Atome d'hydrogène

2 1] Hamiltonien $\hat{H} = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{4\pi\varepsilon_0 r}$ 0,5

Valeurs propres $\hat{H} : E_n = -\frac{13,6}{n^2}$ (eV) 0,5

$\hat{L}^2 : \ell(\ell+1)\hbar^2$ 0,5

$\hat{L}_z : m\hbar$ 0,5

2 2) $n \in \mathbb{N}^*$; $0 \leq \ell \leq n-1$; $-\ell \leq m \leq +\ell$

2 3/ $\psi_{1s} = \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}$ $a_0 = 0,53 Å$ fct normée

Densité volumique 1 $\rho_{v\,1s}(r,\theta,\varphi) = |\psi_{1s}|^2 = \frac{1}{\pi a_0^3} e^{-\frac{2r}{a_0}}$

Densité radiale 1 $\rho_{r\,1s}(r) = \int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} \rho_{v1s}(r,\theta,\varphi)\, r^2 \sin\theta\, d\theta\, d\varphi$
$= 4\pi r^2 \rho_{v1s}(r)$

2 4) $\langle r \rangle, \langle r^2 \rangle, \Delta r$

$\langle r \rangle = \int_0^\infty r \rho_{r1s}(r)\,dr = \frac{1}{\pi a_0^3} \cdot 4\pi \underbrace{\int_0^\infty r^3 e^{-\frac{2r}{a_0}}\,dr}_{\frac{3!}{(2/a_0)^4}} = \frac{3}{2}a_0$ 0,5

$\langle r^2 \rangle = \int_0^\infty r^2 \rho_{r1s}(r)\,dr = \frac{1}{\pi a_0^3} 4\pi \underbrace{\int_0^\infty r^4 e^{-\frac{2r}{a_0}}\,dr}_{\frac{4!}{(2/a_0)^5}} = 3a_0^2$ 0,5

$\rightarrow (\Delta r)^2 = \langle r^2 \rangle - \langle r \rangle^2 = \frac{3}{4}a_0^2 \Rightarrow \Delta r = \frac{a_0\sqrt{3}}{2}$ 1

2 5) Distance au noyau où la densité radiale de probabilité de présence est maximale.

$\frac{d\rho_{r1s}(r)}{dr} = \frac{4}{a_0^3} r e^{-\frac{2r}{a_0}}\left[1 - \frac{r}{a_0}\right] = 0$ 1

$\Rightarrow r = a_0$ 1

2 6) Nombres quantiques $n\,\ell\,m$ $\begin{cases} n = 1 \\ \ell = 0 \\ m = 0 \end{cases}$ 2

Particule chargée dans un champ magnétique

$$\vec{f} = q\vec{v} \wedge \vec{B} \quad ; \quad \vec{B} = B\vec{e_3} \quad ; \quad \vec{A} = \frac{1}{2}\vec{B} \wedge \vec{r}$$

1) $m\vec{a} = q\vec{v} \wedge \vec{B}$ $\quad \vec{a}\begin{vmatrix} \ddot{x} \\ \ddot{y} \\ \ddot{z} \end{vmatrix} \quad \vec{v}\begin{vmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{vmatrix} \quad \vec{B}\begin{vmatrix} 0 \\ 0 \\ B \end{vmatrix}$

on néglige le poids

particule à l'origine du repère en $t=0$

syst d'éqs couplées
$$\begin{cases} m\ddot{x} = q\dot{y}B \\ m\ddot{y} = -q\dot{x}B \\ m\ddot{z} = 0 \end{cases} \Rightarrow \dot{z} = cste = v_{0z} \Rightarrow z(t) = v_{0z}t \quad (z(t=0)=0)$$

Résolution des 2 équations couplées $\quad u = x+iy \; ; \; \dot{u} = \dot{x}+i\dot{y} \; ; \; \ddot{u} = \ddot{x}+i\ddot{y}$

$$m\ddot{u} = m(\ddot{x}+i\ddot{y}) = qB(\dot{y}-i\dot{x}) = -iqB(\dot{x}+i\dot{y}) = -iqB\dot{u}$$

soit $\ddot{u} + i\frac{qB}{m}\dot{u} = 0$ ou avec $\omega = \frac{qB}{m}$: $\ddot{u} + i\omega\dot{u} = 0$

$$\dot{u}(t) = Ke^{-i\omega t} = K(\cos(-\omega t) + i\sin(-\omega t))$$
$$= K(\cos(\omega t) - i\sin(\omega t))$$

soit $\begin{cases} \dot{x} = K\cos(\omega t) = v_{0x}\cos(\omega t) \\ \dot{y} = -K\sin(\omega t) = -v_{0x}\sin(\omega t) \end{cases}$

soit $x(t) = \frac{v_{0x}}{\omega}\sin(\omega t) + K' = \frac{v_{0x}}{\omega}\sin(\omega t)$

$y(t) = \frac{v_{0x}}{\omega}\cos(\omega t) + K'' = \frac{v_{0x}}{\omega}(\cos(\omega t) - 1)$

$z(t) = v_{0z}t$

$\rightarrow$ il s'agit d'une hélice

2) $\hat{\vec{u}} = \hat{\vec{p}} - q\hat{\vec{A}}$

$\vec{p}$ impulsion

$\vec{A}$ potentiel vecteur $\quad \vec{A} = \frac{1}{2}\vec{B} \wedge \vec{r}$

composantes : $\quad \hat{\vec{p}}\begin{vmatrix} -i\hbar\frac{\partial}{\partial x} \\ -i\hbar\frac{\partial}{\partial y} \\ -i\hbar\frac{\partial}{\partial z} \end{vmatrix} \quad \hat{\vec{A}}\begin{vmatrix} -\frac{1}{2}By \\ \frac{1}{2}Bx \\ 0 \end{vmatrix}$

$\left[\vec{\hat{A}}, \vec{\hat{P}}\right]$?

$$\left[\hat{A}_x, \hat{P}_x\right] = \hat{A}_x \hat{P}_x - \hat{P}_x \hat{A}_x = -\frac{1}{2}By \times -i\hbar\frac{\partial}{\partial x} + i\hbar\frac{\partial}{\partial x}\left(-\frac{1}{2}By\right)$$

$$= \frac{i\hbar}{2}By\frac{\partial}{\partial x} - \frac{i\hbar By}{2}\frac{\partial}{\partial x} = 0$$

$$\left[\hat{A}_y, \hat{P}_y\right] = \hat{A}_y \hat{P}_y - \hat{P}_y \hat{A}_y = \frac{1}{2}Bx \times -i\hbar\frac{\partial}{\partial y} + i\hbar\frac{\partial}{\partial y}\left(\frac{1}{2}Bx\right)$$

$$= -\frac{i\hbar Bx}{2}\frac{\partial}{\partial y} + \frac{i\hbar Bx}{2}\frac{\partial}{\partial y} = 0$$

$$\left[\hat{A}_z, \hat{P}_z\right] = \hat{A}_z \hat{P}_z - P_z \hat{A}_z = 0 \quad \text{car } \hat{A}_z = 0$$

$\left[\vec{\hat{A}}, \vec{\hat{P}}\right] = 0$
ou $\vec{\hat{p}}\vec{\hat{A}} = \vec{\hat{A}}\vec{\hat{p}}$

Différentes composantes de $\vec{\hat{u}}$: calcul des commutateurs $\qquad \vec{u} = \vec{p} - q\vec{A}$

$\Rightarrow$ on demande

$\left[\hat{u}_x, \hat{u}_x\right] = 0 = (\hat{u}_x^2 - \hat{u}_x^2)$ $\qquad \hat{u}_x = \hat{p}_x - q\hat{A}_x = -i\hbar\frac{\partial}{\partial x} + q\frac{By}{2}$

$\left[\hat{u}_x, \hat{u}_y\right] = i\hbar q B$ (voir plus bas) $\qquad \hat{u}_y = \hat{p}_y - q\hat{A}_y = -i\hbar\frac{\partial}{\partial y} - q\frac{Bx}{2}$

$\left[\hat{u}_x, \hat{u}_z\right] = 0$ $\qquad \hat{u}_z = -i\hbar\frac{\partial}{\partial z}$

$$\left[\hat{u}_x, \hat{u}_z\right] = \hat{u}_x \hat{u}_z - \hat{u}_z \hat{u}_x = -\hbar^2\frac{\partial}{\partial x}\frac{\partial}{\partial z} - i\hbar q\frac{B}{2}y\frac{\partial}{\partial z} - \left(-\hbar^2\frac{\partial}{\partial z}\frac{\partial}{\partial x} - i\hbar\frac{qBy}{2}\frac{\partial}{\partial z}\right)$$

$$\frac{\partial}{\partial z}\frac{\partial}{\partial x} = \frac{\partial}{\partial x}\frac{\partial}{\partial z}$$

$$= 0$$

$$\left[\hat{u}_x, \hat{u}_y\right] = \hat{u}_x \hat{u}_y - \hat{u}_y \hat{u}_x = \left(-i\hbar\frac{\partial}{\partial x} + q\frac{By}{2}\right)\left(-i\hbar\frac{\partial}{\partial y} - q\frac{Bx}{2}\right) - \left(-i\hbar\frac{\partial}{\partial y} - q\frac{Bx}{2}\right)\left(-i\hbar\frac{\partial}{\partial x} + q\frac{By}{2}\right)$$

$$= \cancel{-\hbar^2\frac{\partial^2}{\partial x\partial y}} + i\hbar\frac{qB}{2}\frac{\partial}{\partial x}(x\ ) - \cancel{i\hbar\frac{qBy}{2}\frac{\partial}{\partial y}} \cancel{- q^2\frac{B^2}{4}xy}$$

$$- \left(\cancel{-\hbar^2\frac{\partial}{\partial y}\frac{\partial}{\partial x}} - i\hbar\frac{qB}{2}\frac{\partial}{\partial y}(y) + \cancel{i\hbar\frac{qBx}{2}\frac{\partial}{\partial x}} \cancel{- q^2\frac{B^2}{4}xy}\right)$$

$$= \frac{i\hbar qB}{2}\left(1 + \cancel{x\frac{\partial}{\partial x}} - \cancel{y\frac{\partial}{\partial y}} + 1 + \cancel{y\frac{\partial}{\partial y}} - \cancel{x\frac{\partial}{\partial x}}\right) = i\hbar q B$$

3) $\hat{H} = \frac{1}{2m}(\vec{\hat{p}} - q\vec{\hat{A}})^2 = \frac{1}{2m}\vec{\hat{u}}^2$

Th d'Ehrenfest $\frac{d}{dt}\langle \hat{O} \rangle = \langle \frac{\partial \hat{O}}{\partial t} \rangle + \frac{1}{i\hbar}\langle [\hat{O}, \hat{H}] \rangle$

$[A, B^2] = [\hat{A}, \hat{B}]\hat{B} + \hat{B}[\hat{A}, \hat{B}]$

* ici $\frac{d}{dt}\langle \vec{\hat{r}} \rangle = \cancel{\langle \frac{\partial \vec{\hat{r}}}{\partial t} \rangle} + \frac{1}{i\hbar}\langle [\vec{\hat{r}}, \hat{H}] \rangle$

- il faut calculer $[\vec{\hat{r}}, \hat{H}]$ soit $[\hat{x}, \hat{H}] = \frac{1}{2m}\{[\hat{x}, \hat{u}_x^2] + [\hat{x}, \hat{u}_y^2] + [\hat{x}, \hat{u}_z^2]$

calculons $[\hat{x}, \hat{u}_x^2] = [\hat{x}, \hat{u}_x]\hat{u}_x + \hat{u}_x[\hat{x}, \hat{u}_x] = 2i\hbar\hat{u}_x$

avec $[\hat{x}, \hat{u}_x] = i\hbar$; $[\hat{x}, \hat{u}_y] = 0$; $[\hat{x}, \hat{u}_z] = 0$

$[\hat{x}, \hat{u}_y^2] = [\hat{x}, \hat{u}_y]\hat{u}_y + \hat{u}_y[\hat{x}, \hat{u}_y] = 0$

$[\hat{x}, \hat{u}_z^2] = 0$

soit $[\hat{x}, \hat{H}] = \frac{i\hbar}{m}\hat{u}_x$

- $[\hat{y}, \hat{H}] = \frac{1}{2m}\{[\hat{y}, \hat{u}_x^2] + [\hat{y}, \hat{u}_y^2] + [\hat{y}, \hat{u}_z^2]\}$

avec $[\hat{y}, \hat{u}_x] = 0$; $[\hat{y}, \hat{u}_y] = i\hbar$; $[\hat{y}, \hat{u}_z] = 0$

soit $[\hat{y}, \hat{H}] = \frac{1}{2m}\{2i\hbar\hat{u}_y\} = \frac{i\hbar}{m}\hat{u}_y$

- $[\hat{z}, \hat{H}] = \frac{1}{2m}\{[\hat{z}, \hat{u}_x^2] + [\hat{z}, \hat{u}_y^2] + [\hat{z}, \hat{u}_z^2]$

avec $[\hat{z}, \hat{u}_x] = 0$; $[\hat{z}, \hat{u}_y] = 0$; $[\hat{z}, \hat{u}_z] = i\hbar$

$[\hat{z}, \hat{H}] = \frac{i\hbar}{m}\hat{u}_z$

au final $[\vec{\hat{r}}, \hat{H}] = \frac{i\hbar}{m}\vec{u} \Rightarrow \frac{d}{dt}\langle \vec{\hat{r}} \rangle = \langle \frac{\vec{u}}{m} \rangle$

$*\quad \frac{d}{dt}\langle \hat{\vec{u}}\rangle = \cancel{\left\langle \frac{\partial \vec{u}}{\partial t}\right\rangle} + \frac{1}{i\hbar}\langle[\hat{\vec{u}},\hat H]\rangle$

• il faut calculer $[\hat{\vec{u}},\hat H]$ $\quad *$ soit $[\hat u_x,\hat H]=\frac{1}{2m}\left\{\cancel{[\hat u_x,\hat u_x^2]}+\underbrace{[\hat u_x,\hat u_y^2]}_{2i\hbar qB\hat u_y}+\cancel{[\hat u_x,\hat u_z^2]}\right\}$

$\longrightarrow [\hat u_x,\hat H] = i\hbar\frac{qB}{m}\hat u_y$

$*$ soit $[\hat u_y,\hat H]=\frac{1}{2m}\left\{\underbrace{[\hat u_y,\hat u_x^2]}_{\underbrace{[\hat u_y,\hat u_x]\hat u_x+\hat u_x[\hat u_y,\hat u_x]}_{-2i\hbar qB\hat u_x}}+\cancel{[\hat u_y,\hat u_y^2]}+[\hat u_y,\hat u_z^2]\right\}$

$\longrightarrow [\hat u_y,\hat H] = -i\hbar\frac{qB}{m}\hat u_x$

$*$ soit $[\hat u_z,\hat H]=\frac{1}{2m}\left\{\cancel{[\hat u_z,\hat u_x^2]}+\cancel{[\hat u_z,\hat u_y^2]}+\cancel{[\hat u_z,\hat u_z^2]}\right\}$

$\longrightarrow [\hat u_z,\hat H] = 0$

finalement $[\hat{\vec{u}},\hat H] = \frac{i\hbar q}{m}\vec{u}\wedge\vec{B}$ $\Rightarrow$ $\frac{d}{dt}\langle\vec{u}\rangle = \frac{q}{m}\langle\vec{u}\wedge\vec{B}\rangle$

<u>En résumé</u> $\quad \frac{d}{dt}\langle\vec{r}\rangle = \frac{1}{m}\langle\vec{u}\rangle$ et $\frac{d}{dt}\langle\vec{u}\rangle = \frac{q}{m}\langle\vec{u}\wedge\vec{B}\rangle$

Méca classique $\rightarrow$ $\vec{f} = q\vec{v}\wedge\vec{B} = m\frac{d^2\vec{r}}{dt^2}$ $\Rightarrow$ $\frac{d^2\vec{r}}{dt^2} = \frac{q}{m}\left(\frac{d\vec{r}}{dt}\right)\wedge\vec{B}$

ici $\frac{d^2}{dt^2}\langle\vec{r}\rangle = \frac{1}{m}\frac{d\langle\vec{u}\rangle}{dt} = \frac{q}{m^2}\langle\vec{u}\wedge\vec{B}\rangle = \frac{q}{m^2}\langle\vec{u}\rangle\wedge\vec{B} = \frac{q}{m}\frac{d}{dt}\langle\vec{r}\rangle\wedge\vec{B}$

donc $\frac{d^2}{dt^2}\langle\vec{r}\rangle = \frac{q}{m}\frac{d}{dt}\langle\vec{r}\rangle\wedge\vec{B}$ $\quad$ identique à $\frac{d^2\vec{r}}{dt^2} = \frac{q}{m}\left(\frac{d\vec{r}}{dt}\right)\wedge\vec{B}$

4) Observable vitesse $\vec{v}$ en fct de $\vec{u}$ $\quad \vec{v} = \frac{d\vec{r}}{dt} = \frac{\vec{u}}{m}$

$\hat H = \frac{\hat{\vec{u}}^2}{2m} = \frac{m^2\hat{\vec{v}}^2}{2m} = \frac{1}{2}m\hat{\vec{v}}^2$ $\Rightarrow$ forme classique d'énergie cinétique

En présence d'un champ magnétique, il ne faut pas confondre l'impulsion $\vec{p}$ (sens lagrangien du terme) avec la $q^{té}$ de mouvement $m\vec{v} = \vec{p} - q\vec{A}$

De ce qui précède $\left[\hat{u}_x, \hat{u}_y\right] = i\hbar q B$

$$\left[\hat{u}_x, \hat{u}_z\right] = \left[\hat{u}_y, \hat{u}_z\right] = 0$$

$\Rightarrow$ $\hat{u}_x$ et $\hat{u}_y$ (resp $\hat{v}_x$ et $\hat{v}_y$) ne peuvent pas être simultanément bien mesurées (commutateur non nul !)

<u>Th de Schwartz</u> : $\Delta \hat{M} \cdot \Delta \hat{N} \geq \frac{1}{2} \left|\langle[\hat{M}, \hat{N}]\rangle\right|$

ici $$\Delta v_x \cdot \Delta v_y \geq \frac{1}{2} \left|\langle \underbrace{[\hat{v}_x, \hat{v}_y]}_{\frac{i\hbar q B}{m^2}} \rangle\right| = \frac{1}{2} \frac{\hbar q B}{m^2}$$