Mécanique Quantique I

séance d'exercices 7

Exercice 1

$$\hat{A}(t) = \frac{1}{i\hbar} \int_{t_0}^{t} \hat{H}(t')\,dt'$$

$$\frac{d\hat{A}}{dt} = \frac{1}{i\hbar} \hat{H}(t)$$

$$\left[\frac{d\hat{A}}{dt}, \hat{A}(t)\right] = -\frac{1}{i\hbar} \cdot \frac{1}{i\hbar} \left[\hat{H}(t), \int_{t_0}^{t} \hat{H}(t')\,dt'\right]$$

$$= \frac{1}{\hbar^2} \int_{t_0}^{t} \underbrace{[\hat{H}(t), \hat{H}(t')]}_{=0 \ \forall t' \in [t_0, t]} dt'$$

$$= 0$$

Exercice 2

a)

$\hat{P}$: projecteur $\Rightarrow P^+ = P$, $\hat{P}^2 = P$

$e^{ix\hat{P}} = \hat{A}$. On voit que $A^+A = e^{-ix\hat{P}} \cdot e^{ix\hat{P}} = \mathbb{1} \Rightarrow A$ unitaire

$$e^{ix\hat{P}} = \sum_{k=0}^{\infty} \frac{(ix\hat{P})^k}{k!} = \mathbb{1} + ix\hat{P} + \frac{(ix\hat{P})^2}{2!} + \frac{(ix\hat{P})^3}{3!} + \ldots \Rightarrow$$

$P^2 = P \Rightarrow P^3 = P^2 = P \Rightarrow P^k = P \ \forall k \in \mathbb{N}$

$$\Rightarrow e^{ix\hat{P}} = \mathbb{1} + \hat{P}\left(ix + \frac{(ix)^2}{2!} + \frac{(ix)^3}{3!} + \ldots\right)$$

$$\Rightarrow e^{ix\hat{P}} = \mathbb{1} + \hat{P}(e^{ix} - 1)$$

On voit aussi que si $\hat{A} = e^{ix\hat{P}} = \mathbb{1} + \hat{P}(e^{ix} - 1)$

$$A \cdot A^+ = (\mathbb{1} + \hat{P}(e^{ix} - 1)) \cdot (\mathbb{1} + \hat{P}(e^{ix} - 1))^+ = \ldots = \mathbb{1}$$

b)

$$\hat{H} = \hbar\omega |1\rangle\langle 1| \quad , \quad |\psi(0)\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

L'opérateur d'évolution est :

$$U(t) = e^{\frac{i}{\hbar}\hat{H}\cdot t} = \exp\left(\frac{i}{\hbar}\hat{H}t\right) = \exp\left(\frac{i}{\hbar}\hbar\omega|1\rangle\langle 1|\right) = \exp\left(i\omega t|1\rangle\langle 1|\right)$$

on voit que, si on poser $x = \omega t$ et $\hat{P} = |1\rangle\langle 1|$

on a $U(t) = \exp(ix\hat{P}) \overset{a)}{=} \mathbb{1} + |1\rangle\langle 1|(e^{i\omega t} - 1)$

L'opérateur $U(t)$ permet de déterminer l'état du système $|\varphi(t)\rangle$, $\forall t > t_0$, à partir de la connaissance de l'état $|\varphi(t_0)\rangle$ au temps t_0.

$$|\varphi(t)\rangle = U(t)\,|\varphi(0)\rangle$$

$$|\varphi(t)\rangle = \left(\mathbb{1} + |1\rangle\langle 1|\,(e^{i\omega t} - 1)\right) \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$|\varphi(t)\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} + \underbrace{|1\rangle\langle 1|\,(|0\rangle + |1\rangle)}_{B} \frac{(e^{i\omega t} - 1)}{\sqrt{2}}$$

$B = |1\rangle\langle 1|\,(|0\rangle + |1\rangle) \Rightarrow$

$B = |1\rangle(\langle 1|0\rangle + \langle 1|1\rangle) = |1\rangle\,(0 + 1) = |1\rangle$

Donc $|\varphi(t)\rangle = \dfrac{|0\rangle + |1\rangle}{\sqrt{2}} + |1\rangle \dfrac{(e^{i\omega t} - 1)}{\sqrt{2}}$

$$|\varphi(t)\rangle = \frac{|0\rangle + e^{i\omega t}\,|1\rangle}{\sqrt{2}}$$

$e^{i\omega t}$: facteur de phase entre les états $|0\rangle$ et $|1\rangle$.

Exercice 3

a)

$$\frac{\partial \rho(r,t)}{\partial t} = \frac{\partial}{\partial t}\left(\varphi^*(r,t)\cdot\varphi(r,t)\right)$$

$$= \frac{\partial \varphi^*(r,t)}{\partial t}\,\varphi(r,t) + \varphi^*(r,t)\,\frac{\partial \varphi(r,t)}{\partial t}$$

L'équation Shr. dépendent du temps est

$$i\hbar \frac{\partial}{\partial t}\varphi(r,t) = \hat{H}\varphi(r,t) \Rightarrow -i\hbar\frac{\partial}{\partial t}\varphi^*(r,t) = \varphi^*(r,t)\hat{H}$$

$$(\hat{H}^+ = \hat{H})$$

$$\left.\begin{array}{l} \text{Alors } \dfrac{\partial \rho(r,t)}{\partial t} = \dfrac{1}{-i\hbar}\left(\hat{H}\varphi^*(r,t)\right)\cdot\varphi(r,t) + \varphi^*(r,t)\cdot\dfrac{1}{i\hbar}\hat{H}\varphi(r,t) \\ \hat{H} = -\dfrac{\hbar^2}{2m}\nabla^2 + V \end{array}\right\} \Rightarrow$$

$$\Rightarrow \frac{\partial \rho(r,t)}{\partial t} = \frac{1}{-i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2\varphi^*(r,t) + V\varphi^*(r,t)\right)\varphi(r,t) +$$

$$\varphi^*(r,t)\,\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2\varphi(r,t) + V\varphi(r,t)\right)$$

Mécanique Quantique I
Séance d'exercices 7

Exercice 3, a) (cont.)

$$\frac{\partial \rho(r,t)}{\partial t} = \frac{\hbar}{2mi}\Big((\nabla^2 \psi^*(r,t))\psi(r,t) - \cancel{V\psi^*(r,t)\psi(r,t)}$$
$$- \psi^*(r,t)\cdot\nabla^2\psi(r,t) + \cancel{V\psi^*(r,t)\psi(r,t)}\Big)$$
$$= \frac{\hbar}{2mi}\Big[(\nabla^2\psi^*(r,t))\cdot\psi(r,t) - \psi^*(r,t)\cdot\nabla^2\psi(r,t)\Big]$$

b)
Il faut qu'on ecrit l'expression

$$\frac{\hbar}{2mi}\left[\nabla^2\psi^*(r,t)\cdot\psi(r,t) - \psi^*(r,t)\nabla^2\psi(r,t)\right] = C$$

dans la forme $\nabla\cdot f$

On remarque que

$$\nabla\left(\nabla\psi^*(r,t)\psi(r,t) - \psi^*(r,t)\nabla\psi(r,t)\right) =$$
$$= \nabla^2\psi^*(r,t)\cdot\psi(r,t) + \cancel{\nabla\psi^*(r,t)\nabla\psi(r,t)}$$
$$- \cancel{\nabla\psi^*(r,t)\nabla\psi(r,t)} - \psi^*(r,t)\cdot\nabla^2\psi(r,t)$$
$$= \nabla^2\psi^*(r,t)\psi(r,t) - \psi^*(r,t)\nabla^2\psi(r,t)$$

Donc $C = \frac{\hbar}{2mi}\nabla\left(\nabla\psi^*(r,t)\psi(r,t) - \psi^*(r,t)\nabla\psi(r,t)\right)$

$$\frac{\partial\rho(r,t)}{\partial t} = C \Rightarrow \frac{\partial\rho(r,t)}{\partial t} + (-C) = 0 \Rightarrow$$

$$\frac{\partial\rho(r,t)}{\partial t} + \nabla\left[\frac{\hbar}{2mi}\left(\psi^*(r,t)\nabla\psi(r,t) - \nabla\psi^*(r,t)\psi(r,t)\right)\right] = 0$$

$$\Rightarrow \frac{\partial\rho(r,t)}{\partial t} + \nabla J = 0$$

avec $J = \frac{\hbar}{2mi}\left(\psi^*(r,t)\nabla\psi(r,t) - \nabla\psi^*(r,t)\psi(r,t)\right)$

c)

$$J(r,t) = \frac{1}{2}\left[\frac{\hbar}{mi}\varphi^*(r,t)\nabla\varphi(r,t) - \frac{\hbar}{mi}\varphi(r,t)\nabla\varphi^*(r,t)\right]$$

On voit que $\left(\frac{\hbar}{mi}\varphi^*(r,t)\nabla\varphi(r,t)\right)^* = -\frac{\hbar}{mi}\varphi(r,t)\nabla\varphi^*(r,t) = z$

Alors $\left.\begin{array}{l} J(r,t) = \frac{1}{2}(z^* + z) \\ z + z^* = 2\,\mathrm{Re}\{z\} \end{array}\right\} \Rightarrow J(r,t) = \mathrm{Re}(z) \Rightarrow$

$$J(r,t) = \mathrm{Re}\left(\frac{i\hbar}{m}\varphi^*\nabla\varphi\right)$$

$$\Leftrightarrow J(r,t) = \mathrm{Re}\left(\frac{\varphi^*}{m}\hat{p}\varphi\right)$$

$$\Leftrightarrow J(r,t) = \mathrm{Re}\{\underbrace{\varphi^*\hat{v}\varphi}\}$$

$\Leftrightarrow$ comparé avec cas classique : $j(\vec{r},t) = \vec{v}\cdot\rho$