |\ell m\rangle$$

$$\hat{L}^z (\hat{L}^\pm)^n |\ell m\rangle = \hbar(m \pm n)(\hat{L}^\pm)^n |\ell m\rangle$$

$$(\hat{L}^+)^{n_1} |\ell m\rangle \qquad (\hat{L}^-)^{n_2} |\ell m\rangle$$

$\sim |\ell, m+n_1\rangle$

$$\|(\hat{L}^+)^{n_1+1} |\ell m\rangle\|^2 = \langle \ell m| (\hat{L}^-)^{n_1} \underbrace{(\hat{L}^- \hat{L}^+)}_{\hat{L}^2 - \hat{L}^z(\hat{L}^z + \hbar)} (\hat{L}^+)^{n_1} |\ell m\rangle$$

$-n_1^2$

$$= \|(\hat{L}^+)^{n_1} |\ell m\rangle\|^2 \, \hbar^2 [\ell(\ell+1) - (m+n_1)(m+n_1+1)]$$

$$\|(\hat{L}^-)^{n_2+1} |\ell m\rangle\|^2 = \dots = \|(\hat{L}^-)^{n_2} |\ell m\rangle\|^2 \, \hbar^2 [\ell(\ell+1) - (m-n_2)(m-n_2-1)]$$

$-n_2^2$

$\exists \; n_1, n_2$

$$\ell(\ell+1) - (m+n_1)(m+n_1+1) = \overset{=0}{(\ell - m - n_1)}(\ell + m + n_1 + 1) = 0$$

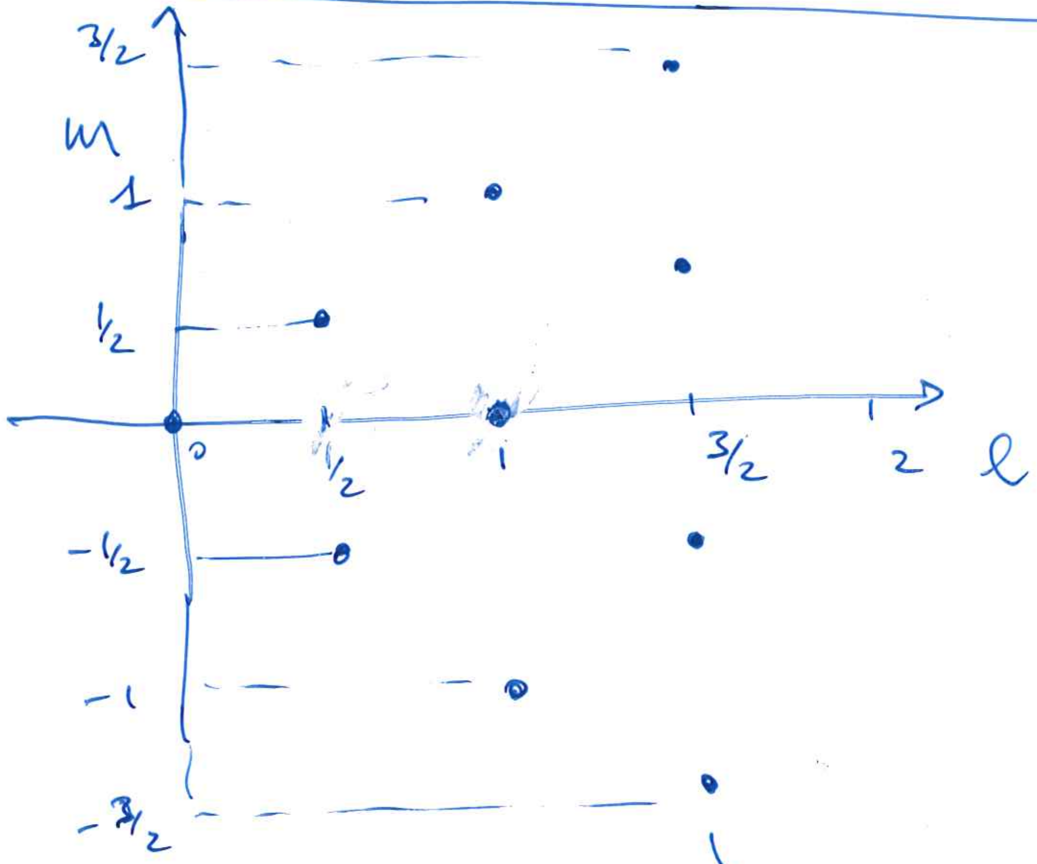
$$\ell(\ell+1) - (m-n_2)(m-n_2-1) = \underset{=0}{(\ell + m - n_2)}(\ell - m + n_2 + 1) = 0$$

$$\begin{cases} l = m + n_1 \\ l = -m + n_2 \end{cases}$$

$$\boxed{l = \frac{n_1 + n_2}{2}} = \begin{cases} p \in \mathbb{N} \\ \dfrac{2p+1}{2} \qquad p \in \mathbb{N} \end{cases}$$

$n_1, n_2 \in \mathbb{N}$

$\boxed{l \text{ entier ou demi entier}}$



$$\begin{cases} m = l - n_1 \\ m = -l + n_2 \end{cases}$$

$-l, -l+1, -l+2, \dots, l-2, l-1, l$

$(2l+1)$ valeurs possibles de m

$\vec{L}$

$\boxed{S = 1/2}$

Spin : moment angulaire intrinsèque $\hat{\vec{S}}$:

$$\hat{\vec{S}}^2 |S m_s\rangle = \hbar^2 S(S+1) |S m_s\rangle$$

$$\hat{S}_z |S m_s\rangle = \hbar m_s |S m_s\rangle$$

Fonctions propres du moment angulaire ORBITALAIRE

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \longrightarrow -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]$$

$$\hat{L}^2 \Longrightarrow -\hbar^2\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)^2 + \left(x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x}\right)^2 + \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)^2\right]$$

$$\vec{r} = (x, y, z) = r(\cos\phi\sin\vartheta,\ \sin\phi\sin\vartheta,\ \cos\vartheta) \qquad \phi \in [0, 2\pi]$$

$$r, \vartheta, \phi \qquad \vartheta \in [0, \pi]$$

$$\hat{L}_z \to -i\hbar\frac{\partial}{\partial\phi}$$

$$\hat{L}^2 \to -\hbar^2\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}(.)\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\phi^2}\right)$$

pas de r

$\nearrow mr^2$

$$L = I\omega$$

$$E = \frac{1}{2}I\omega^2$$

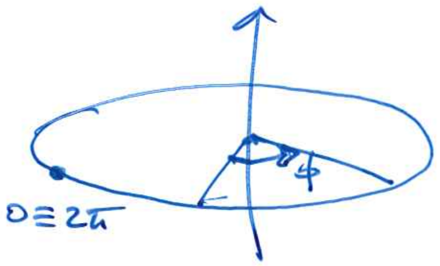
$$|lm\rangle \to \psi_{lm}(r, \vartheta, \phi) = \langle r, \vartheta, \phi | lm\rangle$$

$$= R_{nlm}(r)\ \varphi_{lm}(\vartheta, \phi)$$

$$\varphi_{lm}(\vartheta, \phi) = \langle\vartheta\phi | lm\rangle$$

$$-i\cancel{\hbar}\frac{\partial}{\partial\phi}\varphi_{lm}(\vartheta, \phi) = \cancel{\hbar}m\ \varphi_{lm}(\vartheta, \phi) \qquad \varphi_{lm}(\vartheta, \phi) = \Theta_{lm}(\vartheta)\ \Phi_m(\phi)$$

$$\Phi_m(\phi) = A\, e^{im\phi}$$



$$\Phi_m(0) = \Phi_m(2\pi)$$

$$1 = e^{i2\pi m}$$

$$\begin{cases} m \text{ entier} \ / \ \cancel{\text{demi-entier}} \\ \underline{\underline{l \text{ entier}}} \quad \text{moment angulaire orbitalaire} \end{cases}$$

$$\hat{L}^2$$

$$-\hbar^2 \left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\vartheta}(\cdot)\right) + \frac{1}{\sin^2\vartheta}\underbrace{\left(\frac{\partial^2}{\partial\phi^2}\right)}_{-m^2}\right) \Theta_{lm}(\vartheta)\, e^{im\phi} = \hbar^2\, l(l+1)\, \Theta_{lm}(\vartheta)\, e^{im\phi}$$

$$-\hbar^2 \left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\vartheta}(\cdot)\right) - \frac{m^2}{\sin^2\vartheta} + l(l+1)\right) \Theta_{lm}(\vartheta) = 0$$

$$\underline{\Theta_{lm}(\vartheta)\, e^{im\phi} = Y_{lm}(\vartheta,\phi)} \in \mathbb{C}$$ harmonique sphérique

$$\langle lm | l'm' \rangle = \delta_{ll'}\,\delta_{mm'} = \int_0^{\pi} d\vartheta \sin\vartheta \int_0^{2\pi} d\phi \; Y^*_{lm}(\vartheta,\phi)\, Y_{l'm'}(\vartheta,\phi)$$

$$f(\vartheta,\phi) = \sum_{lm} c_{lm}\, Y(\vartheta,\phi)$$

$\hat{L}^{+} | l, l\rangle = 0 \qquad \hat{L}^{\pm} \rightarrow \hbar e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\vartheta} + i\cot\vartheta \frac{\partial}{\partial\phi}\right)$

$\Theta_{ll}(\vartheta)\, e^{il\phi} \qquad \left(\frac{\partial}{\partial\vartheta} - l\cot\vartheta\right)\Theta_{ll}(\vartheta)\, \cancel{e^{il\phi}} = 0 \qquad \boxed{m = l}$

$\frac{\partial}{\partial\vartheta}\Theta_{ll} = l\,\frac{\cos\vartheta}{\sin\vartheta}\,\Theta_{ll} \qquad \Theta_{ll} = A\,(\sin\vartheta)^{l}$ $\boxed{\text{solution unique}}$

$\Theta_{l-l} = A\,(\sin\vartheta)^{l}$

$\ulcorner Y_{lm} \urcorner$

$\Theta_{lm}(\vartheta)\, e^{im\phi} \sim \left[e^{-i\phi}\left(-\frac{\partial}{\partial\vartheta} + i\cot\vartheta\,\frac{\partial}{\partial\phi}\right)\right]^{l-m} \Theta_{ll}\, e^{il\phi}$

$\llcorner\ Y_{ll}\ \lrcorner$

<u>Exemples de harmoniques sphériques</u>

$l=0,\ m=0 \quad Y_{00}(\vartheta,\phi) = \frac{1}{\sqrt{4\pi}}$

$l = 1 \begin{cases} m=0) \quad Y_{10}(\vartheta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\vartheta \\ m=\pm1) \quad Y_{1\pm1} = \sqrt{\frac{3}{8\pi}}\, e^{\pm i\phi}\sin\vartheta \end{cases}$

$l = 2 \begin{cases} m=0) \quad Y_{20} = \sqrt{\frac{5}{16\pi}}\,(3\cos^2\vartheta - 1) \\ m=\pm1) \quad Y_{2\pm1} = \sqrt{\frac{15}{8\pi}}\,\sin\vartheta\cos\vartheta\, e^{\pm i\phi} \\ m=\pm2) \quad Y_{2\pm2} = \sqrt{\frac{15}{32\pi}}\,\sin^2\vartheta\, e^{\pm i2\phi} \end{cases}$

etc...

$\underline{m=0}$: Θ_{l0}

$$\left[+ \frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\, \frac{\partial(\cdot)}{\partial\vartheta}\right) + l(l+1) \right] \Theta_{l0} = 0$$

$u = \cos\vartheta$ $\qquad \dfrac{\partial}{\partial u} = -\dfrac{1}{\sin\vartheta}\dfrac{\partial}{\partial\vartheta}$

$$\sin\vartheta \frac{\partial}{\partial\vartheta} = -\sin^2\vartheta \frac{\partial}{\partial u} = -(1-u^2)\frac{\partial}{\partial u} \qquad \Theta_{l0}(\vartheta) = P_l(u)$$

$$\left[\frac{\partial}{\partial u}\left((1-u^2)\frac{\partial}{\partial u}(\cdot)\right) + l(l+1)\right] P_l(u) = 0$$

<u>équation de Legendre</u>

P_l polynômes de Legendre (ordre l)

$P_0 = 1$, $\quad P_1 = u$, $\quad P_2 = \frac{1}{2}(3u^2-1)$ ---

$$\boxed{Y_{l0}(\vartheta,\phi) = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\vartheta)}$$

$m \neq 0$ $\quad \Theta_{lm}$ $\qquad$ polynômes associés de Legendre

$$P_{lm}(u) = \sqrt{(1-u^2)^m}\, \frac{d^m}{du^m} P_l(u)$$

$$Y_{lm}(\vartheta,\phi) \sim P_{lm}(\cos\vartheta)\, e^{im\phi}$$

<u>propriété de parité</u> $\qquad \vec r \to -\vec r \qquad \vartheta \to \pi-\vartheta$, $\quad \phi \to \phi+\pi$

$$\boxed{Y_{lm}(\pi-\vartheta, \phi+\pi) = (-1)^l\, Y_{lm}(\vartheta,\phi)}$$

$$\psi_{n\ell m}(r,\ell m) = R(r)\, Y_{\ell m}(\vartheta,\phi)$$

$$\|\psi\|^2 = \left(\int_0^\infty dr\, r^2\, |R(r)|^2\right)\left(\int d\Omega\, |Y_{\ell m}|^2\right)$$

Potential central

$$V(\vec{r}) = V(r) = \frac{q q'}{4\pi\varepsilon_0 r}$$

$O_{\bullet}\, +q$

$\mu\; q'$

$$\hat{H} = \frac{\hat{\vec{P}}^2}{2\mu} + \hat{V}(r)$$

$$[\hat{H}, \hat{L}] = 0$$

$$\frac{\hat{\vec{p}}^2}{2\mu} \longrightarrow -\frac{\hbar^2}{2\mu}\nabla^2 = -\frac{\hbar^2}{2\mu}\left\{\frac{1}{r}\frac{\partial^2}{\partial r^2} r(\cdot) + \frac{1}{r^2}\left[\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}(\cdot)\right)\right.\right.\right.$$

$$\left.\left.\left. + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\phi^2}\right)\right]\right\}$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

$$-\frac{\hat{L}^2}{\hbar^2}$$

$$\boxed{\hat{H} = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} r(\cdot) + \frac{\hat{L}^2}{2\mu r^2} + V(r)}$$