Densidade de probabilidade e Fluxo

* Fluxo de probabilidade: $\rho = |\psi(\vec{r},t)|^2$

$$\vec{J}(\vec{r},t) = -\frac{i\hbar}{2m}\left[\psi(\vec{r},t)^*\nabla\psi(\vec{r},t) - \psi(\vec{r},t)\nabla\psi(\vec{r},t)^*\right]$$

$$\frac{d}{dt}\int_V \rho\, dV = -\oint_S \vec{J}\cdot d\vec{S}$$

se fluxo > 0 (sai), probabilidade diminui

↓ T. divergência

$$\int_V \frac{\partial}{\partial t}\rho\, dV = -\int_V \nabla\cdot\vec{J}\, dV$$

arbit.

$$\int_V \Big(\underbrace{\frac{\partial}{\partial t}\rho + \nabla\cdot\vec{J}}_{=0}\Big)\, dV = 0$$

Equação da continuidade

$$\boxed{\frac{\partial}{\partial t}\rho + \nabla\cdot\vec{J} = 0}$$

* Eq. Schrödinger satisfaz a eq. continuidade:

$$\psi^* \times \left[-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}\right]$$

$$-\left[-\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^* = -i\hbar\frac{\partial\psi^*}{\partial t}\right]\times\psi$$

$$-\frac{\hbar^2}{2m}\left[\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right] = i\hbar\frac{\partial(\psi^*\psi)}{\partial t}$$

$$-\frac{\hbar^2}{2m}\nabla\Big[\underbrace{\psi^*\nabla\psi - \psi\nabla\psi^*}_{=\frac{\vec{J}}{-\frac{i\hbar}{2m}}}\Big] = i\hbar\frac{\partial(\overbrace{\psi^*\psi}^{\rho})}{\partial t} \Rightarrow \boxed{\frac{\partial}{\partial t}\rho + \nabla\cdot\vec{J} = 0}$$

* Notação

→ $dV = dx\,dy\,dz = d^3r = r^2\,\text{sen}\theta\, d\theta\, d\varphi$

→ $\int d^3r\,|\psi(\vec{r},t)|^2 = \int d^3r\,\psi(\vec{r},t)^*\psi(\vec{r},t) = 1$

→ $\delta^3(\vec{r}-\vec{r}_0) = \delta(x-x_0)\,\delta(y-y_0)\,\delta(z-z_0)$

* Corolário:

$$\int_V \frac{\partial}{\partial t}\rho\, dV = -\int_V \nabla\cdot\vec{J}\, dV \quad \Big\}\ \text{versão integral}$$

$$\frac{\partial}{\partial t}\rho + \nabla\cdot\vec{J} = 0 \quad \Big\}\ \text{versão diferencial}$$

$V\to\infty$

$\vec{J}\to 0$

$$\Rightarrow \frac{d}{dt}\int_{V\to\infty}\rho\, dV = 0 \Rightarrow \int_{V\to\infty}\rho\, dV = \text{cte no tempo}$$

$$\int_{V\to\infty}|\psi(\vec{r},t)|^2\, dV = \text{cte} = 1$$

∴ Uma vez normalizada, a função de onda permanecerá normalizada

Para potenciais reais

Porque: partículas que decaem → $V\in\mathbb{C}$

Médias em Mecânica Quântica

* Médias (valor esperado): $\langle x \rangle = \int_{-\infty}^{+\infty} x |\psi|^2 dV$

$P = |\psi|^2 \rightarrow$ densidade de probabilidade

Média sobre um ensemble, não sobre o mesmo sistema

generalizando: $\langle f(x,y,z) \rangle = \int f(x,y,z) |\psi(\vec{r})|^2 dV$ → pode depender do tempo

$\langle f(x,y,z,t) \rangle = \int f(x,y,z,t) |\psi(\vec{r},t)|^2 dV$

* Exemplo: $\langle f(x,p) \rangle = \int f(x,p) |\psi(\vec{r},t)|^2 dx = ?$

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = m \frac{d}{dt} \int_{-\infty}^{+\infty} x |\psi(x,t)|^2 dV \quad \Bigg| \quad \frac{\partial}{\partial t}|\psi|^2 + \nabla \vec{J} = 0$$

$$= m \int_{-\infty}^{+\infty} x \frac{\partial}{\partial t} |\psi|^2 dV$$

$$= -m \int_{-\infty}^{+\infty} x \nabla \vec{J} dV$$

$$= -m \int \Big[x \frac{\partial}{\partial x} J_x \, dx + \overset{0}{\cancel{x \int \frac{\partial}{\partial y} J_y \, dy}} + \overset{0}{\cancel{x \int \frac{\partial}{\partial z} J_z \, dz}} \Big] dV$$

$$\int_{-\infty}^{+\infty} \underbrace{x}_{u} \cdot \underbrace{\frac{\partial}{\partial x} J_x dx}_{dv} = \overset{0}{\cancel{x J_x \Big|_{-\infty}^{+\infty}}} - \int_{-\infty}^{+\infty} J_x \frac{\partial}{\partial x} x \, dx = \int_{-\infty}^{+\infty} -J_x \, dx \qquad \vec{J}(x,y,z) \rightarrow J_x(x,y,z)$$

$$\therefore x \frac{\partial}{\partial x} J_x = -J_x$$

$$= -m \int [-J_x] dV, \quad J_x = -\frac{i\hbar}{2m}\left(\psi^* \frac{\partial}{\partial x}\psi - \psi \frac{\partial}{\partial x}\psi^*\right)$$

$$= \int -\frac{i\hbar}{2}\left(\psi^* \frac{\partial}{\partial x}\psi - \psi \frac{\partial}{\partial x}\psi^*\right) dV$$

int. partes em x

$$= \int -i\hbar \left(\psi^* \frac{\partial}{\partial x}\psi\right) dV$$

$$\langle p_x \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, dV$$

↳ operador $\hat{p}_x$: $\vec{p} \rightarrow -i\hbar \vec{\nabla}(\cdot\cdot)$

* Generalizando: Função de operador: $\langle f(\vec{r},\vec{p}) \rangle = \int \psi^*(\vec{r},t) f(\vec{r}, -i\hbar\vec{\nabla}) \psi(\vec{r},t) dV$

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$$\psi(\vec r,t)\begin{cases}\text{Densidade de probabilidade: } \rho=|\psi(\vec r,t)|^2 \\ \text{Corrente de probabilidade: } \vec J = -\frac{i\hbar}{2m}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right) \\ \text{Médias: } \langle\vec r\rangle=\int \vec r\,\rho\, d^3r=\int\psi^*\vec r\,\psi\, d^3r,\quad \langle f(p)\rangle=\int dk\,A^* f(p)\,A\end{cases}$$

$$\left.\begin{matrix}\rho \\ \vec J\end{matrix}\right\}\ \frac{\partial\rho}{\partial t}+\nabla\cdot\vec J=0$$

* Funções: $\langle f(\vec r)\rangle=\int d^3r\,\psi^*(\vec r,t)\,f(\vec r)\,\psi(\vec r,t)$

* Operadores: $\langle g(\vec p)\rangle=\int d^3r\,\psi^*(\vec r,t)\,g(-i\hbar\nabla)\,\psi(\vec r,t)$ → função de operador

↳ Função de operador: $F(\hat O)=\sum_n a_n \hat O^n$

↳ Ex.: $e^{\frac{d}{dx}}f(x)=\left(I+\frac{d}{dx}+\frac{1}{2}\frac{d^2}{dx^2}+\cdots\right)f(x)$

$$\operatorname{sen}\left(\frac{d}{dx}\right)x^5=\left(\frac{d}{dx}-\frac{1}{3!}\frac{d^3}{dx^3}+\frac{1}{5!}\frac{d^5}{dx^5}-\cdots\right)x^5=5x^4-10x^2+1 \ //$$

$$-i\hbar\vec\nabla u(\vec r)=\vec p\,u(\vec r)$$
$$u(\vec r)=e^{i\frac{\vec p\cdot\vec r}{\hbar}}$$
$$u(\vec r)=e^{i\vec k\cdot\vec r} \ //$$

$$e^{i\vec k\cdot\vec r}e^{-\frac{iEt}{\hbar}}=e^{i\left(\vec k\cdot\vec r-\frac{E}{\hbar}t\right)}=e^{i(\vec k\cdot\vec r-\omega t)}$$

↳ Autofunções: $\hat O u_i(x)=\lambda_i u_i(x)$ → $H\varphi_i(x)=E_i\varphi_i(x)$

$$\boxed{F(\hat O)\,u_i(x)=F(\lambda_i)\,u_i(x)}$$

↳ $F(\hat O)f(x)=F(\hat O)\sum_i c_i u_i(x)=\sum_i c_i F(\hat O)u_i(x)=\sum_i c_i F(\lambda_i)u_i(x)$

↳ Autofunções do momento: $p=-i\hbar\frac{d}{dx}$ → $-i\hbar\frac{d}{dx}u(x)=p\,u(x)$ → $\boxed{u(x)=e^{\frac{ipx}{\hbar}}=e^{ikx}}$

Onda plana

$$\text{1D: }\begin{cases}\psi(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}dk\,A(k)\,e^{ikx} \\ A(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}dx\,\psi(x)\,e^{-ikx}\end{cases}$$

~ prob. de medir a posição

→ Transformada de Fourier ~ prob. de medir o momento

$$\langle p\rangle=\int dx\,\psi^*(x)\left(\frac{d}{dx}\right)\psi(x)=\int dx\,\psi^*(x)\left(-i\hbar\frac{d}{dx}\right)\int_{-\infty}^{+\infty}dk\,A(k)\frac{e^{ikx}}{\sqrt{2\pi}}=$$

$$=\int dx\,\psi^*(x)\int_{-\infty}^{+\infty}dk\,A(k)\left(-i\hbar\frac{d}{dx}\right)\frac{e^{ikx}}{\sqrt{2\pi}}$$

$$=\int dx\,\psi^*(x)\int_{-\infty}^{+\infty}dk\,A(k)\,\hbar k\frac{e^{ikx}}{\sqrt{2\pi}}$$

$$=\int_{-\infty}^{+\infty}dk\,A(k)\,\hbar k\int dx\,\psi^*(x)\frac{e^{ikx}}{\sqrt{2\pi}} \quad A^*(k)$$

$$=\int_{-\infty}^{+\infty}dk\,A(k)\,\hbar k\,A^*(k)$$

$$\therefore\boxed{\langle p\rangle=\int_{-\infty}^{+\infty}\hbar k\,|A(k)|^2\,dk} \qquad \boxed{\langle f(p)\rangle=\int_{-\infty}^{+\infty}f(\hbar k)\,|A(k)|^2\,dk=\int_{-\infty}^{+\infty}\frac{dp}{\hbar}\left|A\left(\frac{p}{\hbar}\right)\right|^2 f(p)}$$

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→ Obter informações: expandir $\psi(\vec{r},t)$

→ $\psi(\vec{r}) = \sum_E c_E \underline{\phi_E}(\vec{r})$ → estados estacionários

$$\rightarrow \begin{cases} -\dfrac{\hbar^2}{2m}\nabla^2\phi_E + V(\vec{r})\,\phi_E = E\phi_E(\vec{r}) \\ + c.c. \end{cases}$$

→ ortogonais

$V(\vec{r})$ → conservativo

+c.c. → espectro de E

$$\begin{cases} -\dfrac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi = i\hbar\dfrac{\partial\psi}{\partial t} \\ +c.c. \\ +c.i. \rightarrow \psi(\vec{r},0) = g(\vec{r}) \end{cases}$$

→ $\psi(\vec{r},t) = \text{"}\sum_E\text{"} c_E \phi_E(\vec{r}) e^{-i\frac{Et}{\hbar}}$ → estado estacionário } depende do tempo apenas de forma "trivial" por meio da exponencial complexa
↳ fase

→ $\psi(\vec{r},0) = \text{"}\sum_E\text{"} c_E \phi_E(\vec{r}) = g(\vec{r})$

→ Ortogonal: $\int d^3r\, \phi_E^*(\vec{r})\,\phi_{E'}(\vec{r}) = 0 \quad \forall\ E \neq E'$

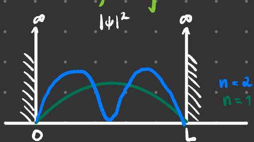
$$\int d^3r\, \phi_E^*(\vec{r})\,\phi_{E'}(\vec{r}) = \begin{cases} \delta_{E,E'} \rightarrow \text{discreto} \\ \delta(E-E') \rightarrow \text{contínuo} \end{cases}$$

$$\int d^3r\, \phi_{E'}^*(\vec{r})\,\psi(\vec{r},0) = \text{"}\sum_E\text{"} c_E \int \phi_{E'}^*(\vec{r})\,\phi_E(\vec{r}) = c_{E'}$$

* Problema de Sturm-Liouville: $\begin{cases} \mathcal{D}f(\vec{r}) = \lambda f(\vec{r}) \\ +c.c. \end{cases} \longrightarrow \begin{cases} \mathcal{H}\phi_E(\vec{r}) = E\phi_E(\vec{r}) \\ +c.c. \end{cases}$

* Exemplo:

① Poço infinito



$\phi(0) = \phi(L) = 0$

$$\boxed{E_n = \frac{\hbar^2\pi^2}{2mL} n^2} \qquad \boxed{\phi_{E_n} = \sqrt{\frac{2}{L}}\, \text{sen}\left(\frac{n\pi}{L}x\right)}$$

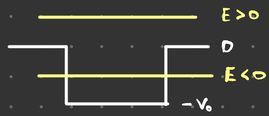
$$\boxed{\psi(\vec{r},t) = \sum_{n=1}^{\infty} \underbrace{c_n}_{\text{condição inicial}} \sqrt{\frac{2}{L}}\, \text{sen}\left(\frac{n\pi}{L}x\right) e^{-\frac{i\hbar\pi^2 n^2 t}{2m}}}$$

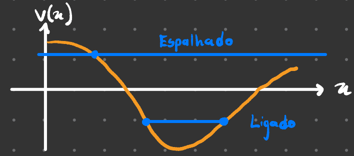
② Partícula livre (apenas energia cinética)

→ E é qualquer $(0, \dots, \infty)$

$$\boxed{\phi_E = \frac{1}{\sqrt{2\pi}} e^{-ikx}} \qquad \boxed{\psi(x,t) = \int_{-\infty}^{+\infty} dk\, \underbrace{c(k)}_{\text{condição inicial}} \frac{1}{\sqrt{2\pi}} e^{ikx} e^{-\frac{i\hbar k^2 t}{2m}}}$$

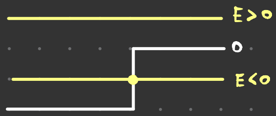
③ Poço finito





$$\boxed{\psi(x,t) = \sum_n^{\text{ligado}} c_n \phi_n(x) e^{-\frac{iE_n t}{\hbar}} + \int_0^\infty dE\, c(E)\, \phi_E(x)\, e^{-\frac{iEt}{\hbar}}}$$

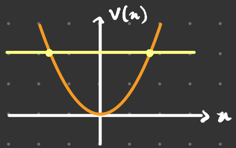
④ Barreira



$$\boxed{\phi_E = \begin{cases} A e^{ikx} + B e^{-ikx} & <0 \\ C e^{ikx} & >0 \end{cases}}$$

→ E contínuo

⑤ Oscilador harmônico



$$\boxed{E_n = \hbar\omega\left(n + \tfrac{1}{2}\right)}$$

$$\boxed{\phi_n = \text{gauss} \times \text{hermite}}$$

$$\boxed{\psi(x,t) = \sum_{n=0}^{\infty} c_n \phi_n(x) e^{-\frac{iE_n t}{\hbar}}}$$

→ $\psi(\vec{r}) = \text{"}\sum_E\text{"}\, \underset{?}{c(E)}\, \phi_E(\vec{r})$

$$\langle H \rangle = \int d^3r\, \psi^* H \psi = \int d^3r\, \psi^* H \text{"}\sum_E\text{"} c(E) \phi_E(\vec{r}) = \int d^3r\, \psi^* \text{"}\sum_E\text{"} c(E) H \phi_E(\vec{r}) = \int d^3r\, \psi^* \text{"}\sum_E\text{"} c(E) E \phi_E(\vec{r})$$

$$= \text{"}\sum_E\text{"} c(E) E \int d^3r\, \psi^*(\vec{r}) \phi_E(\vec{r}) = \text{"}\sum_E\text{"} c(E) E \left(\overbrace{\int d^3r\, \psi(\vec{r}) \phi_E^*(\vec{r})}^{c(E)}\right)^* = \text{"}\sum_E\text{"} c(E) E c^*(E)$$

$\therefore \langle H \rangle = \text{"}\sum_E\text{"} E\, |c(E)|^2$

↳ probabilidade de encontrar a partícula com energia E

* Resumo

$\psi(\vec{r}) = \int d^3r_0\, \delta(\vec{r}_0 - \vec{r})\, \psi(\vec{r}_0)$

$|\psi(\vec{r})|^2$ → densidade de probabilidade de encontrar a partícula em $\vec{r}$
↳ expansão de $\psi(\vec{r})$ nos estados $\delta(\vec{r} - \vec{r}_0)$ → posição bem definida

$|c(k)|^2$ ou $|A(k)|^2$ → densidade de probabilidade de encontrar a partícula com $\vec{p} = \hbar\vec{k}$
↳ expansão de $\psi(\vec{r})$ nos estados $e^{i\vec{k}\cdot\vec{r}}/\sqrt{2\pi}$ → momento bem definido

$|c(E)|^2$ → densidade de probabilidade de encontrar a partícula com energia E
↳ expansão de $\psi(\vec{r})$ nos estados estacionários → energia bem definida

↳ Geral: $\psi(\vec{r}) = \sum_{uga} c_{uga} \phi_{uga}$ → $|c_{uga}|^2$ → (densidade de) probabilidade de encontrar a partícula em uga

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Espaço vetorial $\mathcal{F}$

a) Definição de $\mathcal{F}$: $\psi_1(\vec{r}) \in \mathcal{F}$, $\psi_2(\vec{r}) \in \mathcal{F}$ $\Rightarrow \lambda_1\psi_1(\vec{r}) + \lambda_2\psi_2(\vec{r}) \in \mathcal{F}$ $\Big|$ $\int d^3r\, |\psi|^2 < \infty$ (L^2) + contínua

b) Produto interno: $(\psi_1, \psi_2) \equiv \int d^3r\, \psi_1^*(\vec{r})\, \psi_2(\vec{r})$

↳ Propriedades:
- $(\psi_2, \psi_1) = (\psi_1, \psi_2)^*$
- $(\psi_2, \lambda_1\varphi_1 + \lambda_2\varphi_2) = \lambda_1(\psi_2, \varphi_1) + \lambda_2(\psi_2, \varphi_2)$ $\Big\}$ $\lambda_1, \lambda_2 \in \mathbb{C}$
- $(\lambda_1\varphi_1 + \lambda_2\varphi_2, \psi_1) = \lambda_1^*(\varphi_1, \psi_1) + \lambda_2^*(\varphi_2, \psi_1)$
- $(\psi_1, \psi_2) = 0 \Rightarrow \psi_1$ e ψ_2 são ortogonais
- Norma de uma função: $\|\psi(\vec{r})\| = \sqrt{(\psi, \psi)} \geq 0 \rightarrow (\psi, \psi) = 0 \Leftrightarrow \psi = 0$

→ Estado físico $\begin{cases} \text{normalizável: definido a menos de uma constante} \\ \text{normalizado: definido a menos de uma fase} \end{cases}$

↳ Desigualdade de Schwartz: $(\varphi_1, \varphi_2) \leq \sqrt{(\varphi_1, \varphi_1)(\varphi_2, \varphi_2)}$

c) Operadores lineares: $\tilde{\psi}(\vec{r}) = A\psi(\vec{r})$

$A(\lambda_1\varphi_1(\vec{r}) + \lambda_2\varphi_2(\vec{r})) = \lambda_1 A\varphi_1(\vec{r}) + \lambda_2 A\varphi_2(\vec{r})$

↳ Produto de operadores: $A\overbrace{B\varphi(\vec{r})}^{\tilde{\varphi}(\vec{r})} = A(B\varphi(\vec{r}))$

$A\tilde{\varphi}(\vec{r}) = \tilde{\tilde{\varphi}}(\vec{r})$

$AB\varphi(\vec{r}) \neq BA\varphi(\vec{r})$

↳ Operador comutador: $[A, B] = AB - BA$

1) $[B, A] = -[A, B]$
2) $[A, BC] = B[A, C] + [A, B]C$
3) $[A, [B, C]] + [C, [B, A]] + [A, [C, B]] = 0$

↳ $[X, D] = -I$, $P = -i\hbar D$ $\Big\}$ $\boxed{[X, P] = i\hbar}$ → Quantidades físicas não comutam
Limite clássico: $\hbar \to 0 \Rightarrow$ comutam

d) Bases: $\{u_i(\vec{r})\}$, $i \in \mathbb{N}$ → discreta

→ Ortonormal: $(u_i, u_j) = \delta_{ij}$

→ $\psi(\vec{r}) = \sum_j c_j u_j(\vec{r}) \Rightarrow \int d^3r\, u_i^*(\vec{r})\psi(\vec{r}) = \sum_j c_j \int u_i^* u_j\, d^3r = \sum_j c_j \delta_{ij} \Rightarrow c_i = (u_i, \psi(\vec{r}))$

→ Exemplo: $\vec{v} = \sum_{i=1}^{3} c_i \hat{e}_i \rightarrow \hat{e}_i \cdot \vec{v} = \sum_{j=1}^{3} c_j \hat{e}_j \cdot \hat{e}_i \Rightarrow c_i = \vec{v} \cdot \hat{e}_i$

$\{u_\alpha(\vec{r})\}$, $\alpha \in \mathbb{R}$ → contínua

→ $\psi(\vec{r}) = \int_{-\infty}^{+\infty} d\alpha\, c_\alpha u_\alpha(\vec{r})$

→ $(u_\alpha, u_\beta) = \delta(\alpha - \beta) \rightarrow c_\alpha = (u_\alpha, \psi(\vec{r}))$

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* Operador hermitiano: $(f, Ag) = (Af, g)$

$$\int f^*(\vec{r}) A g(\vec{r})\, d^3r = \int (Af(\vec{r}))^* g(\vec{r})\, d^3r$$

* Bases $\begin{cases} \text{Discreta: } \{u_i(\vec{r})\},\ i = 1, 2, 3, \ldots \rightarrow \psi(\vec{r}) = \sum_i c_i u_i(\vec{r}) \\ \text{Contínua: } \{u_\alpha(\vec{r})\},\ \alpha \in \mathbb{R} \rightarrow \psi(\vec{r}) = \int d\alpha\, c(\alpha)\, u_\alpha(\vec{r}) \end{cases}$

↳ Ortonormais: $(u_i, u_j) = \delta_{ij}$, $(u_\alpha, u_\beta) = \delta(\alpha - \beta)$ | $\left.\begin{array}{l} \psi(\vec{r}) = \sum_i c_i u_i(\vec{r}) \\ \varphi(\vec{r}) = \sum_i b_i u_i(\vec{r}) \end{array}\right\}$ $(\varphi, \psi) = \sum_{i,j} b_i^* c_j \underbrace{(u_i, u_j)}_{\delta_{ij}} = \sum_i b_i^* c_i$

↳ Relação de clausura:

$$\psi(\vec{r}) = \sum_i c_i u_i(\vec{r}) = \sum_i (u_i, \psi)\, u_i(\vec{r}) = \sum_i \int d^3r'\, u_i^*(\vec{r}\,')\, \psi(\vec{r}\,')\, u_i(\vec{r}) = \int d^3r' \left(\sum_i u_i^*(\vec{r}\,')\, u_i(\vec{r})\right) \psi(\vec{r}\,')$$

$$\psi(\vec{r}) = \int d^3r' \left(\sum_i u_i^*(\vec{r}\,')\, u_i(\vec{r})\right) \psi(\vec{r}\,') \Leftrightarrow \boxed{\sum_i u_i^*(\vec{r}\,')\, u_i(\vec{r}) = \delta^{(3)}(\vec{r}\,' - \vec{r})}$$

	Base discreta	Base contínua
Ortonormalidade	$(u_i, u_j) = \delta_{ij}$	$(u_\alpha, u_\beta) = \delta(\alpha - \beta)$
Clausura	$\sum_i u_i^*(\vec{r}\,')\, u_i(\vec{r}) = \delta^{(3)}(\vec{r}\,' - \vec{r})$	$\int d\alpha\, u_\alpha^*(\vec{r}\,')\, u_\alpha(\vec{r}) = \delta^{(3)}(\vec{r}\,' - \vec{r})$
Expansão	$\psi(\vec{r}) = \sum_i c_i u_i(\vec{r})$	$\psi(\vec{r}) = \int d\alpha\, c(\alpha)\, u_\alpha(\vec{r})$
Produto interno	$(\varphi, \psi) = \sum_i b_i^* c_i$	$(\varphi, \psi) = \int d\alpha\, b^*(\alpha)\, c(\alpha)$
Norma ao quadrado	$\sum_i \lvert c_i \rvert^2 = 1$	$\int d\alpha\, \lvert c(\alpha) \rvert^2 = 1$

* Exemplos (1D)

1. Onda plana

$$u_k(x) = e^{ikx}, \quad \lambda \equiv \frac{2\pi}{k}$$

$$\int_{-\infty}^{+\infty} |u_k|^2 dk = \int |e^{ikx}| dk = \int_{-\infty}^{+\infty} dk \to \infty$$

↳ Interpretação – fluxo

densidade de partículas

$$\vec{J} = -\frac{i\hbar}{2m}\left(u_k^* \frac{d}{dk} u_k - u_k \frac{d}{dk} u_k^*\right) = -\frac{i\hbar}{2m}\left(e^{-ikx}\, ike^{ikx} - e^{ikx}(-ik)e^{-ikx}\right) = -\frac{i\hbar}{2m}(2ik) = \frac{\hbar k}{m} = \frac{p}{m} \Rightarrow \boxed{J = \rho v}$$

→ Onda plana: estado com momento bem definido

↳ Ortonormalidade

$$(u_k, u_{k'}) = \int_{-\infty}^{+\infty} dx\, e^{-ikx} e^{ik'x} = \int_{-\infty}^{+\infty} dx\, e^{i(k'-k)x}$$

↳ $\int_{-\infty}^{+\infty} dx\, e^{i\alpha x} \text{ `` = '' } 2\pi\delta(\alpha)$ → distribuição

$$\lim_{\varepsilon\to 0} \int_{-\infty}^{+\infty} dx\, e^{-\varepsilon x^2} e^{i\alpha x} = \lim_{\varepsilon \to 0} e^{-\frac{\alpha^2}{4\varepsilon}}\sqrt{\frac{\pi}{\varepsilon}}$$

$$F_\varepsilon(\alpha) \to \int_{-\infty}^{+\infty} e^{-\frac{\alpha^2}{4\varepsilon}}\sqrt{\frac{\pi}{\varepsilon}}\, d\alpha = \sqrt{\frac{\pi}{\varepsilon}} \int_{-\infty}^{+\infty} e^{-\frac{1}{4\varepsilon}\alpha^2} d\alpha^2 = \sqrt{\frac{\pi}{\varepsilon}}\sqrt{4\varepsilon\pi} = 2\pi \,//$$

↳ $\int_{-\infty}^{+\infty} e^{-ax^2+bx} dx = \int_{-\infty}^{+\infty} e^{-a[(x-x_0)^2+\Delta]}$

$$\left(x^2 + \frac{b}{a}x\right) = (x-x_0)^2 + \Delta$$
$$x^2 + \frac{b}{a}x = x^2 - 2xx_0 + x_0^2 + \Delta$$

$$-2x_0 = \frac{b}{a}, \quad x_0^2 + \Delta = 0 \Rightarrow \Delta = -x_0^2 = -\left(\frac{b}{2a}\right)^2$$

$$\int_{-\infty}^{+\infty} e^{-ax^2-bx} dx = e^{a\left(\frac{b}{2a}\right)^2}\sqrt{\frac{\pi}{a}} = e^{\frac{b^2}{4a}}\sqrt{\frac{\pi}{a}}$$

$$\therefore (e^{ikx}, e^{ik'x}) = 2\pi\delta(k'-k) \to \left(\frac{1}{\sqrt{2\pi}}e^{ikx}, \frac{1}{\sqrt{2\pi}}e^{ik'x}\right) = \delta(k'-k)$$

↳ Clausura

$$\int dk\, u_k^*(x')\, u_k(x) = \int dk \frac{e^{-ikx'}}{\sqrt{2\pi}} \frac{e^{ikx}}{\sqrt{2\pi}} = \int dk \frac{e^{ik(x-x')}}{2\pi} = \delta(x-x')$$

$\therefore \left\{\frac{1}{\sqrt{2\pi}}e^{ikx}\right\}$, $k \in \mathbb{R}$ é base ortonormal e completa

2. Deltas: $\delta(x-x_0)$

$$u_{x_0}(x) = \delta(x-x_0)$$

$\psi(x) = \int \psi(x_0)\,\delta(x-x_0)\, dx_0$ → as componentes são as próprias funções

↳ Ortonormalidade

$$(u_\alpha, u_\beta) = \delta(\alpha-\beta)$$
$$(u_{x_0}, u_{x_0'}) = \delta(x_0-x_0') \to (u_{x_0}, u_{x_0'}) = \int_{-\infty}^{+\infty} dx\, \delta(x-x_0)\,\delta(x-x_0') = \delta(x_0-x_0') \to \text{ortonormal}$$

↳ Clausura

$$\int d\alpha\, u_\alpha^*(x')\, u_\alpha(x) = \delta(x-x')$$
$$\int dx_0\, u_{x_0}^*(x')\, u_{x_0}(x) = \int dx_0\, \delta^*(x_0-x')\,\delta(x_0-x) = \delta(x-x') \to \text{completa}$$

Aproximação Clássica

Princípio da correspondência

i) Teorema de Ehrenfest

ii) Relação entre comutadores e parênteses de Poisson

iii) WKB ou aproximação semiclássica

iv) Bohm - de Broglie

v) Integral de caminho de Feynman

Teorema de Ehrenfest

→ Observável A

→ $\langle A\rangle(t) = \int d^3r\, \psi(r,t)^* A\, \psi(r,t)$

$$\frac{d}{dt}\langle A\rangle(t) = \frac{d}{dt}(\psi, A\psi) = \int d^3r\left(\frac{\partial\psi^*}{\partial t}A\psi + \psi^* A\frac{\partial\psi}{\partial t} + \psi^*\frac{\partial A}{\partial t}\psi\right)$$

$H\psi = i\hbar\frac{\partial\psi}{\partial t}, \quad H\psi^* = -i\hbar\frac{\partial\psi^*}{\partial t}$

$$= \int d^3r\left[\frac{(H\psi)^*}{-i\hbar}A\psi + \psi^* A\frac{H\psi}{i\hbar} + \psi^*\frac{\partial A}{\partial t}\psi\right]$$

$$= \frac{1}{-i\hbar}(H\psi, A\psi) + \frac{1}{i\hbar}(\psi, AH\psi) + \left(\psi, \frac{\partial A}{\partial t}\psi\right)$$

$H = H^\dagger$

$$= \frac{1}{-i\hbar}(\psi, HA\psi) + \frac{1}{i\hbar}(\psi, AH\psi) + \left\langle\frac{\partial A}{\partial t}\right\rangle$$

$$= \frac{1}{i\hbar}\Big[(\psi, AH\psi) - (\psi, HA\psi)\Big] + \left\langle\frac{\partial A}{\partial t}\right\rangle$$

$$= \frac{1}{i\hbar}\Big[(\psi, [A,H]\psi)\Big] + \left\langle\frac{\partial A}{\partial t}\right\rangle$$

$$\therefore \boxed{\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle[A,H]\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle}$$

→ geral: vale para diferentes formalismos

clássico

→ $f(q,p,t) \rightarrow \frac{df}{dt} = \frac{\partial f}{\partial q}\dot q + \frac{\partial f}{\partial p}\dot p + \frac{\partial f}{\partial t} = \frac{\partial f}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial f}{\partial t}$

→ Parênteses de Poisson: $\{f,g\} \equiv \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial q}$

$$\boxed{\frac{df}{dt} = \{f, H\} + \frac{\partial f}{\partial t}}$$

↳ $\{A,B\} = \lim_{\hbar\to 0}\frac{[A,B]}{i\hbar}$

* Propriedades do comutador:

- $[A,B] = -[B,A]$
- $[A, B+C] = [A,B] + [A,C]$
- $\alpha[A,B] = [\alpha A, B] = [A, \alpha B]$
- $[A, BC] = B[A,C] + [A,B]C$

* Exemplo: $A = X$

$$\frac{d\langle X\rangle}{dt} = \frac{1}{i\hbar}\langle [X,H]\rangle = \frac{1}{i\hbar}\left\langle \frac{2i\hbar P}{2m}\right\rangle$$

$$\therefore \frac{d\langle X\rangle}{dt} = \frac{1}{m}\langle P\rangle$$

$$[X,H] = \left[X, \frac{P^2}{2m} + V(X)\right] = \left[X, \frac{P^2}{2m}\right] + [X, V(X)] = \left[X, \frac{PP}{2m}\right] + [X, V(X)] = \frac{1}{2m}\left(P\underbrace{[X,P]}_{i\hbar} + \underbrace{[X,P]}_{i\hbar}P\right) + \underbrace{\cancel{[X, V(X)]}}_{0}$$

$$XV(X) = \sum_n a_n X^n X = V(X)X$$

* Exemplo: $A = P$

$$\frac{d\langle P\rangle}{dt} = \frac{1}{i\hbar}\langle [P,H]\rangle = \frac{1}{i\hbar}\left\langle -i\hbar\frac{\partial V}{\partial X}\right\rangle = \left\langle -\frac{\partial V}{\partial X}\right\rangle$$

$$\therefore \boxed{\frac{d\langle P\rangle}{dt} = \langle F(X)\rangle}$$

$$[P,H] = \left[P, \frac{P^2}{2m} + V(X)\right] = [P, V(X)]$$

$$[P, X^n] = -ni\hbar X^{n-1}$$

$$[P, V(X)] = \left[P, \sum_n a_n X^n\right] = \sum_n a_n [P, X^n] = \sum_n (-i\hbar) a_n n X^{n-1} = -i\hbar\frac{\partial V}{\partial X}$$

Eq. Newton: $\frac{d\langle P\rangle}{dt} = F(\langle X\rangle)$ → Casos em que se recupera a 2ª lei: $\begin{cases} F(X) = 0 \to \text{partícula livre} \\ F(X) = -KX \to \text{oscilador harmônico}\end{cases}$

→ Casos aproximados: pacotes estreitos $(\langle X\rangle^2 \approx \langle X^2\rangle)$

→ Largura do pacote: $\sigma = \sqrt{\langle X^2\rangle - \langle X\rangle^2}$

$\langle X\rangle(t) \to A = X$

$\langle X^2\rangle(t) \to A = X^2 \to \frac{d\langle X^2\rangle}{dt} = \frac{1}{i\hbar}\langle [X^2, H]\rangle$

Partícula livre: $H = \frac{P^2}{2m}$

$$\frac{d^2\langle X^2\rangle}{dt^2} = \frac{4}{m}\left\langle \frac{P^2}{2m}\right\rangle \to \langle X^2\rangle(t) = \langle X^2\rangle(0) + \mu t + \frac{a}{2}t^2 = \langle X^2\rangle(0) + \mu t + \frac{\langle P^2\rangle}{m^2}t^2$$

$$\langle X\rangle(t) = \langle X\rangle(0) + v_0 t \to \langle X\rangle^2(t) = \langle X\rangle^2(0) + 2\langle X\rangle(0)v_0 t + v_0^2 t^2$$

$$\langle X^2\rangle(t) - \langle X\rangle^2(t) = \sigma_0^2 + \left(\frac{\langle P^2\rangle}{m^2} - \underbrace{v_0^2}_{\left(\frac{\langle P\rangle}{m}\right)^2}\right)t^2 + \Theta(t)$$

$$= \sigma_0^2 + \frac{\langle \Delta P^2\rangle}{m^2}t$$

alargamento mínimo: $\Theta(t) \to 0$

$\sigma^2 = \sigma_0^2 + \Delta V^2 t^2$ → princípio da incerteza

$$\left.\begin{aligned} \Delta V^2 &= \frac{\langle \Delta P\rangle^2}{m^2} \\ \Delta P &= \frac{\hbar}{2\Delta X} = \frac{\hbar}{2\sigma_0}\end{aligned}\right\} \boxed{\sigma^2 = \sigma_0^2 + \frac{\hbar^2}{4\sigma_0^2}t^2}$$

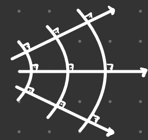
Limite clássico da Eq. Schrödinger
$\hbar \to 0$

$\to$ $-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r},t)\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$

$\to$ Para calcular o limite $\hbar \to 0$: forma polar dos complexos

$\to$ $\psi(\vec{r},t) = Ae^{\frac{iS(\vec{r},t)}{\hbar}} = \psi_1(\vec{r},t) + i\psi_2(\vec{r},t)$ $\Big|$ $A(\vec{r},t),\ S(\vec{r},t),\ \psi_1, \psi_2 \in \mathbb{R}$

$\to$ $P = |\psi|^2 = |Ae^{i\frac{S}{\hbar}}|^2 = A^2$



p fase relacionada ao momento

$\to$ $\vec{J} = -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*)$

$\nabla\psi = (\nabla A)e^{i\frac{S}{\hbar}} + \frac{iA\nabla S}{\hbar}e^{i\frac{S}{\hbar}}$

$\psi^*\nabla\psi = A\nabla A + \frac{iA^2\nabla S}{\hbar}$, $\quad \psi\nabla\psi^* = A\nabla A - \frac{iA^2\nabla S}{\hbar}$

$$\left.\right\} \vec{J} = \frac{-i\hbar}{2m}\left(\frac{2iA^2\nabla S}{\hbar}\right) \Rightarrow \boxed{\vec{J} = A^2\frac{\nabla S}{m}}$$

$$\begin{cases}\nabla S = p \\ \frac{\nabla S}{m} = v\end{cases}$$

$\to$ $-\frac{\hbar^2}{2m}\nabla^2\left[Ae^{i\frac{S}{\hbar}}\right] + V(\vec{r},t)Ae^{i\frac{S}{\hbar}} = i\hbar\left(\dot{A} + \frac{iA\dot{S}}{\hbar}\right)e^{i\frac{S}{\hbar}}$

$$\nabla^2\psi = \nabla\left[(\nabla A)e^{i\frac{S}{\hbar}} + \frac{iA\nabla S}{\hbar}e^{i\frac{S}{\hbar}}\right] = \left[\nabla^2 A + \frac{2i}{\hbar}\nabla A\cdot\nabla S + \frac{i}{\hbar}A\nabla^2 S - \frac{1}{\hbar}A(\nabla S)^2\right]e^{i\frac{S}{\hbar}}$$

$\to$ $-\frac{\hbar^2}{2m}\left[\nabla^2 A + \frac{2i}{\hbar}\nabla A\cdot\nabla S + \frac{i}{\hbar}A\nabla^2 S - \frac{A(\nabla S)^2}{\hbar^2}\right] + V(\vec{r},t)A = i\hbar\left(\dot{A} + \frac{iA\dot{S}}{\hbar}\right)$

Parte real: $\quad -\frac{\hbar^2}{2m}\nabla^2 A + \frac{1}{2m}A(\nabla S)^2 + V(\vec{r},t)A = -A\frac{\partial S}{\partial t}$

Parte imaginária: $\boxed{-\frac{1}{2m}(2\nabla A\cdot\nabla S + A\nabla^2 S) = \frac{\partial A}{\partial t}}$ $\Big\}$ eq. continuidade

$$2A\frac{\partial A}{\partial t} + 2A\frac{A\nabla^2 S + 2\nabla A\cdot\nabla S}{2m} = 0 \Rightarrow \frac{\partial(A^2)}{\partial t} + \frac{A^2\nabla^2 S + 2A\nabla A\cdot\nabla S}{m} = 0$$

$$\nabla\vec{J} = \frac{2A\nabla A\cdot\nabla S}{m} + \frac{A^2\nabla^2 S}{m}$$

$$\left.\right\} \frac{\partial(A^2)}{\partial t} + \nabla\vec{J} = 0$$

$$\boxed{\frac{\partial P}{\partial t} + \nabla\vec{J} = 0}$$

Equação da continuidade

$\to$ Voltando à parte real e dividindo por A: $\quad \frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V(\vec{r},t) = \frac{\hbar^2}{2m}\nabla^2 A$

$\hbar \to 0$:

fase da função de onda

$$\boxed{\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V(\vec{r},t) = 0}$$

Função principal de Hamilton–Jacobi

Fluido clássico

$$\left.\begin{array}{l} \rightarrow \vec{J} = P\vec{v} \\ \rightarrow \vec{v} = \dfrac{\nabla S}{m} \end{array}\right\} \quad \begin{array}{l} \dfrac{\partial}{\partial t}(\nabla S) + \dfrac{\nabla(\nabla S)^2}{2m} + \nabla V = 0 \\ \dfrac{\partial}{\partial t} m\vec{v} + \dfrac{\nabla m^2 v^2}{2m} = -\nabla V \end{array}$$

$$\Rightarrow m\left(\frac{\partial}{\partial t}\vec{v} + \frac{\nabla v^2}{2}\right) = \vec{F}$$

$$m\left(\frac{\partial}{\partial t}\vec{v} + \vec{v}\cdot\nabla\vec{v}\right) = \vec{F}$$

$$m\left(\frac{\partial}{\partial t} + \vec{v}\cdot\nabla\right)\vec{v} = \vec{F}$$

$$m\frac{d\vec{v}}{dt} = \vec{F} \Rightarrow \boxed{\vec{F} = m\vec{a}}$$

Interpretação de Bohm

→ Potencial quântico: $V_{qm} = Q = -\dfrac{\hbar^2}{2m}\dfrac{\nabla^2 A}{A}$ } originado pela onda piloto

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + \underbrace{V(\vec{r}) + V_{qm}(\vec{r})}_{V_{eff}} = 0 \Rightarrow \boxed{\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V_{eff}(\vec{r}) = 0}$$

Notação de Dirac

Componentes	Base		
c_i	$\{\phi_i(\vec{r})\}$	$\rightarrow \psi(\vec{r}) = \sum_i c_i \phi_i(\vec{r})$	Energia bem definida
$A(\vec{k})$	$(2\pi)^{-\frac{1}{2}}\{e^{i\vec{k}\cdot\vec{r}}\}$	$\rightarrow \psi(\vec{r}) = \int d^3k\, A(k) \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{2\pi}}$	Momento bem definido
$\psi(\vec{r}_0)$	$\{\delta^{(3)}(\vec{r}-\vec{r}_0)\}$	$\rightarrow \psi(\vec{r}) = \int d^3r_0\, \psi(\vec{r}_0)\, \delta^{(3)}(\vec{r}-\vec{r}_0)$	Posição bem definida

$$\int |\psi(\vec{r})|^2 d^3r < \infty$$

$$\int |A(\vec{k})|^2 d^3k < \infty$$

$$\sum_i |c_i|^2 < \infty$$

$|\psi\rangle \rightarrow$ ortodoxa

$|\psi\rangle, \lambda \rightarrow$ realista

* Vantagens $\begin{cases} \text{simplifica o formalismo} \\ \text{generaliza} \end{cases}$

i) Vetores ket e bra:

a) Ket: $|\psi\rangle$ $\quad |\psi\rangle = \int d^3r\, \psi(\vec{r})\, |\vec{r}\rangle = \int d^3k\, A(\vec{k})\, |\vec{k}\rangle = \sum_i c_i |E_i\rangle = \dots$

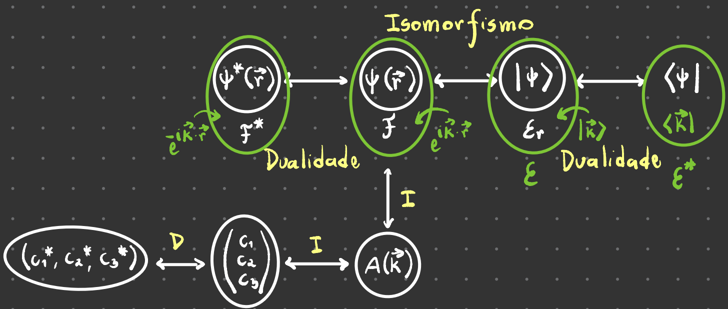
$$|\psi\rangle \in \mathcal{E}_r \Leftrightarrow \psi(\vec{r}) \in \mathcal{F}$$

$$(|\psi\rangle, |\varphi\rangle) = (\psi(\vec{r}), \varphi(\vec{r})) = \int d^3r\, \psi^*(\vec{r})\, \varphi(\vec{r})$$

b) Bra: $\langle\chi|$ $\rightarrow$ funcional linear

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

$$\langle\chi|\psi\rangle \equiv (|\chi\rangle, |\psi\rangle) \equiv \int d^3r\, \chi^*(\vec{r})\, \psi(\vec{r})$$



$$\langle\chi|\psi\rangle = \int d^3r\, \chi^*(\vec{r})\, \psi(\vec{r}) = \sum_i b_i^* c_i = (b_1, \dots, b_n)^* \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}$$

ii) Correspondência Ket $\leftrightarrow$ bra

$$|\chi\rangle \longleftrightarrow \langle\chi|$$

$$c|\chi\rangle \longleftrightarrow c^*\langle\chi|$$

$$c_1|\chi_1\rangle + c_2|\chi_2\rangle \longleftrightarrow c_1^*\langle\chi_1| + c_2^*\langle\chi_2|$$

$$|c\psi\rangle = c|\psi\rangle$$

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

iii) Nova notação para produto interno: $\langle\varphi|\psi\rangle = (|\varphi\rangle, |\psi\rangle)$

Propriedades
$$\begin{cases} \langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle^* \\ \langle\varphi|c_1\psi_1 + c_2\psi_2\rangle = c_1\langle\varphi|\psi_1\rangle + c_2\langle\varphi|\psi_2\rangle \\ \langle c_1\varphi_1 + c_2\varphi_2|\psi\rangle = c_1^*\langle\varphi_1|\psi\rangle + c_2^*\langle\varphi_2|\psi\rangle \\ \langle\psi|\psi\rangle \geq 0 \longrightarrow \langle\psi|\psi\rangle = 0 \Leftrightarrow |\psi\rangle = 0 \end{cases}$$

iv) Operadores $|\tilde{\psi}\rangle = A|\psi\rangle$

1. $A = I \rightarrow I|\psi\rangle = |\psi\rangle$

2. $A^{-1}A = AA^{-1} = I$

3. $F(A) = \sum_{n=0}^{\infty} a_n A^n$

4. Comutador: $[A, B] = AB - BA$

5. Projetor P: $\boxed{P^n = P}$, $n \geq 1$

$\langle\chi|\psi\rangle$ = número
$|\psi\rangle\langle\chi|$ = operador

$$(|\psi\rangle\langle\chi|)|\varphi\rangle = |\psi\rangle\langle\chi|\varphi\rangle = c|\psi\rangle$$

$$\left.\begin{matrix}\langle\psi|\psi\rangle = 1 \\ |\psi\rangle\langle\psi| = P\end{matrix}\right\} \quad P^2 = |\psi\rangle\langle\psi|\,|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = P$$

$$P|\chi\rangle = |\psi\rangle\langle\psi|\chi\rangle = \langle\psi|\chi\rangle|\psi\rangle$$

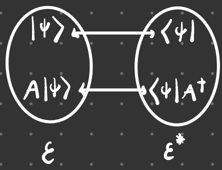
→ Seja um conjunto ortonormal de kets: $\{|\psi_i\rangle\}$, $i = 1, \dots, n$ e $\langle\psi_j|\psi_i\rangle = \delta_{ij}$

$P = \sum_{i=1}^{n}|\psi_i\rangle\langle\psi_i|$ → projetor no subespaço gerado por $\{|\psi_i\rangle\}$

$$P^2 = \left(\sum_{i=1}^{n}|\psi_i\rangle\langle\psi_i|\right)\left(\sum_{j=1}^{n}|\psi_j\rangle\langle\psi_j|\right) = \sum_{i,j}|\psi_i\rangle\overbrace{\langle\psi_i|\psi_j\rangle}^{\delta_{ij}}\langle\psi_j| = \sum_{i=1}^{n}|\psi_i\rangle\langle\psi_i| = P$$

Relação de clausura: $P = \sum_{i=1}^{\infty}|\psi_i\rangle\langle\psi_i| = I$

6. Operador adjunto (conjugação hermitiana)



$(|\psi\rangle)^\dagger \Leftrightarrow \langle\psi|$

$(A|\psi\rangle)^\dagger \Leftrightarrow \langle\psi|A^\dagger$

$A \leftrightarrow A^\dagger$

$(AB)^\dagger = B^\dagger A^\dagger$

$(A+B)^\dagger = A^\dagger + B^\dagger$

$(A^\dagger)^\dagger = A$

$|\tilde{\psi}\rangle = A|\psi\rangle$

$\langle\tilde{\psi}| = \langle\psi|A^\dagger$

$\langle\varphi|\tilde{\psi}\rangle = \langle\tilde{\psi}|\varphi\rangle^*$

$\langle\varphi|A|\psi\rangle = \langle\psi|A^\dagger|\varphi\rangle^*$

7. Operador autoadjunto: $A = A^\dagger$

$\langle\varphi|A|\psi\rangle = \langle\psi|A|\varphi\rangle^*$

$(|\varphi\rangle, A|\psi\rangle) = (|\psi\rangle, A|\varphi\rangle)^*$

$(\varphi, A\psi) = (A\varphi, \psi)$

hermitiano $\rightarrow$ observável

01/11/23

Representação

→ Base discreta: $\{|u_i\rangle\}$, $i \in \mathbb{Z}, \mathbb{Q}$ (enumerável)

$\langle u_i|u_j\rangle = \delta_{ij}$ (ortonormal)

$\sum_{i=1}^{\infty} |u_i\rangle\langle u_i| = I$ (completa)

→ Base contínua: $\{|u_\alpha\rangle\}$, $\alpha \in \mathbb{R}$

$\langle u_\alpha|u_\beta\rangle = \delta(\alpha-\beta)$

$\int_{-\infty}^{+\infty} d\alpha\, |u_\alpha\rangle\langle u_\alpha| = I$

i) Ket: $|\psi\rangle = I|\psi\rangle = \left(\sum_i |u_i\rangle\langle u_i|\right)|\psi\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle = \sum_i \langle u_i|\psi\rangle |u_i\rangle$

$$|\psi\rangle = \sum_i c_i |u_i\rangle, \quad c_i = \langle u_i|\psi\rangle$$

$|\psi\rangle = I|\psi\rangle = \left(\int d\alpha\, |u_\alpha\rangle\langle u_\alpha|\right)|\psi\rangle = \int d\alpha\, |u_\alpha\rangle\langle u_\alpha|\psi\rangle = \int d\alpha\, \langle u_\alpha|\psi\rangle |u_\alpha\rangle$

$$|\psi\rangle = \int d\alpha\, c(\alpha)|u_\alpha\rangle, \quad c(\alpha) = \langle u_\alpha|\psi\rangle$$

ii) Bra: $\langle\psi| = \langle\psi|I = \langle\psi|\sum_i |u_i\rangle\langle u_i| = \sum_i \langle\psi|u_i\rangle\langle u_i|$

$$\langle\psi| = \sum_i c_i^* \langle u_i|, \quad c_i^* = \langle\psi|u_i\rangle$$

$\langle\psi| = \langle\psi|I = \langle\psi|\int d\alpha\, |u_\alpha\rangle\langle u_\alpha| = \int d\alpha\, \langle\psi|u_\alpha\rangle\langle u_\alpha| = \int d\alpha\, \langle\psi|u_\alpha\rangle\langle u_\alpha|$

$$\langle\psi| = \int d\alpha\, c^*(\alpha)\langle u_\alpha|, \quad c^*(\alpha) = \langle\psi|u_\alpha\rangle$$

iii) Produto interno: $\langle\varphi|\psi\rangle = \langle\varphi|\left(\sum_i |u_i\rangle\langle u_i|\right)|\psi\rangle = \sum_i \underbrace{\langle\varphi|u_i\rangle}_{b_i^*}\underbrace{\langle u_i|\psi\rangle}_{c_i}$

$$\langle\varphi|\psi\rangle = \sum_i b_i^* c_i$$

representação

base vetor

1) $\langle x|x_0\rangle = \delta(x-x_0)$ 2) $\langle x|p_0\rangle = \frac{1}{\sqrt{2\pi}} e^{i\frac{p_0}{\hbar}x}$ 3) $\langle p|p_0\rangle = \delta(p-p_0)$ 4) $\langle p|x_0\rangle = \frac{1}{\sqrt{2\pi}} e^{-i\frac{p}{\hbar}x_0}$

iv) Operador: $A = IAI = \sum_i |u_i\rangle\langle u_i| A \sum_j |u_j\rangle\langle u_j| = \sum_{i,j} \langle u_i|A|u_j\rangle |u_i\rangle\langle u_j|$

$$A = \sum_{i,j} A_{ij} |u_i\rangle\langle u_j|, \quad A_{ij} = \langle u_i|A|u_j\rangle$$

$C = AB \rightarrow C_{ij} = \langle u_i|C|u_j\rangle = \langle u_i|AIB|u_j\rangle = \langle u_i|A\sum_k |u_k\rangle\langle u_k|B|u_j\rangle = \sum_k \langle u_i|A|u_k\rangle\langle u_k|B|u_j\rangle$

$$C_{ij} = \sum_k A_{ik}B_{kj}$$

$A^\dagger \rightarrow \langle u_i|A^\dagger|u_j\rangle = \langle u_j|A^{\dagger\dagger}|u_i\rangle^* = \langle u_j|A|u_i\rangle^* \rightarrow A_{ij}^\dagger = A_{ji}^* = (A_{ij})^{\dagger *}$

↳ Autoadjunto: $A^\dagger = A \rightarrow A_{ij} = A_{ji}^*$

↳ Unitário: $A^\dagger = A^{-1} \rightarrow AA^\dagger = I$

v) Mudança de base: Sejam duas bases $\begin{cases} 1) \{|u_i\rangle\}: \langle u_i|u_j\rangle = \delta_{ij}, & \sum_i |u_i\rangle\langle u_i| = I \\ 2) \{|t_i\rangle\}: \langle t_i|t_j\rangle = \delta_{ij}, & \sum_i |t_i\rangle\langle t_i| = I \end{cases}$

$$\left.\begin{array}{l} |\psi\rangle = \sum_j \langle u_j|\psi\rangle |u_j\rangle \\ |\psi\rangle = \sum_j \langle t_j|\psi\rangle |t_j\rangle \end{array}\right\} \begin{array}{l} \sum_j \langle u_j|\psi\rangle\langle u_i|u_j\rangle = \sum_j \langle t_j|\psi\rangle\langle u_i|t_j\rangle \\ \qquad \langle u_i|\psi\rangle = \sum_j \langle u_i|t_j\rangle\langle t_i|\psi\rangle \end{array}$$

$$\left.\begin{array}{l} c_i = \langle u_i|\psi\rangle \\ b_i = \langle t_i|\psi\rangle \end{array}\right\} \boxed{S_{ij} = \langle u_i|t_j\rangle}, \quad c_i = \sum_j S_{ij} b_j$$

$$\left.\begin{array}{l} S_{ij} = \langle u_i|t_j\rangle \\ S_{ij}^* = \langle t_j|u_i\rangle \end{array}\right\} \begin{array}{l} \sum_j S_{ij}S_{kj}^* = \sum_j \langle u_i|t_j\rangle\langle t_j|u_k\rangle = \langle u_i|\sum_j |t_j\rangle\langle t_j|u_k\rangle = \langle u_i|u_k\rangle = \delta_{ik} \\ \sum_j S_{ij}S_{kj}^* = \sum_j S_{ij}(S_{kj}^T)^* = \delta_{ik} \Rightarrow (S_{jk}^T)^* = S_{jk}^{-1} \Rightarrow S^{-1}S = I \end{array}$$

$$\rightarrow \langle u_i|A|u_j\rangle = \langle u_i|IAI|u_j\rangle = \dots = \langle t_i|A|t_j\rangle$$

$$\boxed{A_{ij}^u = \sum_{l,k} S_{ik} A_{kl}^t S_{kj}^{-1}} \quad \text{Transformação de similaridade}$$

$$A^u = SA^tS^{-1}$$

$$\det(AB) = \det(A)\det(B)$$

$$\det(A_u) = \det(S)\det(A_t)\underbrace{\det(S^{-1})}_{\frac{1}{\det S}} = \det(A_t) \rightarrow \text{determinante é invariante sob transformação de similaridade}$$

03/11/23

Autovalores e autovetores

$e^{A}|\psi\rangle = e^{\lambda}|\psi\rangle$

→ $|\psi\rangle$ é um autovetor (eigenvector, eigenket) de A se $\underbrace{A}_{\text{operador}}|\psi\rangle = \overbrace{\lambda}^{\text{número}}|\psi\rangle$ $\left\{\begin{array}{l}\text{Vários } |\psi\rangle \text{ L.I.} \\ \text{Degenerado } (\geq 2\ |\psi_i\rangle \text{ p/ mesmo } \lambda) \\ |\psi\rangle \neq 0\end{array}\right.$

→ Não degenerado: $A|\psi_n\rangle = \lambda_n|\psi_n\rangle$

→ Degenerado: $A|\psi_n^i\rangle = \lambda_n|\psi_n^i\rangle$, $i = 1, \dots, g_n$ → dimensão do subespaço vetorial degenerado

$$\{|\psi_n^i\rangle\} \to \lambda_n$$

* Exemplo: $g = 2$

$$A|\psi_1\rangle = \lambda|\psi_1\rangle \qquad A|\psi_2\rangle = \lambda|\psi_2\rangle$$

$|\psi_1\rangle$ e $|\psi_2\rangle$ são L.I.

$|\psi\rangle = \alpha_1|\psi_1\rangle + \alpha_2|\psi_2\rangle$ é autovetor

Representação discreta

→ $A|\psi\rangle = \lambda|\psi\rangle \to \boxed{\sum_j A_{ij}c_j = \lambda c_i}$ $\quad c_i = \langle u_i|\psi\rangle$, $A_{ij} = \langle u_i|A|u_j\rangle$

→ $A\vec{c} = \lambda\vec{c} = \lambda I\vec{c} \Rightarrow \overbrace{(A-\lambda I)}^{M}\vec{c} = 0$

$$\begin{pmatrix} A_{11}-\lambda & A_{12} & \cdots & \cdots \\ A_{21} & A_{22}-\lambda & \cdots & \cdots \\ \vdots & \vdots & \ddots & \\ \vdots & \vdots & & \ddots \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ \vdots \end{pmatrix} = 0$$

Solução trivial: $\vec{c} = M^{-1}0 = 0$

Solução não trivial: $\det(M^{-1}) = \dfrac{1}{\det(M)}$

$\det(M) = 0$

→ $\begin{vmatrix} A_{11}-\lambda & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22}-\lambda & & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & \vdots & & A_{nn} \end{vmatrix} = 0 \to N\times N \to$ equação polinomial de grau N

equação característica → N soluções

Representação contínua $\{|u_\alpha\rangle\}$

→ $A|\psi\rangle = \lambda|\psi\rangle \to \left\{\begin{array}{l} D_\alpha\psi(\alpha) = \lambda\psi(\alpha) \\ + \text{c.c.}\end{array}\right.$

→ $\left.\begin{array}{l}\psi_\alpha = \langle u_\alpha|\psi\rangle \\ A_{\alpha\beta} = \langle u_\alpha|A|u_\beta\rangle\end{array}\right\}$ $\int d\beta\, A_{\alpha\beta}\psi(\beta) = D_\alpha\psi(\alpha)$

Observáveis

→ $A^\dagger = A$: hermitiano

i) autovalores de A são reais

$$\left.\begin{aligned} \langle\psi|A|\psi\rangle &= \langle\psi|\lambda|\psi\rangle = \lambda\langle\psi|\psi\rangle = \lambda \\ \langle\psi|A^\dagger|\psi\rangle &= \langle\psi|\lambda^*|\psi\rangle = \lambda^*\langle\psi|\psi\rangle = \lambda^* \end{aligned}\right\} \langle\psi|A|\psi\rangle = \langle\psi|A^\dagger|\psi\rangle \Rightarrow \lambda = \lambda^* \in \mathbb{R}$$

ii) autovetores são ortogonais (para autovalores distintos)

→ Não degenerado:

$$A|\psi_1\rangle = \lambda_1|\psi_1\rangle \to \langle\psi_1|A^\dagger = \langle\psi_1|A = \lambda_1^*\langle\psi_1| = \lambda_1\langle\psi_1|$$
$$A|\psi_2\rangle = \lambda_2|\psi_2\rangle \to \langle\psi_2|A^\dagger = \langle\psi_2|A = \lambda_2^*\langle\psi_2| = \lambda_2\langle\psi_2|$$

$$\langle\psi_2|A|\psi_1\rangle = \lambda_1\langle\psi_2|\psi_1\rangle = \lambda_2\langle\psi_2|\psi_1\rangle$$
$$\underbrace{(\lambda_1-\lambda_2)}_{\neq 0}\langle\psi_2|\psi_1\rangle = 0$$
$$\langle\psi_2|\psi_1\rangle = 0$$
$$\therefore |\psi_1\rangle \perp |\psi_2\rangle$$

$$\begin{aligned} A|\psi_n\rangle &= \lambda_n|\psi_n\rangle \\ \langle\psi_{n'}|\psi_n\rangle &= \delta_{nn'} \end{aligned} \to \begin{aligned} &\{|\psi_n\rangle\}: \text{ base} \\ &\{\lambda_n\}: \text{ quantidade física (medida)} \end{aligned}$$

Notação: $A|a\rangle = a|a\rangle$

↳ Degenerado: $A|a_i\rangle = a|a_i\rangle$, $i = 1, \dots, g_a$

ou

$B|b_j\rangle = b|b_j\rangle \to \begin{aligned} A|a,b\rangle &= a|a,b\rangle \\ B|a,b\rangle &= b|a,b\rangle \end{aligned} \Leftrightarrow$ Teorema fundamental da MQ $[A,B] = 0$

Exemplo: $\nexists\ |x,p\rangle$

✱ 1D: $A = X$, $a = x$, $X = X^\dagger$

$X|x\rangle = x|x\rangle$, $x \in \mathbb{R} \to -\infty < x < \infty$

$$|\psi\rangle \xrightarrow[x_0]{\text{medida}} |x_0\rangle$$

$$\langle x|\psi\rangle \xrightarrow[x_0]{} \langle x|x_0\rangle$$

$$\begin{aligned} \int dx\, |x\rangle\langle x| &= I \\ \langle x|x'\rangle &= \delta(x-x') \end{aligned} \quad \Big| \quad \psi(x) = \langle x|\psi\rangle \quad \Big|$$

$$\psi(x) \xrightarrow[x_0]{} \delta(x-x_0)$$

$A = P$, $a = p$, $P = P^\dagger$

$P|p\rangle = p|p\rangle$

$$|\psi\rangle \xrightarrow[p_0]{\text{medida}} |p_0\rangle$$

$$\langle p|\psi\rangle \xrightarrow[p_0]{} \langle p|p_0\rangle$$

$$\begin{aligned} \int dp\, |p\rangle\langle p| &= I \\ \langle p|p'\rangle &= \delta(p-p') \end{aligned} \quad \Big| \quad \tilde{\psi}(p) = \langle p|\psi\rangle \quad \Big|$$

$$\tilde{\psi}(p) \xrightarrow[p_0]{} \delta(p-p_0)$$

$$\langle x|p_0\rangle = \frac{1}{\sqrt{2\pi}} e^{i\frac{p_0}{\hbar}x} \longleftrightarrow [X,P] = i\hbar$$

Postulado de De Broglie — Postulado de Heisenberg

06/11/23

$$\rightarrow \langle x|\overset{\downarrow I}{P}|\psi\rangle = \int \langle x|P|p\rangle\langle p|\psi\rangle\, dp = \int p\,\langle x|p\rangle\langle p|\psi\rangle\, dp = \int dp \left(p\,\frac{1}{(2\pi)^{\frac{1}{2}}}e^{\frac{ip}{\hbar}x}\right)\langle p|\psi\rangle \qquad \frac{\hbar}{i}\frac{\partial}{\partial x}\frac{e^{\frac{ip}{\hbar}x}}{\sqrt{2\pi}}$$

$$= \frac{\hbar}{i}\frac{d}{dx}\int dp\,\frac{e^{\frac{ipx}{\hbar}}}{(2\pi)^{\frac{1}{2}}}\langle p|\psi\rangle = \frac{\hbar}{i}\frac{d}{dx}\int dp\,\langle x|p\rangle\langle p|\psi\rangle = \frac{\hbar}{i}\frac{d}{dx}\langle x|\psi\rangle$$

$$\therefore \langle x|P|\psi\rangle = -i\hbar\frac{d}{dx}\psi(x) \qquad \langle x|P \rightarrow -i\hbar\frac{d}{dx}\langle x|$$

$$\rightarrow \langle p|P|\psi\rangle = p\langle p|\psi\rangle = \int p\langle p|x\rangle\langle x|\psi\rangle\, dx = p\,\frac{1}{(2\pi)^{\frac{1}{2}}}\int e^{-\frac{ipx}{\hbar}}\psi(x)\, dx$$

$$\rightarrow \langle x|X|\psi\rangle = x\langle x|\psi\rangle = x\psi(x)$$

$$\rightarrow \langle p|\overset{x\psi}{\widehat{X|\psi}}\rangle = \int dx\, x\langle p|x\rangle\langle x|\psi\rangle = \int dx\, \underbrace{x\,\frac{1}{(2\pi)^{\frac{1}{2}}}e^{-\frac{ip}{\hbar}x}}_{-\frac{\hbar}{i}\frac{\partial}{\partial p}\left(\frac{1}{\sqrt{2\pi}}e^{-\frac{ix}{\hbar}p}\right) \rightarrow \langle p|x\rangle}\langle x|\psi\rangle = -\frac{\hbar}{i}\frac{d}{dp}\int dx\,\langle p|x\rangle\langle x|\psi\rangle = -\frac{\hbar}{i}\frac{d}{dp}\langle p|\psi\rangle$$

$$\therefore \langle p|X|\psi\rangle = i\hbar\frac{d}{dp}\tilde{\psi}(p) \qquad \langle p|X \rightarrow i\hbar\frac{d}{dp}$$

$$\rightarrow H|\psi\rangle = i\hbar\frac{d}{dt}|\psi\rangle$$

$$\rightarrow \langle x|\frac{P^2}{2m}+V(x)|\psi\rangle = i\hbar\frac{\partial}{\partial t}\langle x|\psi\rangle$$

$$\langle x|\frac{P^2}{2m}|\psi\rangle + \langle x|V(x)|\psi\rangle = i\hbar\frac{\partial}{\partial t}\psi(x)$$

$$\frac{1}{2m}(-i\hbar)\frac{\partial}{\partial x}\langle x|P|\psi\rangle + V(x)\langle x|\psi\rangle = i\hbar\frac{\partial}{\partial t}\psi(x)$$

$$\therefore \boxed{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = i\hbar\frac{\partial}{\partial t}\psi(x)}$$

$$\rightarrow \langle p|H|\psi\rangle = ?\ \frac{p^2\tilde{\psi}(p)}{2m} + \int \tilde{V}(p-p')\tilde{\psi}(p')\,dp' = i\hbar\frac{\partial}{\partial t}\tilde{\psi}(p)$$

$$\rightarrow \langle \phi_E|H|\psi\rangle = i\hbar\frac{d}{dt}\langle\phi_E|\psi\rangle$$

$$E\langle\phi_E|\psi\rangle = i\hbar\frac{d}{dt}\langle\phi_E|\psi\rangle$$

$$E c_E = i\hbar\frac{d}{dt}c_E(t) \Rightarrow \boxed{c_E = Ae^{-\frac{iEt}{\hbar}}}$$

Conjunto de Observáveis Comutantes

* **Teorema 1:** $[A,B]=0$, $A|\psi\rangle = a|\psi\rangle$ $\Rightarrow$ $B|\psi\rangle$ é autovetor de A com o mesmo autovalor a

↳ $A|\psi\rangle = a|\psi\rangle$

$BA|\psi\rangle = a\,BA|\psi\rangle$ //

$$B|\psi\rangle = \begin{cases} |\psi'\rangle \text{ LI } |\psi\rangle \rightarrow \text{deg} \\ |\psi'\rangle = c|\psi\rangle \end{cases}$$

* **Teorema 2:** $[A,B]=0$

$A|\psi_1\rangle = a_1|\psi_1\rangle$

$A|\psi_2\rangle = a_2|\psi_2\rangle$, $a_1 \neq a_2$ $\Rightarrow$ $\langle\psi_1|B|\psi_2\rangle = 0$

↳ $AB - BA = 0$

$\langle\psi_1|AB|\psi_2\rangle - \langle\psi_1|BA|\psi_2\rangle = 0 \Rightarrow a_1\langle\psi_1|B|\psi_2\rangle - a_2\langle\psi_1|B|\psi_2\rangle = 0$

$(a_1 - a_2)\langle\psi_1|B|\psi_2\rangle = 0$

$\neq 0 \swarrow$ $\langle\psi_1|B|\psi_2\rangle = 0$

* **Teorema 3:** $[A,B]=0 \Leftrightarrow$ É possível construir uma base ortogonal de autovetores comuns a A e B

($\exists\{|a,b\rangle\} \rightarrow$ $A|a,b\rangle = a|a,b\rangle$, $B|a,b\rangle = b|a,b\rangle$

↳ $A|u_n^i\rangle = a_n|u_n^i\rangle$, $i = 1, \dots, g_n$

$\langle u_n^i|u_{n'}^j\rangle = \delta_{nn'}\delta_{ij}$

↳ Pelo T2 $\Rightarrow \langle u_n^i|B|u_{n'}^j\rangle = 0$, $n \neq 0$

$$A = \begin{pmatrix} \begin{pmatrix} a_1 & 0 \\ 0 & a_1 \end{pmatrix} & & & \\ & a_2 & & 0 \\ & 0 & \begin{pmatrix} a_3 & 0 & 0 & 0 \\ 0 & a_3 & 0 & 0 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & a_3 \end{pmatrix} & \\ & & & \ddots \end{pmatrix} \rightarrow B = \begin{array}{c|c} & \varepsilon_1 \quad \varepsilon_2 \quad \varepsilon_3 \\ \begin{matrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{matrix} & \begin{pmatrix} \blacksquare & 0 & 0 \\ 0 & \blacksquare & 0 \\ 0 & 0 & \blacksquare \end{pmatrix} \end{array} \rightarrow \text{diagonalizar blocos}$$

↳ B é diagonal fora dos blocos

↗ base comum

$B|v_n^i\rangle = b_n^i|v_n^i\rangle$

$A|v_n^i\rangle = a_n|v_n^i\rangle$

↳ $[A,B] \neq 0 \Leftrightarrow \nexists\ |a,b\rangle$ t.q. $A|a,b\rangle = a|a,b\rangle$ e $B|a,b\rangle = b|a,b\rangle$

↳ **Teorema fundamental da MQ:**

$[A,B] \neq 0 \Leftrightarrow$ não existe estado físico com a e b bem definidos $\rightarrow$ princípio da incerteza

08/11/23

Princípio da incerteza

$\rightarrow A \rightarrow \hat{A} = A - \langle A \rangle \Rightarrow \langle \hat{A} \rangle = 0$ | $A^\dagger = A, \ \hat{A}^\dagger = \hat{A}$ | $[A,B] = [\hat{A}, \hat{B}]$

$\rightarrow B \rightarrow \hat{B} = B - \langle B \rangle \Rightarrow \langle \hat{B} \rangle = 0$ | $B^\dagger = B, \ \hat{B}^\dagger = \hat{B}$

$\rightarrow |\psi_1\rangle = \hat{A}|\psi\rangle \quad \rightarrow \quad \langle \psi_1| = \langle \psi | \hat{A}$

$\rightarrow |\psi_2\rangle = \hat{B}|\psi\rangle \quad \rightarrow \quad \langle \psi_2| = \langle \psi | \hat{B}$

$\rightarrow$ Desigualdade de Schwarz: $\langle \psi_1|\psi_1\rangle \langle \psi_2|\psi_2\rangle \geq |\langle \psi_1|\psi_2\rangle|^2$

$\langle \hat{O} \rangle \equiv \langle \psi | \hat{O} | \psi \rangle$

$$\langle \psi|\hat{A}\hat{A}|\psi\rangle \langle \psi|\hat{B}\hat{B}|\psi\rangle \geq |\langle \psi|\hat{A}\hat{B}|\psi\rangle|^2 \Rightarrow \langle (\hat{A})^2\rangle \langle (\hat{B})^2 \rangle \geq |\langle \hat{A}\hat{B}\rangle|^2 = |z|^2 \geq \frac{|z-z^*|^2}{4}$$

$$\rightarrow |z|^2 = (Re\, z)^2 (Im\, z)^2 \geq (Im\, z)^2 \geq \left(\frac{z-z^*}{2}\right)^2 = \frac{|z-z^*|}{4}$$

$(\hat{A}\hat{B})^\dagger = B^\dagger A^\dagger = \hat{B}\hat{A}$

$$\rightarrow \langle \hat{A}^2\rangle\langle \hat{B}^2\rangle \geq \frac{|\langle \hat{A}\hat{B}\rangle - \langle \hat{A}\hat{B}\rangle^*|^2}{4} = \frac{|\langle \hat{A}\hat{B}\rangle - \langle (\hat{A}\hat{B})^\dagger\rangle|^2}{4} \Rightarrow \langle \hat{A}^2\rangle\langle \hat{B}^2\rangle \geq \frac{|\langle [\hat{A}, \hat{B}]\rangle|^2}{4}$$

Desvio padrão

$$\left.\begin{aligned} \rightarrow \langle \hat{A}^2 \rangle &= \langle (A - \langle A\rangle)^2\rangle = \sigma_A^2 \\ \rightarrow \langle \hat{B}^2 \rangle &= \langle (B - \langle B\rangle)^2\rangle = \sigma_B^2 \end{aligned}\right\} \ \underbrace{\sigma_A^2 \sigma_B^2}_{} \geq \frac{|\langle [A,B]\rangle|^2}{4} \Rightarrow \boxed{\sigma_A \sigma_B \geq \frac{|\langle [A,B]\rangle|}{2}}$$

Princípio da incerteza generalizado

* Princípio da incerteza energia - tempo

$\rightarrow A = H \Rightarrow \sigma_H \rightarrow \Delta E$ | $\Delta E \Delta B \geq |\langle [H, B]\rangle|$

$\rightarrow B =$ "relógio"

$\rightarrow$ Teorema de Ehrenfest:

$$\left.\begin{aligned} \frac{d\langle \hat{A}\rangle}{dt} &= \frac{1}{i\hbar}\langle [\hat{A}, H]\rangle + \left\langle \frac{\partial \hat{A}}{\partial t}\right\rangle \\ \frac{d\langle B\rangle}{dt} &= \frac{1}{i\hbar}\langle [B, H]\rangle + 0 \\ \left|\frac{d\langle B\rangle}{dt}\right| &= \frac{1}{\hbar}|\langle [B, H]\rangle| \end{aligned}\right\}$$

$$\Delta E \Delta B \geq \frac{\hbar}{2}\left|\frac{d\langle B\rangle}{dt}\right|$$

$$\Delta E \left|\underbrace{\frac{\Delta B}{\frac{d\langle B\rangle}{dt}}}_{\Delta t}\right| \geq \frac{\hbar}{2} \Rightarrow \boxed{\Delta E \Delta t \geq \frac{\hbar}{2}}$$

Conjunto Completo de Observáveis Comutantes (CCOC)

→ Teorema fundamental: $[A,B] \Leftrightarrow \exists\, |a,b\rangle$ t.q. $A|a,b\rangle = a|a,b\rangle$ e $B|a,b\rangle = b|a,b\rangle$

* CCOC: Um conjunto de observáveis $\{A, B, C, \dots\}$ é CCOC se existe uma base ortonormal única a menos de uma constante de fase

* Exercício: $|u_1\rangle, |u_2\rangle, |u_3\rangle, \quad \langle u_i|u_j\rangle = \delta_{ij}$

$$H = \hbar\omega_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad B = b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

a) H e B são observáveis? Sim → $(B^T)^* = B, \ (H^T)^* = H$

b) Mostrar que $[H,B]=0$ e encontrar uma base comum

$$HB = \hbar\omega_0 b \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \hbar\omega_0 b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$$

$$BH = \hbar\omega_0 b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \hbar\omega_0 b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$$

$$[H,B] = HB - BH = 0$$

Autovalores de H: $\hbar\omega_0, -\hbar\omega_0, -\hbar\omega_0$
Autovetores de H:

$$\hbar\omega_0 \rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |u_1\rangle \quad \Big| \quad -\hbar\omega_0 \rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = |u_2\rangle, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = |u_3\rangle \rightarrow a|u_2\rangle + b|u_3\rangle$$

Autovalores de B: $b, +b, -b$
Autovetores de B:

$$b \rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |u_1\rangle$$

$$B\begin{pmatrix} 0 \\ \alpha \\ \beta \end{pmatrix} = \lambda \begin{pmatrix} 0 \\ \alpha \\ \beta \end{pmatrix}$$

$$\begin{vmatrix} 0-\lambda & b \\ b & 0-\lambda \end{vmatrix} = 0 \Rightarrow \begin{matrix} \lambda^2 = b^2 \\ \lambda = \pm b \end{matrix} \rightarrow b\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \lambda\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \Rightarrow \begin{matrix} \lambda = b \Rightarrow \beta = \alpha \nearrow \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \\ \lambda = -b \Rightarrow \beta = -\alpha \searrow \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \end{matrix}$$

→ H: $|u_1\rangle, |u_2\rangle, |u_3\rangle$

→ B: $|u_1\rangle, |u_2\rangle + |u_3\rangle, |u_2\rangle - |u_3\rangle$

Base comum: $|u_1\rangle, \frac{1}{\sqrt{2}}(|u_2\rangle + |u_3\rangle), \frac{1}{\sqrt{2}}(|u_2\rangle - |u_3\rangle)$

$$\underbrace{|\hbar\omega_0, b\rangle \quad |-\hbar\omega_0, b\rangle \quad |-\hbar\omega_0, -b\rangle}_{\text{únicos}}$$

c) Quais formam um CCOC? $\{H\}, \{B\}, \{H,B\}, \{H^2, B\}$

✗ ✗ ✓ ✗

→ Exercício: Calcule Δ do seguinte estado: $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\hbar\omega_0, b\rangle + |-\hbar\omega_0, b\rangle\right)$

→ $\langle H\rangle^2 = 0$

→ $\langle H^2\rangle = \frac{1}{2}\langle \hbar\omega_0, b|H^2|\hbar\omega_0, b\rangle + \frac{1}{2}\langle -\hbar\omega_0, b|H^2|-\hbar\omega_0, b\rangle = \frac{1}{2}\hbar^2\omega_0^2 + \frac{1}{2}\hbar^2\omega_0^2 = \hbar^2\omega_0^2$

⋮

* Exercício: Mostrar que $X^\dagger = X$, $P^\dagger = P$

→ $\langle f|Xg\rangle = \langle Xf|g\rangle$

$\int dx\, f^* x g = \int dx (xf)^* g \Rightarrow X = X^\dagger$

→ $\langle f|Pg\rangle \overset{?}{=} \langle Pf|g\rangle$

$\int dx\, f^*(-i\hbar)\frac{d}{dx} g = -i\hbar\left(\cancel{f^* g\Big|_{-\infty}^{+\infty}}^{0} - \int dx \left(\frac{d}{dx}f^*\right) g\right)$

$\int dx \left(-i\hbar\frac{d}{dx}f\right)^* g = \int dx \left(-i\hbar\frac{d}{dx}f\right)^* g$

I

↓

$\langle f|Pg\rangle \overset{?}{=} \langle Pf|g\rangle$

$\int dx\, f^*(-i\hbar)\frac{\partial}{\partial x} g =$

$-i\hbar\left[\cancel{f^* g\Big|_{-\infty}^{+\infty}} - \int dx \frac{\partial f^*}{\partial x} g\right] =$

$i\hbar \int dx\, g \frac{\partial f^*}{\partial x} =$

$\int dx \left(-i\hbar\frac{\partial}{\partial x}f\right)^* g = \langle Pf|g\rangle$

10/11/23

Postulados da Mecânica Quântica

1. Para um certo tempo t_0, o **estado físico** de um sistema é definido pelo ket $|\psi(t_0)\rangle \in \mathcal{E}_r$

2. Toda quantidade física mensurável $\mathcal{A}$ é descrita por um operador A que atua em $\mathcal{E}_r$. A é dito um **observável**: $A^\dagger = A$

3. Os únicos valores de medida possíveis de uma quantidade física $\mathcal{A}$ são os **autovalores** a do observável correspondente A.

4. A **probabilidade** de medir um certo valor do observável A, quando o sistema está no estado $|\psi\rangle$, é dada por
   $P(a) = |\langle a|\psi\rangle|^2$ discreto
   $dP = |\langle a|\psi\rangle|^2 da$ contínuo
   $\langle\psi|\psi\rangle = 1$
   → medida é projeção, não aplicação
   No caso degenerado, $A|u_i\rangle = a|u_i\rangle$, $i = 1, \dots, n$ → $P(a) = \sum_{i=1}^{n} |\langle u_i|\psi\rangle|^2$

   Exemplo: $A = X$, $a = x$: $|\langle x|\psi\rangle|^2$ → densidade de probabilidade de encontrar a partícula em x

5. Colapso/Redução:

   Antes: $|\psi\rangle = c_1|a=1\rangle + c_2|a=3\rangle + c_3|a=7\rangle + c_4|a=12\rangle$, $\sum_{i=1}^{4} |c_i|^2 = 1$

   Depois: $a = 3 \rightarrow |\psi\rangle = 1|a=3\rangle$

6. Evolução temporal:

   $|\psi(t_0)\rangle \rightarrow |\psi(t)\rangle$ $\boxed{\begin{array}{l} H|\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle \\ |\psi(t_0)\rangle = |a\rangle \end{array}}$

7. Regras de quantização: $\{A, B\}_{PB} \longleftrightarrow i\hbar[A, B]$

$$\begin{array}{ll|l|l} R_1 = X & P_1 = P_x & [R_i, R_j] = 0 & \\ R_2 = Y & P_2 = P_y & [P_i, P_j] = 0 & \langle \vec{r}|\vec{p}\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{\vec{p}\cdot\vec{r}}{\hbar}} \\ R_3 = Z & P_3 = P_z & [R_i, P_j] = i\hbar\delta_{ij} & \end{array}$$

* Operador evolução temporal:

$\rightarrow i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle \rightarrow \frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = \left(\frac{d}{dt}\langle\psi(t)|\right)|\psi(t)\rangle + \langle\psi(t)|\left(\frac{d}{dt}|\psi(t)\rangle\right)$

$= \frac{1}{-i\hbar}\langle\psi(t)|H|\psi(t)\rangle + \frac{1}{i\hbar}\langle\psi(t)|H|\psi(t)\rangle$

$= 0$

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle$$

$\rightarrow$ Operador unitário: $UU^\dagger = U^\dagger U = I$, $U^{-1} = U^\dagger$

$A^\dagger = A \rightarrow$ hermitiano $\leftrightarrow$ simétrica
$U^\dagger = U^{-1} \rightarrow$ unitário $\leftrightarrow$ ortogonal

$\left.\begin{array}{l} |\psi\rangle = U|\varphi\rangle \\ \langle\psi| = \langle\varphi|U^\dagger \end{array}\right\} \langle\psi|U^\dagger U|\psi\rangle = \langle\varphi|\varphi\rangle \rightarrow$ preserva a norma

$\rightarrow |\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle$

$\rightarrow$ Propriedades:

a) $U(t_0,t_0) = 1$

b) $U(t,t_0) = U(t,t')\,U(t',t_0)\,, \quad t_0 \leq t' \leq t$

c) $U(t_0,t) = U^{-1}(t,t_0) = U^\dagger(t,t_0)$

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

$i\hbar\frac{\partial}{\partial t}U(t,t_0)|\psi(t_0)\rangle = HU(t,t_0)|\psi(t_0)\rangle \Rightarrow i\hbar\frac{\partial}{\partial t}U(t,t_0) = HU(t,t_0)$

$\int_{t_0}^{t} i\hbar\frac{\partial}{\partial t}U\,dt' = \int_{t_0}^{t} dt' HU \Rightarrow i\hbar\,U(t,t_0)\Big|_{t_0}^{t} = \int_{t_0}^{t} dt'\,H(t')U(t',t_0) \Rightarrow i\hbar\left[U(t,t_0) - U(t_0,t_0)\right] = \int_{t_0}^{t'} dt'\,H(t')\,U(t',t_0)$

$\boxed{U(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,H(t')\,U(t',t_0)}$ recorrência, c.i.

$\rightarrow$ Se $H(t) = H$: $\boxed{U(t,t_0) = e^{-\frac{iH}{\hbar}(t-t_0)}}$

$\rightarrow F(A)|a_n\rangle = F(a_n)|a_n\rangle \rightarrow$ expandir $|\psi(t_0)\rangle$: $|\psi(t_0)\rangle = \sum_n c_n|\phi_n\rangle$, $c_n = \langle\phi_n|\psi(t_0)\rangle$

$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle = U(t,t_0)\sum_n c_n|\phi_n\rangle = \sum_n c_n e^{-i\frac{H(t-t_0)}{\hbar}}|\phi_n\rangle$

$$\boxed{|\psi(t)\rangle = \sum_n c_n e^{-i\frac{E_n(t-t_0)}{\hbar}}|\phi_n\rangle}$$

Picture de Schrödinger e de Heisenberg

→ Transformação unitária genérica: $U^{-1} = U^\dagger$

$U^\dagger U = UU^\dagger = I$

→ $|\psi\rangle = U|\varphi\rangle \rightarrow \langle\psi| = \langle\varphi|U^\dagger$

→ $\langle\psi|\psi\rangle = \langle\varphi|\varphi\rangle$

→ $\langle\chi|A|\phi\rangle \rightarrow \overbrace{\langle\chi|U^\dagger}^{\langle\tilde{\chi}|}\underbrace{UAU^\dagger}_{\tilde{A}}\overbrace{U|\phi\rangle}^{|\tilde{\phi}\rangle} = \langle\tilde{\chi}|\tilde{A}|\tilde{\phi}\rangle \Big\} \; \langle\chi|A|\phi\rangle = \langle\tilde{\chi}|\tilde{A}|\tilde{\phi}\rangle$

Invariância frente a transf. unitária

Evolução temporal

* Schrödinger

→ $\dfrac{d\langle A\rangle}{dt} = \dfrac{1}{i\hbar}\langle[A,H]\rangle + \left\langle\dfrac{\partial A}{\partial t}\right\rangle$

$I = UU^\dagger$

$\dfrac{d}{dt}\langle\psi|\overset{\downarrow I}{}A\overset{\downarrow I}{}|\psi\rangle = \dfrac{1}{i\hbar}\langle\psi|AH - HA|\psi\rangle + \left\langle\psi\left|\dfrac{\partial A}{\partial t}\right|\psi\right\rangle$

$\dfrac{d}{dt}\langle\psi|UU^\dagger A\, UU^\dagger|\psi\rangle = \dfrac{1}{i\hbar}\langle\psi|UU^\dagger AH\,UU^\dagger - UU^\dagger HA\,UU^\dagger\rangle + \left\langle\psi\left|UU^\dagger\dfrac{\partial A}{\partial t}UU^\dagger\right|\psi\right\rangle$

$\dfrac{d}{dt}\langle\psi|UU^\dagger A\, UU^\dagger|\psi\rangle = \dfrac{1}{i\hbar}\Big\{\langle\psi|UU^\dagger AUU^\dagger HUU^\dagger\rangle - \langle UU^\dagger HUU^\dagger AUU^\dagger\rangle\Big\} + \left\langle\psi\left|UU^\dagger\dfrac{\partial A}{\partial t}UU^\dagger\right|\psi\right\rangle$

↳ $|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle \rightarrow U^\dagger(t,t_0)|\psi(t)\rangle = |\psi(t_0)\rangle \rightarrow$ retira dependência temporal

$|\psi(t_0)\rangle_s = |\psi\rangle_H$

* Heisenberg: $A_H = U^\dagger A_s U \;\big|\; |\psi\rangle_s = U^\dagger(t,t_0)|\psi(t)\rangle_s$

→ $\dfrac{d}{dt}\langle\psi|_H A_H|\psi\rangle_H = \left\langle\psi\right|_H \dfrac{d}{dt}A_H|\psi\rangle_H$

→ $\langle\psi|_H\left(\dfrac{d}{dt}A_H\right)|\psi\rangle_H = \dfrac{1}{i\hbar}\langle\psi|_H[A_H, H_H]|\psi_H\rangle + \langle\psi|_H\left(\dfrac{\partial A}{\partial t}\right)|\psi\rangle_H$

Equação de Heisenberg: $\boxed{\dfrac{d}{dt}A_H(t) = \dfrac{1}{i\hbar}[A_H, H_H] + \dfrac{\partial A_H}{\partial t}}$ $\longrightarrow$ Teorema de Ehrenfest: $\dfrac{d}{dt}\langle A\rangle = i\hbar\langle[A,H]\rangle + \left\langle\dfrac{\partial A}{\partial t}\right\rangle$

$\dfrac{dA}{dt} = \{A, H\} + \dfrac{\partial A}{\partial t} \longrightarrow$ Clássico: $\{\cdots,\cdots\} \longleftrightarrow \dfrac{1}{i\hbar}[\cdots,\cdots]$

* S: {
  - vetor de estado depende do tempo: $|\psi(t)\rangle_s$
  - operadores são fixos: X, P
  - base é fixa: $A|a\rangle = a|a\rangle$

* H: {
  - vetor de estado é fixo: $|\psi\rangle_H$
  - operadores dependem do tempo: $X(t), P(t)$
  - base depende do tempo: $A|a(t)\rangle = a|a(t)\rangle$
    ↳ "gira"

Operador densidade de probabilidade

→ Estado físico pode ser representado por um **operador** (ao invés de um vetor)

→ Todo estado quântico é determinado a menos de uma constante: $|\psi\rangle = e^{i\theta}|\psi\rangle$

↳ invariante frente a uma transformação de calibre

* Mistura estatística:

$$|\psi\rangle = c_1|a_1\rangle + c_2|a_2\rangle$$

$p_1 = |c_1|^2$, $p_2 = |c_2|^2$ → mistura estatística pois não sabemos $e^{i\theta_1}$, $e^{i\theta_2}$

$$c_1 = \sqrt{p_1}\, e^{i\theta_1}, \quad c_2 = \sqrt{p_2}\, e^{i\theta_2}$$

→ Informação incompleta: Conhecemos apenas o vínculo $\sum_i p_i = 1$

Define-se $\boxed{\rho = \sum_i p_i |u_i\rangle\langle u_i|}$ $\quad |u_i\rangle\langle u_i| = e^{i\theta}|\psi\rangle\langle\psi|e^{-i\theta} = |\psi\rangle\langle\psi|$

$$\begin{pmatrix} p_1 & & 0 \\ & p_2 & \\ 0 & & p_3 \end{pmatrix}$$

① $\mathrm{Tr}\,\rho = 1$: $\quad \mathrm{Tr}\,\rho = \sum_j \langle u_j|\rho|u_j\rangle = \sum_i\sum_j p_i \langle u_j|u_i\rangle\langle u_i|u_j\rangle = \sum_i p_i = 1$ //

② $\langle A\rangle = \mathrm{Tr}\,\rho A$: $\quad \langle A\rangle = \sum_i p_i \langle u_i|A|u_i\rangle = \sum_i\sum_j p_i \langle u_i|A|u_j\rangle \delta_{ij} = \sum_i\sum_j p_i \langle u_i|A|u_j\rangle\langle u_j|u_i\rangle$

$$= \sum_i\sum_j \underline{p_i}\langle u_j|\underline{u_i\rangle\langle u_i|}A|u_j\rangle = \sum_j \langle u_j|\rho A|u_j\rangle = \mathrm{Tr}\,\rho A$$

③ $\dfrac{d\rho}{dt} = \dfrac{1}{i\hbar}[\rho, H]$: evolução temporal é dado pela eq. Heisenberg

→ Estado puro: $\rho = |\psi\rangle\langle\psi| \rightarrow \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$

↳ $\mathrm{Tr}\,\rho = \sum_i \langle u_i|\rho|u_i\rangle = \sum_i \langle u_i|\psi\rangle\langle\psi|u_i\rangle = \langle\psi|\overbrace{\sum_i |u_i\rangle\langle u_i|}^{1}|\psi\rangle = 1$

↳ $\langle A\rangle = \langle\psi|A|\psi\rangle = \sum_j c_j^* \langle u_j|A|\sum_i c_i|u_i\rangle = \sum_{i,j} c_i c_j^* \langle u_j|A|u_i\rangle$

$$= \sum_{i,j,k} c_i c_j^* \delta_{k,i} \langle u_j|A|u_k\rangle = \sum_{i,j,k} \underbrace{c_i c_j^*}_{\rho} \langle u_k|\underline{u_i\rangle\langle u_j|}A|u_k\rangle = \sum_k \langle u_k|\rho A|u_k\rangle$$

$$\therefore \langle A\rangle = \mathrm{Tr}(\rho A)$$

↳ $\rho = |\psi\rangle\langle\psi|$ é projetor: $\rho^2 = \rho$

$$\begin{cases} \text{Estado puro: } \rho^2 = \rho, \text{ não diagonal} \\ \text{Mistura estatística: } \rho^2 \neq \rho, \text{ diagonal} \end{cases}$$