Evolution temporelle d'un état quantique

$|\psi(0)\rangle$ $\quad t=0 \quad$ $E \to \hat{\mathcal{H}}$

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{\mathcal{H}}|\psi(t)\rangle$$

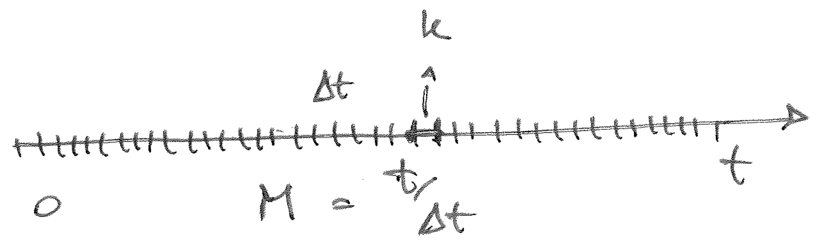
$$|\psi(t)\rangle = \hat{U}(t,0)\,|\psi(0)\rangle$$

1) cas de $\hat{\mathcal{H}}$ indépendant de t

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}$$

2) $\hat{\mathcal{H}}$ dépendant du temps $\quad \hat{\mathcal{H}} = \hat{\mathcal{H}}(t)$

I) $[\hat{\mathcal{H}}(t), \hat{\mathcal{H}}(t')] = 0$



$$\hat{U}(t) \underset{\substack{\Delta t \to 0 \\ M \to \infty}}{\cong} \prod_{k=1}^{M} e^{-\frac{i}{\hbar}\hat{\mathcal{H}}(k\Delta t)\,\Delta t}$$

$$[\hat{\mathcal{H}}(k\Delta t), \hat{\mathcal{H}}(k'\Delta t)] = 0$$

$$e^{\hat{A}}\, e^{\hat{B}} \underset{[\hat{A},\hat{B}]=0}{=} e^{\hat{A}+\hat{B}}$$

$$= e^{-\frac{i}{\hbar}\sum_{k=1}^{M}\hat{\mathcal{H}}(k\Delta t)\,\Delta t} = e^{-\frac{i}{\hbar}\int_0^t dt'\,\hat{\mathcal{H}}(t')}$$

$$\boxed{\hat{U} = e^{-\frac{i}{\hbar}\int_0^t dt'\,\hat{\mathcal{H}}(t')}}$$

$$\hat{\mathcal{H}}(t) = -\frac{g\mu_B}{\hbar}\, B_z(t)\, \hat{S}_z$$

II) $[\hat{H}(t), \hat{H}(t')] \neq 0$

$$\hat{U} = T\left[e^{-\frac{i}{\hbar}\int_0^t dt' \hat{H}(t')} \right]$$

↳ opérateur d'ordonnement temporel

$$\left(\int dt' \hat{H}(t) \right)^2 = \int dt' H(t') \int dt'' H(t'')$$

$$= \int dt' \int dt'' H(t') H(t'')$$

$$= T \left[\sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \left(\hat{H}(t_1) \hat{H}(t_2) \cdots \hat{H}(t_n) \right) \right]$$

$$= \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-2}} dt_{n-1} \int_0^{t_{n-1}} dt_n \; \hat{H}(t_1) \hat{H}(t_2) \cdots \hat{H}(t_n)$$

Points de vue sur l'évolution
("picture")

Point de vue de $\boxed{\text{Schrödinger}}$ $\quad |\psi(0)\rangle \to |\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$$

$$\langle \hat{A} \rangle_t = \langle \psi(t)| \hat{A} |\psi(t)\rangle$$

$$= \langle \psi(0)| \underbrace{\hat{U}^\dagger(t) \; \hat{A} \; \hat{U}(t)} |\psi(0)\rangle$$

$$\hat{A}_H(t) = \hat{U}^\dagger(t) \hat{A} \hat{U}(t)$$

point de vue d'$\boxed{\text{Heisenberg}}$

les opérateurs évoluent
les états non

[$\hat{A}(t)$ si fonction dépendante du temps]

③

$$i\hbar \frac{d\hat{A}_H}{dt} = i\hbar \frac{d\hat{U}^+}{dt}\hat{A}\hat{U} + \hat{U}^+\hat{A}\left(i\hbar\frac{d\hat{U}}{dt}\right)$$

$$+ i\hbar\, \underbrace{\hat{U}^+\left(\frac{\partial \hat{A}}{\partial t}\right)\hat{U}}_{} \rightarrow \left(\frac{\partial \hat{A}}{\partial t}\right)_H$$

$$i\hbar \frac{d}{dt}\hat{U}\cancel{|\psi(0)\rangle} = \hat{H}\hat{U}\cancel{|\psi(0)\rangle}$$

$$i\hbar \frac{d}{dt}\hat{U} = \hat{H}\hat{U}$$

$$-i\hbar \frac{d}{dt}\hat{U}^+ = \hat{U}^+\hat{H}$$

$$\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}$$

$\hat{H}$ indépendant de t

$$= -\hat{U}^+\hat{H}\underset{\hat{U}\hat{U}^+}{\wedge}\hat{A}\hat{U} + \hat{U}^+\hat{A}\underset{\hat{U}\hat{U}^+}{\wedge}\hat{H}\hat{U} + i\hbar\left(\frac{\partial \hat{A}}{\partial t}\right)_H$$

$$= \hat{A}_H\hat{H}_H - \hat{H}_H\hat{A}_H + i\hbar\left(\frac{\partial \hat{A}}{\partial t}\right)_H \Rightarrow$$

$$\boxed{i\hbar\frac{d}{dt}\hat{A}_H = [\hat{A}_H, \hat{H}_H] + i\hbar\left(\frac{\partial \hat{A}}{\partial t}\right)_H}$$

$\langle\psi(0)|$ $\quad$ $|\psi(0)\rangle = \langle\psi(0)|$ $\quad$ $|\psi(0)\rangle$

$$i\hbar\frac{d}{dt}\langle\psi(0)|A_H|\psi(0)\rangle = \langle\psi(0)|[\quad]|\psi(0)\rangle + i\hbar\langle\psi(0)|\frac{\partial \hat{A}}{\partial t}|\psi(0)\rangle$$

$$\hat{A} = \hat{\vec{S}}\cdot\vec{u}(t)$$

$$\frac{\partial \hat{A}}{\partial t} = \hat{\vec{S}}\cdot\frac{\partial \vec{u}}{\partial t}$$

Point de l'interaction (ou de Dirac)

$$\hat{H}(t) = \hat{H}_0 + \hat{W}(t)$$

$$|\psi(t)\rangle \rightarrow |\psi_I(t)\rangle = e^{+\frac{i}{\hbar}\hat{H}_0 t}|\psi(t)\rangle$$

état dans le point de vue de l'interaction

$$i\hbar\frac{d}{dt}|\psi_I(t)\rangle = -\hat{H}_0|\psi_I(t)\rangle + e^{\frac{i}{\hbar}H_0 t}\,\hat{H}\, e^{-\frac{i}{\hbar}H_0 t} e^{\frac{i}{\hbar}H_0 t}|\psi(t)\rangle$$

$$e^{\frac{i}{\hbar}H_0 t}\hat{H}e^{-\frac{i}{\hbar}H_0 t} = \hat{H}_0 + \hat{W}_I(t)$$

$$\boxed{\hat{W}_I(t) = e^{\frac{i}{\hbar}H_0 t}\hat{W}(t)e^{-\frac{i}{\hbar}H_0 t}}$$

$$= [\cancel{-\hat{H}_0} + \cancel{\hat{H}_0} + \hat{W}_I(t)]|\psi_I(t)\rangle$$

$$= \hat{W}_I(t)|\psi_I(t)\rangle$$

$$\boxed{i\hbar\frac{d}{dt}|\psi_I(t)\rangle = \hat{W}_I(t)|\psi_I(t)\rangle}$$

Opérateur d'évolution temporelle (Schrödinger)

$$\hat{U}(t_3, t_2)\ \hat{U}(t_2, t_1) = \hat{U}(t_3, t_1)$$ propriété de semi-groupe

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<u>Application</u> : principe de la résonance magnétique nucléaire (RMN)

Spin $-\frac{1}{2}$:

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

base de ses vecteurs propres

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

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

$$(\sigma^\alpha)^2 = \mathbb{1} \qquad (\sigma^\alpha)^n = \begin{cases} \mathbb{1} & n \text{ pair} \\ \sigma^\alpha & n \text{ impair} \end{cases}$$

$\alpha = x, y, z$

$$(\hat{S}^\alpha)^2 = \hat{\mathbb{1}} \cdot \frac{\hbar^2}{4}$$

$$\hat{S}^+ = \hat{S}^x + i\hat{S}^y \rightarrow \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \rightarrow \hbar\ |\uparrow_z\rangle\langle\downarrow_z|$$ montée

$$\hat{S}^- = (\hat{S}^+)^\dagger = \hat{S}^x - i\hat{S}^y \rightarrow \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \rightarrow \hbar\ |\downarrow_z\rangle\langle\uparrow_z|$$ descente

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

$$\hat{S}^+\hat{S}^- = \hbar^2 (|\uparrow\rangle\langle\downarrow|)(|\downarrow\rangle\langle\uparrow|) = \hbar^2 |\uparrow\rangle\langle\uparrow|$$

$$\hat{S}^-\hat{S}^+ = \quad -- \quad = \hbar^2 |\downarrow\rangle\langle\downarrow|$$

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\boxed{[\hat{S}^+, \hat{S}^-] = \hbar\, 2\hat{S}^z} \rightarrow \boxed{[\sigma^+, \sigma^-] = \sigma^z}$$

$$\sigma^+ = \sigma^x + i\sigma^y \qquad \sigma^- = \sigma^x - i\sigma^y$$

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

$$\hat{S}^-\hat{S}^z = \quad -- \quad = \frac{\hbar}{2}\hat{S}^-$$

$\ominus$

$$(\hat{S}^+\hat{S}^z)^\dagger = \hat{S}^z\hat{S}^- = -\frac{\hbar}{2}\hat{S}^-$$

$\ominus$

$$(\hat{S}^-\hat{S}^z)^\dagger = \hat{S}^z\hat{S}^+ = \frac{\hbar}{2}\hat{S}^+$$

$$\boxed{[\hat{S}^z, \hat{S}^\pm] = \pm\hbar\hat{S}^\pm} \qquad \boxed{[\sigma^z, \sigma^\pm] = \pm 2\sigma^\pm}$$

$$e^{-i\frac{\phi}{2}\sigma^z}\,\sigma^\pm\, e^{i\frac{\phi}{2}\sigma^z} = \tilde{\sigma}^\pm(\phi) \qquad \phi \in \mathbb{R}$$

→ ~~transformation~~ unitaire

$$\frac{d\tilde{\sigma}^\pm}{d\phi} = e^{-i\frac{\phi}{2}\sigma^z}\left(-\frac{i}{2}\sigma^z\sigma^\pm + \frac{i}{2}\sigma^\pm\sigma^z\right) e^{i\phi\sigma^z}$$

$$= e^{-i\frac{\phi}{2}\sigma^z}\,\frac{i}{2}[\sigma^\pm, \sigma^z]\, e^{i\frac{\phi}{2}\sigma^z} = \mp i\,\tilde{\sigma}^\pm$$

$$\frac{d\tilde{\sigma}^\pm}{d\phi} = \mp i\,\tilde{\sigma}^\pm$$

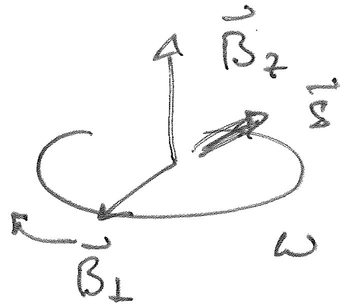
$$\tilde{\sigma}^\pm(\phi) = \sigma^\pm e^{\mp i\phi} \Longrightarrow$$

$$e^{-i\frac{\phi}{2}\sigma^z}$$

↑

$$\boxed{e^{-\frac{i}{\hbar}\hat{S}^z\phi}\,\hat{S}^\pm\, e^{\frac{i}{\hbar}\hat{S}^z\phi} = \hat{S}^\pm e^{\mp i\phi}}$$

RMN :



$$\vec{B}(t) = B_z \vec{e}_z + B_\perp \left[\cos(\omega t)\, \vec{e}_x - \sin(\omega t)\, \vec{e}_y \right]$$

$$\begin{cases} \hat{S}^+ = \hat{S}^x + i \hat{S}^y \\ \hat{S}^- = \hat{S}^x - i \hat{S}^y \end{cases} \qquad \hat{S}^x = \frac{\hat{S}^+ + \hat{S}^-}{2} \qquad \hat{S}^y = \frac{\hat{S}^+ - \hat{S}^-}{2i}$$

$$\hat{H} = -\frac{g\mu_B}{\hbar} \vec{B}(t) \cdot \vec{S} = -\underbrace{\frac{g\mu_B B_z}{\hbar}}_{\omega_0} S^z - \underbrace{\frac{g\mu_B B_\perp}{\hbar}}_{\omega_1} \Big[\cos(\omega t) \hat{S}^x - \sin(\omega t) \hat{S}^y \Big]$$

$$\cos(\omega t) \to \frac{e^{i\omega t} + e^{-i\omega t}}{2} \qquad \sin(\omega t) \to \frac{e^{i\omega t} - e^{-i\omega t}}{2i}$$

$$= \ldots = -\omega_0 S^z - \frac{\omega_1}{2} \left[e^{+i\omega t} \hat{S}^+ + e^{-i\omega t} \hat{S}^- \right]$$

Référentiel tournant

$$|\tilde{\psi}(t)\rangle = e^{-\frac{i}{\hbar}\omega \hat{S}^z t} |\psi(t)\rangle$$

état vu d'un référentiel qui tourne d'une façon solidaire au champ $\vec{B}_\perp$

$$i\hbar \frac{d}{dt} |\tilde{\psi}(t)\rangle = \omega \hat{S}^z |\tilde{\psi}(t)\rangle + e^{-\frac{i}{\hbar}\omega \hat{S}^z t} \Big[-\omega_0 \hat{S}^z - \frac{\omega_1}{2} \left(e^{i\omega t} S^+ + e^{-i\omega t} S^- \right) \Big] e^{\frac{i}{\hbar}\omega \hat{S}^z t} \tilde{\psi}(t)$$

$$1 = e^{\frac{i}{\hbar}\omega S^z t} e^{-\frac{i}{\hbar}\omega S^z t}$$

$$\phi = \omega t$$

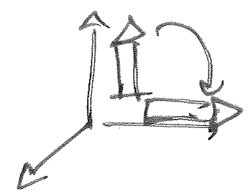
$$= \Big[-\overbrace{(\omega_0 - \omega)}^{\delta} \hat{S}^z - \frac{\omega_1}{2} (S^+ + S^-) \Big] |\tilde{\psi}(t)\rangle$$

$$= \left[-\delta \hat{S}^z - \omega_1 \hat{S}^x \right] |\tilde{\psi}(t)\rangle$$

$\delta = 0$

$$|\tilde{\psi}(0)\rangle = |\psi(0)\rangle = |\uparrow_z\rangle \qquad |\tilde{\psi}(t)\rangle = \cos\left(\frac{\omega_1 t}{2}\right) |\uparrow_z\rangle + i \sin\left(\frac{\omega_1 t}{2}\right) |\downarrow_z\rangle$$

$$T_{\pi/2} = \frac{\pi}{2\omega_1} \qquad \tilde{\psi}(T_{\pi/2}) = \frac{1}{\sqrt{2}} \left(|\uparrow_z\rangle + i |\downarrow_z\rangle \right) = |\uparrow_y\rangle$$



référentiel tournant

référentiel du labo

$$|\psi(t)\rangle = e^{\frac{i}{\hbar}\omega \hat{S}^z t}\,|\tilde{\psi}(t)\rangle \qquad \omega = 2\omega_1$$

$T_{\pi/2} = \frac{\pi}{2\omega_1}$

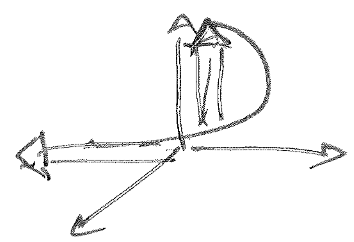
$$= e^{\frac{i}{\hbar}\frac{\pi}{2\omega_1}\cancel{2\omega_1}\hat{S}^z}\,|\tilde{\psi}(t)\rangle$$

$t = T_{\pi/2}$

$$= e^{\frac{i}{\hbar}\pi \hat{S}^z}\,\frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle + i\,|\downarrow_z\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\Big(\underbrace{e^{+i/2\,\pi}}_{i}\,|\uparrow_z\rangle + i\,\underbrace{e^{-i\pi/2}}_{-i}\,|\downarrow_z\rangle\Big)$$

$$= \frac{i}{\sqrt{2}}\left(|\uparrow_z\rangle - i\,|\downarrow_z\rangle\right) = i\,|\downarrow_y\rangle$$



Espaces d'Hilbert de dimension infinie

$D = 2$ spin $\frac{1}{2}$

$D = \infty$

$$|\psi\rangle = \sum_{n=1}^{\infty} \psi_n |\alpha_n\rangle \to \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \\ \vdots \end{pmatrix}$$

$\{|\alpha_n\rangle\}$ $\quad \langle\alpha_n|\alpha_m\rangle = \delta_{nm}$

$n = 1, \ldots, \infty$

$\approx$ $\mathbb{C}^{\infty}$

infini de coefficients

$|\psi\rangle$ état physique $\|\psi\|^2 = \langle\psi|\psi\rangle = 1$

$|\psi\rangle \to$ état physique $\dfrac{|\psi\rangle}{\|\psi\|}$

$$\|\psi\|^2 = \langle\psi|\psi\rangle = \sum_{n=1}^{\infty} |\psi_n|^2$$

Sous-espace physique de l'espace d'Hilbert $\quad H_{\Phi} \subset H \qquad \dim(H) = \infty$

H_{Φ} : $|\psi\rangle \in H$: $\|\psi\| < \infty$

$|\psi\rangle, \; |\phi\rangle \in H_{\Phi} \Rightarrow \lambda|\psi\rangle + \mu|\phi\rangle \in H_{\Phi}$

$\langle\psi|\psi\rangle, \; \langle\phi|\phi\rangle < \infty \qquad \lambda, \mu \in \mathbb{C} \quad |\lambda|, |\mu| < \infty$

$\| \lambda|\psi\rangle + \mu|\phi\rangle \|^2$

$= (\lambda^* \langle\psi| + \mu^* \langle\phi|)(\lambda|\psi\rangle + \mu|\phi\rangle)$

$= |\lambda|^2 \|\psi\|^2 + |\mu|^2 \|\phi\|^2 + \lambda^*\mu\langle\psi|\phi\rangle + \mu^*\lambda\langle\phi|\psi\rangle \; < \infty$

$|\langle\psi|\phi\rangle|^2 \leq \|\psi\|^2 \, \|\phi\|^2 < \infty$ (9)

$|\psi\rangle \in \mathcal{H}_\Phi \rightarrow \hat{A}|\psi\rangle \in \mathcal{H}_\Phi$? NON

$$\hat{A} : |\psi\rangle = \sum_{n=1}^{\infty} \psi_n |\alpha_n\rangle \longrightarrow |\psi\rangle = \sum_{n=1}^{\infty} n\,\psi_n |\alpha_n\rangle$$

$|\psi\rangle \in \mathcal{H}_\Phi$

$$\begin{cases} \sum_{n=1}^{\infty} |\psi_n|^2 < \infty \quad \left(\to \frac{1}{n^{2\alpha}}\right) & \alpha > 1/2 \\ \sum_{n=1}^{\infty} n^2 |\psi_n|^2 = \infty \quad \left(\frac{1}{n^{2\alpha-2}}\right) & 2\alpha - 2 \leq 1 \\ & \alpha \leq 3/2 \end{cases}$$

$\psi_n = \frac{1}{n^\alpha}$

$\frac{1}{2} < \alpha \leq 3/2$

Est-ce que $\hat{A}$ me laisse en $\mathcal{H}_\Phi$ ou pas ?

Norme d'un opérateur sur $\mathcal{H}_\Phi$: $\sup_{\substack{|\psi\rangle \in \mathcal{H}_\Phi \\ \|\psi\|^2 = 1}} \|\hat{A}|\psi\rangle\| = \|A\|_{\mathcal{H}_\Phi}$

$\hat{A} = \hat{A}^\dagger$ admets des valeurs propres réels

$$\|A\|_{\mathcal{H}_\Phi} = \max(\lambda_i)$$

$\hat{A}$ est dit borné si $\|\hat{A}\| < \infty$ (spectre est borné).

Exemple : espaces des fonctions à valeurs complexes au carré sommable sur $[0,1]$

$L^{(2)}[0,1]$ $\qquad \psi(x) \in \mathbb{C} : x \in \mathbb{R}$ $\qquad \psi : x \in \mathbb{R} \to \psi(x) \in \mathbb{C}$

$$\|\psi\|^2 = \int_0^1 dx \, |\psi|^2 < \infty$$ norme $\qquad |\psi\rangle \to \psi(x)$

produit scalaire $\quad \langle \phi | \psi \rangle = \int_0^1 dx \, \phi^*(x)\, \psi(x)$

Base

$$\psi(x) = \sum_{n=-\infty}^{+\infty} e^{i 2\pi n x} \psi_n$$ série de Fourier

$|\alpha_n\rangle \Rightarrow e^{i 2\pi n x}$ $\qquad \psi_n = \langle \alpha_n | \psi \rangle = \int_0^1 dx \, e^{-i 2\pi n x} \psi(x)$

$$\langle \alpha_n | \alpha_m \rangle = \delta_{nm} = \int_0^1 dx \, e^{i 2\pi (m-n) x}$$

à démontrer : opérateur x : $\psi \to x\psi$ $\qquad$ borné

$\frac{d}{dx}$: $\psi \to \frac{d\psi}{dx}$ $\qquad$ pas borné