Etats en MQ et les espaces d'Hilbert

- <u>mécanique classique</u> 1 particule en <u>d=3</u>

$$(\vec{r}(t), \vec{p}(t)) \in \mathbb{R}^6$$

vecteur d'état

toute observable A (quantité à mesurer)

$$A = A(\vec{r}(t), \vec{p}(t))$$

- <u>mécanique quantique</u> vecteur d'état

contient les amplitudes de proba de mesurer une certaine valeur pour une certain observable

Spin $\frac{1}{2}$: $\uparrow_z$ $\quad P(\uparrow_x|\uparrow_z) = |\langle \uparrow_x | \uparrow_z \rangle|^2$ $\quad P(\uparrow_z|\uparrow_x) = |\langle \uparrow_z | \uparrow_x \rangle|^2$

<u>vecteur à composantes complexes</u>

$$|\psi\rangle$$

Espace vectoriel à coeff. $\mathbb{C}$ $\Rightarrow$ espace de <u>Hilbert</u> $\mathcal{H}$

$\dim(\mathcal{H}) = D \neq d$ dimensions de l'espace

$$\boxed{\dim(\mathcal{H}) = D < \infty}$$

spin $\frac{1}{2}$ $\rightarrow$ <u>$D=2$</u>

$\vec{S}$

Propriétés des espaces d'Hilbert de $D < \infty$

1) $|\psi\rangle \in H$ $\boxed{\lambda \in \mathbb{C} \to \text{c-nombre (c-number)}}$ multiplication par un c-nombre

$$\lambda|\psi\rangle \in H$$

2) somme

$|\psi\rangle \in H$ $|\phi\rangle \in H$ $\lambda, \mu \in \mathbb{C}$

$$\lambda|\psi\rangle + \mu|\phi\rangle \in H$$

3) produit scalaire

$|\chi\rangle \in H$ $|\psi\rangle \in H$

$$\langle\chi|\psi\rangle \in \mathbb{C}$$

$$\langle\psi|\chi\rangle = \langle\chi|\psi\rangle^*$$

$|\chi\rangle = |\psi\rangle$ $\langle\psi|\psi\rangle = \|\psi\|^2$

linéarité $\left[\langle\chi|\left(\lambda|\psi\rangle + \mu|\phi\rangle\right)\right]^* = \lambda^*\langle\chi|\psi\rangle^* + \mu^*\langle\chi|\phi\rangle^*$

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

$$\left(\lambda\langle\psi| + \mu\langle\phi|\right)|\chi\rangle = \lambda\langle\psi|\chi\rangle + \mu\langle\phi|\chi\rangle$$

③

$$\langle \chi | \left(\lambda |\psi\rangle + \mu |\phi\rangle \right) = \lambda \langle \chi|\psi\rangle + \mu \langle \chi|\phi\rangle$$

$$(\quad)^* = \left(\lambda^* \langle \psi| + \mu^* \langle \phi| \right) |\chi\rangle = \lambda^* \langle \psi|\chi\rangle + \mu^* \langle \phi|\chi\rangle$$

$$\langle \lambda \psi| = \lambda^* \langle \psi|$$

4) Base orthonormée

$\exists \ \{|\alpha_n\rangle\} \qquad n = 1, \dots, D$

$|\phi\rangle$ ket

$\forall |\psi\rangle \in H$: $\quad |\psi\rangle = \sum_{n=1}^{D} \psi_n |\alpha_n\rangle$

$\langle \phi|$ bra

$$\langle \alpha_n | \alpha_m \rangle = \delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases}$$

$\langle \phi | \psi \rangle$

bracket

$$|\phi\rangle = \sum_{n=1}^{D} \phi_n |\alpha_n\rangle$$

$$\langle \phi | \psi \rangle = \left(\sum_{m=1}^{D} \phi_m^* \langle \alpha_m | \right) \left(\sum_{n=1}^{D} \psi_n |\alpha_n\rangle \right)$$

$$= \sum_{m,n=1}^{D} \phi_m^* \psi_n \delta_{nm} = \sum_{n=1}^{D} \phi_n^* \psi_n = (\phi_1^*, \phi_2^*, \dots, \phi_D^*) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_D \end{pmatrix}$$

base $\{|\alpha_n\rangle\}$

$$|\phi\rangle \rightarrow \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_D \end{pmatrix} \qquad \langle \phi| \rightarrow (\phi_1^*, \phi_2^*, \dots, \phi_D^*)$$

ket $\qquad$ bra

représentation

Inégalité de Cauchy-Schwarz

$$|\langle\phi|\psi\rangle|^2 \le \langle\phi|\phi\rangle \langle\psi|\psi\rangle$$

5) Vecteur nul

$\lambda = 0 \in \mathbb{C}$ $\quad\quad$ $\psi \in \mathcal{H}$

$\lambda|\psi\rangle = 0$

↪ vecteur de norme zéro

$\cancel{|0\rangle}$

Spin $\frac{1}{2}$ $\quad\quad$ $D=2$

$|\uparrow_z\rangle, \ |\downarrow_z\rangle$

$$\boxed{|\uparrow_x\rangle = \frac{|\uparrow_z\rangle + |\downarrow_z\rangle}{\sqrt{2}}}$$

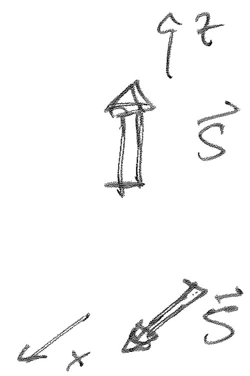
$$|\downarrow_x\rangle = \frac{-|\uparrow_z\rangle + |\downarrow_z\rangle}{\sqrt{2}}$$

$$|\uparrow_y\rangle = \frac{|\uparrow_z\rangle + i|\downarrow_z\rangle}{\sqrt{2}}$$

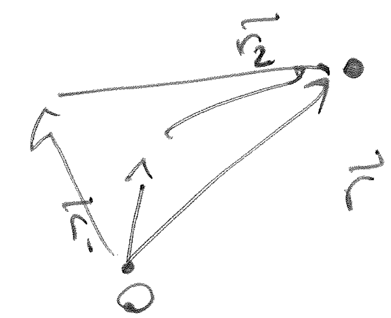
$$|\downarrow_y\rangle = \frac{|\uparrow_z\rangle - i|\downarrow_z\rangle}{\sqrt{2}}$$

$|\uparrow_z\rangle \rightarrow$

$|\uparrow_x\rangle$



Mécanique classique



Changement de base

$|\alpha_n\rangle \qquad |\beta_m\rangle$ deux bases distinctes de $\mathcal{H}$

$$|\psi\rangle = \sum_{n=1}^{D} \psi_n |\alpha_n\rangle \longrightarrow \underline{\psi_n = \langle \alpha_n | \psi \rangle}$$

$$= \sum_{m=1}^{D} \psi'_m |\beta_m\rangle$$

$$|\alpha_n\rangle = \sum_m \underbrace{\langle \beta_m | \alpha_n \rangle}_{M_{mn}} |\beta_m\rangle$$

$$|\psi\rangle = \sum_{m=1}^{D} \underbrace{\sum_{n=1}^{D} M_{mn} \psi_n}_{\psi'_m} |\beta_m\rangle$$

matrice de changement de base

$$\psi'_m = \sum_n M_{mn} \psi_n$$

Ex. $S = 1/2$

$$|\psi\rangle = \alpha |\uparrow_z\rangle + \beta |\downarrow_z\rangle \qquad \begin{pmatrix}1\\0\end{pmatrix} \quad \begin{pmatrix}0\\1\end{pmatrix}$$

$$\Rightarrow \begin{pmatrix}\alpha\\\beta\end{pmatrix}$$

$$|\uparrow_x\rangle = \frac{|\uparrow_z\rangle + |\downarrow_z\rangle}{\sqrt{2}} \qquad |\uparrow_z\rangle = \frac{|\uparrow_x\rangle - |\downarrow_x\rangle}{\sqrt{2}}$$

$$|\downarrow_x\rangle = \frac{-|\uparrow_z\rangle + |\downarrow_z\rangle}{\sqrt{2}} \qquad |\downarrow_z\rangle = \frac{|\uparrow_x\rangle + |\downarrow_x\rangle}{\sqrt{2}}$$

$$M = \begin{pmatrix} \langle \uparrow_x | \uparrow_z \rangle & \langle \uparrow_x | \downarrow_z \rangle \\ \langle \downarrow_x | \uparrow_z \rangle & \langle \downarrow_x | \downarrow_z \rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$|\psi\rangle = \frac{\alpha+\beta}{\sqrt{2}} |\uparrow_x\rangle + \frac{-\alpha+\beta}{\sqrt{2}} |\downarrow_x\rangle \longleftarrow M \begin{pmatrix}\alpha\\\beta\end{pmatrix} = \begin{pmatrix} \frac{\alpha+\beta}{\sqrt{2}} \\ \frac{-\alpha+\beta}{\sqrt{2}} \end{pmatrix}$$

Opérateurs linéaires sur H

$$\hat{A}|\psi\rangle = \underset{\in H}{|\psi'\rangle} \qquad |\psi\rangle \in H$$

$$\hat{A}\left(\lambda|\psi\rangle + \mu|\phi\rangle\right) = \lambda\,\hat{A}|\psi\rangle + \mu\,\hat{A}|\phi\rangle$$

$$\hat{A}|\psi\rangle \neq \lambda|\psi\rangle \quad /\!/\, |\psi\rangle$$

Base de H $\{|\alpha_n\rangle\}$ $\qquad \dim(H) = D < \infty$

$$\hat{A}|\psi\rangle = \sum_{n=1}^{D} \psi_n\, \hat{A}|\alpha_n\rangle = |\psi'\rangle = \sum_m \psi'_m |\alpha_m\rangle$$

élements de matrice d'une matrice A

$$\psi'_m = \langle\alpha_m|\psi'\rangle = \sum_{n=1}^{D} \psi_n \underbrace{\langle\alpha_m|\hat{A}|\alpha_n\rangle}_{A_{mn}}$$

$$\psi'_m = \sum_n A_{mn}\,\psi_n$$

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1D} \\ \vdots & A_{mn} & & \\ A_{D1} & - & \cdots & A_{DD} \end{pmatrix}$$

$\langle\alpha_m|\hat{A}|\alpha_n\rangle$

" sandwich "

$$|\psi'\rangle \Rightarrow \begin{pmatrix} \psi'_1 \\ \psi'_2 \\ \vdots \\ \psi'_D \end{pmatrix} = A \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_D \end{pmatrix}$$

opérateur : projecteur $\hat{P}(|\alpha_n\rangle) = |\alpha_n\rangle\langle\alpha_n| = |\alpha_n\rangle\langle\alpha_n|$

$$\hat{P}(|\alpha_n\rangle)|\psi\rangle = |\alpha_n\rangle \underbrace{\langle\alpha_n|\psi\rangle}_{\psi_n} = \psi_n|\alpha_n\rangle$$

$$\hat{P}^2 = \hat{P} \qquad \hat{P}^n = \hat{P} \qquad n \geq 1$$

projecteur généralisé $\hat{P}(|\alpha_n\rangle, |\alpha_m\rangle) = |\alpha_n\rangle\langle\alpha_m|$

$$\hat{P}(|\alpha_n\rangle, |\alpha_m\rangle)|\psi\rangle = \psi_m|\alpha_n\rangle$$

Tout opérateur $\hat{A}$ peut s'exprimer comme somme de $P(|\alpha_n\rangle, |\alpha_m\rangle)$

projecteurs sur les vecteurs orthonormés d'une base de H $\{|\alpha_n\rangle\}$

$\hat{P}(|\alpha_n\rangle)$

$$\left(\sum_{n=1}^{D}\hat{P}(|\alpha_n\rangle)\right)|\psi\rangle = \left(\sum_{n=1}^{D}|\alpha_n\rangle\langle\alpha_n|\right)|\psi\rangle$$

$(\hat{A}+\hat{B})|\psi\rangle = \hat{A}|\psi\rangle + \hat{B}|\psi\rangle$

$$= \sum_n |\alpha_n\rangle\psi_n = |\psi\rangle$$

$\hat{1\!\!1}|\psi\rangle = |\psi\rangle$

$$\boxed{\sum_{n=1}^{D}|\alpha_n\rangle\langle\alpha_n| = \hat{1\!\!1}}$$

résolution de l'identité sur la base $|\alpha_n\rangle$

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

A_{mn}

$$\hat{P}(|\alpha_m\rangle)\hat{A}|\psi\rangle = \langle\alpha_m|\hat{A}|\psi\rangle|\alpha_m\rangle = \sum_{n=1}^{D}\psi_n\langle\alpha_m|\hat{A}|\alpha_n\rangle|\alpha_m\rangle$$

$\rightarrow \langle\alpha_m|\psi\rangle$

$$= \sum_{n=1}^{D}\langle\alpha_m|\hat{A}|\alpha_n\rangle(|\alpha_n\rangle\langle\alpha_n|)\psi\rangle$$

$$\underbrace{\sum_m |\alpha_m\rangle\langle\alpha_m|}_{\mathbb{1}}\hat{A}|\psi\rangle = \left(\sum_{m,n=1}^{D} A_{mn}\, |\alpha_m\rangle\langle\alpha_n|\right) |\psi\rangle$$

$$\hat{A}|\psi\rangle = \left(\sum_{nm} A_{mn}\, |\alpha_m\rangle\langle\alpha_n|\right)|\psi\rangle$$

$$\boxed{\hat{A} = \sum_{n,m=1}^{D} A_{mn}\, |\alpha_m\rangle\langle\alpha_n|}$$

<u>Adjoint d'un opérateur</u> (conjugué hermitique)

$\hat{A} \rightarrow \hat{A}^{+}$ — dague

$\underbrace{\hat{A}|\psi\rangle}_{} = |\psi'\rangle$ $\qquad\qquad \langle\psi'| = \langle\psi|\hat{A}^{+}$

ket

$$\mathbb{1}\,\hat{A}|\alpha_n\rangle = \sum_m |\alpha_m\rangle\langle\alpha_m|\hat{A}|\alpha_n\rangle = \sum_m A_{mn}\, |\alpha_m\rangle$$

$$\langle\alpha_n|\hat{A}^{+} = \sum_m A^{*}_{mn}\, \langle\alpha_m|$$

<u>conjugaison complexe + transposition</u>

$$\langle\alpha_n|\hat{A}^{+}|\alpha_m\rangle = A^{*}_{mn} = (A^{+})_{nm}$$

$$\hat{A} \rightarrow \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1D} \\ \vdots & & & \\ A_{D1} & & \cdots & A_{DD} \end{pmatrix} \Longrightarrow \hat{A}^{+} \rightarrow \begin{pmatrix} A^{*}_{11} & A^{*}_{21} & \cdots & A^{*}_{D1} \\ \vdots & & & \vdots \\ A^{*}_{1D} & & \cdots & A^{*}_{DD} \end{pmatrix}$$

$$\underline{\left(\langle\alpha_n|\hat{A}|\alpha_m\rangle\right)^*} = A^*_{nm} = (A^\dagger)_{mn} = \underline{\langle\alpha_m|\hat{A}^\dagger|\alpha_n\rangle}$$

hermitiens

<u>opérateurs hermitiques</u> $\boxed{\hat{A} = \hat{A}^\dagger}$

(Hermite)

$$A^*_{mn} = A_{nm}$$

<u>Propriété fondamentale</u>

$\hat{A} = \hat{A}^\dagger$ opérateur hermitique

$\exists \{|\chi_i\rangle\}$ base orthonormée de $\mathcal{H}$

$$\hat{A}|\chi_i\rangle = a_i|\chi_i\rangle \qquad \boxed{a_i \in \mathbb{R}}$$

$$\sum_i |\chi_i\rangle\langle\chi_i| = \hat{\mathbb{1}} \qquad \text{base complète}$$

A_{nm} → diagonalisable sur la base $|\chi_i\rangle$ $\quad \hat{A} \rightarrow \begin{pmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{pmatrix}$

matrice unitaire $\xleftarrow{\text{base } \{|\alpha_n\rangle\}}$ opérateur unitaire $\hat{U}$: $\hat{U}^\dagger\hat{U} = \hat{\mathbb{1}} = \hat{U}\hat{U}^\dagger$

$\hat{U}$ opérateur unitaire $\xrightarrow[\text{base } \{|\alpha_n\rangle\}]{}$ $|\chi_i\rangle = \sum_n \chi_i^{(n)}|\alpha_n\rangle$ $\quad \hat{U} \rightarrow \begin{pmatrix} \chi_1^{(1)} & \chi_2^{(1)} & \cdots & \chi_n^{(1)} \\ \chi_1^{(2)} & & & \vdots \\ \vdots & & & \\ \chi_1^{(n)} & \cdots & & \chi_n^{(n)} \end{pmatrix}$

$$\hat{U}^+ \hat{A} \hat{U} \xrightarrow[\text{base } \{|\alpha_n\rangle\}]{} \begin{pmatrix} a_1 & & & \\ & a_2 & & \\ & & \ddots & \\ & & & a_D \end{pmatrix}$$

Propriétés fondamentales

$$\hat{A}\hat{B}|\psi\rangle = \hat{A}(\underbrace{\hat{B}|\psi\rangle}_{|\psi'\rangle}) = \hat{A}|\psi'\rangle \neq \hat{B}\hat{A}|\psi\rangle$$

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \neq \hat{0}$$ non commutativité

$(\hat{A}\hat{B})^+$

$$\hat{A}\hat{B}|\psi\rangle = |\psi'\rangle$$

$$\langle\psi'| = \langle\psi|(\hat{A}\hat{B})^+ = \langle\psi|\hat{B}^+\hat{A}^+ \Rightarrow (\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+$$

$$(\hat{A}\hat{B}\hat{C})^+ = (\hat{A}(\hat{B}\hat{C}))^+ = (\hat{B}\hat{C})^+\hat{A}^+ = \hat{C}^+\hat{B}^+\hat{A}^+$$

Spin $\frac{1}{2}$ — opérateurs possibles

base $|\uparrow_z\rangle$, $|\downarrow_z\rangle$ → $\begin{pmatrix}1\\0\end{pmatrix}$ $\begin{pmatrix}0\\1\end{pmatrix}$

$|\uparrow_z\rangle\langle\uparrow_z|$, $|\uparrow_z\rangle\langle\downarrow_z|$, $|\downarrow_z\rangle\langle\uparrow_z|$, $|\downarrow_z\rangle\langle\downarrow_z|$

$$\begin{pmatrix}1&0\\0&0\end{pmatrix} \quad \begin{pmatrix}0&1\\0&0\end{pmatrix} \quad \begin{pmatrix}0&0\\1&0\end{pmatrix} \quad \begin{pmatrix}0&0\\0&1\end{pmatrix}$$

opérateurs sur H de $\dim(H) = 2$ → matrice 2×2 à coeff. complexes

$$\hat{\mathbb{1}} \Longleftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \Longleftarrow |\hat{\uparrow}_z\rangle\langle\hat{\uparrow}_z| + |\downarrow_z\rangle\langle\downarrow_z|$$

$$\frac{\hbar}{2}\Big[|\hat{\uparrow}_z\rangle\langle\hat{\uparrow}_z| - |\downarrow_z\rangle\langle\downarrow_z|\Big] \rightarrow \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \hat{S}^z$$

$$\hat{S}^z|\hat{\uparrow}_z\rangle = \frac{\hbar}{2}|\hat{\uparrow}_z\rangle$$

$$\hat{S}^z|\downarrow_z\rangle = -\frac{\hbar}{2}|\downarrow_z\rangle$$

$$|\hat{\uparrow}_x\rangle = \frac{|\hat{\uparrow}_z\rangle + |\downarrow_z\rangle}{\sqrt{2}} \qquad |\downarrow_x\rangle = \frac{-|\hat{\uparrow}_z\rangle + |\downarrow_z\rangle}{\sqrt{2}}$$

$$\frac{\hbar}{2}\Big[|\hat{\uparrow}_x\rangle\langle\hat{\uparrow}_x| - |\downarrow_x\rangle\langle\downarrow_x|\Big] = \frac{\hbar}{4}\Big[\big(|\hat{\uparrow}_z\rangle + |\downarrow_z\rangle\big)\big(\langle\hat{\uparrow}_z| + \langle\downarrow_z|\big) - \big(-|\hat{\uparrow}_z\rangle + |\downarrow_z\rangle\big)\big(-\langle\hat{\uparrow}_z| + \langle\downarrow_z|\big)\Big]$$

$$= \hat{S}^x$$

$$= \frac{\hbar}{4}\Big[\cancel{|\hat{\uparrow}_z\rangle\langle\hat{\uparrow}_z|} + |\hat{\uparrow}_z\rangle\langle\downarrow_z| + |\downarrow_z\rangle\langle\hat{\uparrow}_z| + \cancel{|\downarrow\rangle\langle\downarrow|} - \big(+\cancel{|\hat{\uparrow}\rangle\langle\hat{\uparrow}|} - |\uparrow\rangle\langle\downarrow|$$

$$-|\downarrow\rangle\langle\uparrow| + \cancel{|\downarrow\rangle\langle\downarrow|}\big)$$

$$= \frac{\hbar}{2}\big(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\big) \longrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\frac{\hbar}{2}\Big[|\hat{\uparrow}_y\rangle\langle\hat{\uparrow}_y| - |\downarrow_y\rangle\langle\downarrow_y|\Big] \longrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$= \hat{S}^y$$