Resumo da Aula 1 - Postulados da MQ

① Estados

$|\psi\rangle = \sum_i^n c_i |u_i\rangle$; $c_i = \langle u_i | \psi \rangle$

$\langle \psi | \psi \rangle = 1$

$$\begin{cases} \{u_i\} = \{u_1, u_2 \dots u_n\} \\ \langle u_i | u_j \rangle = \delta_{ij} \\ \sum_i |u_i\rangle\langle u_i| = \mathbb{1} \end{cases}$$

② Observáveis físicos (operadores)

→ op. Hermitianos → $\hat{M} \Rightarrow \mathbf{M} = (M)$: Representação matriz

$\hat{M}^{\dagger} = (M^T)^* = \hat{M}$

③ Medidas : resultados possíveis são autovalores do op observável $\hat{M}$

$\Rightarrow \hat{M} = \sum_i^n \lambda_i |m_i\rangle\langle m_i|$ (decomposição espectral) ; $\hat{M}|m_i\rangle = \lambda_i |m_i\rangle$

autovalores $\in \mathbb{R}$

autovetores

$$\Downarrow$$

$$\hat{M} = \sum_{i,j} M_{ij} |u_i\rangle\langle u_j| \; ; \quad M = \begin{pmatrix} M_{11} & M_{12} & \cdots & M_{1n} \\ \vdots & & & \\ M_{n1} & \cdots & & M_{nn} \end{pmatrix}$$

$\langle u_i | \hat{M} | u_j \rangle$: "elemento de matriz"

④ Prob. das Medidas : regra de Born

$$|\psi\rangle = \begin{cases} c_1|u_1\rangle + c_2|u_2\rangle + \dots c_n|u_n\rangle \\ \alpha_1|a_1\rangle + \alpha_2|a_2\rangle + \dots \alpha_n|a_n\rangle \quad \{a_i\} \\ \beta_1|m_1\rangle + \beta_2|m_2\rangle + \dots \beta_n|m_n\rangle \quad \{m_i\} \end{cases}$$

$\rightarrow P_{c_i} = |\langle c_i | \psi \rangle|^2$

$\lambda_1 \rightarrow |m_1\rangle$

$$\boxed{P_{\lambda_i} = |\langle m_i | \psi \rangle|^2}$$

Cuidado com degenerescências!

$\lambda_g : \{|m_2\rangle, |m_3\rangle, |m_4\rangle\}$ $\qquad P_{\lambda_g} = \sum_{i=2}^{4} |\langle m_i | \psi \rangle|^2$

⑤ Estado pós-medida

⑥ Dinâmica quântica

- Schrödinger

$i\hbar \partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$; "ket"

$\left(\frac{\partial}{\partial t}\right)$

- Heisenberg

$$\boxed{\hat{A}_h(t) = \hat{U}^{\dagger}(t,t_0)\hat{A}_S(t)\hat{U}(t,t_0)}$$

$\Rightarrow \hat{A}_h(t)$, $|\psi\rangle$ $\Rightarrow \frac{d}{dt}\hat{A}_h = \frac{1}{i\hbar}[\hat{A}_h, \hat{H}] + \frac{\partial \hat{A}_h}{\partial t}$

Operador densidade

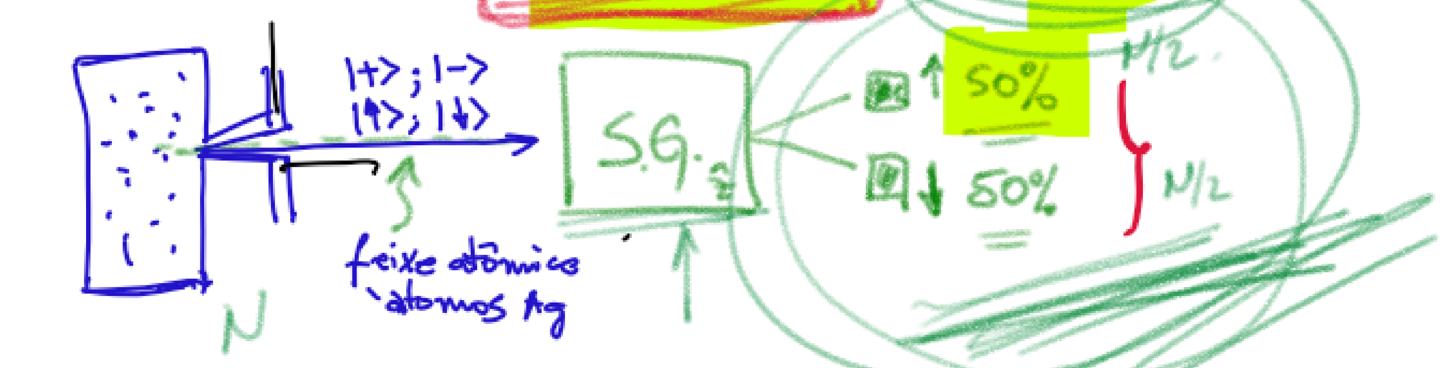
⇒ Exemplo p/ introduzir a "intuição" necessária.

"sistema 2-níveis" $\{|+\rangle, |-\rangle\}$

$|\Psi\rangle = \alpha|+\rangle + \beta|-\rangle$; $\alpha = \beta = \frac{1}{\sqrt{2}}$

$\langle\Psi|\Psi\rangle = (\alpha^*\langle +| + \beta^*\langle -|)(\alpha|+\rangle + \beta|-\rangle)$

$\boxed{|\alpha|^2 + |\beta|^2 = 1}$



↳ feixe n̄ é "spin-polarizado" (ensemble)*
(*distrib. estatística de estados)

$$\begin{cases} |\Psi_+\rangle_{N/2} = |+\rangle & 50\% \\ |\Psi_-\rangle_{N/2} = |-\rangle & 50\% \end{cases}$$

← mistura estatística

Como escrever esse estado?

⇓

Usando o op. densidade!

$$\boxed{\hat{\rho} = \sum_i^m p_i |\Psi_i\rangle\langle\Psi_i|}$$

(estado de mistura estatística)

$\{|\Psi_i\rangle\} = \{|\Psi_+\rangle, |\Psi_-\rangle\}$

vetores da base (vetores de estado)

$\{|\Psi_1\rangle, |\Psi_2\rangle, \dots |\Psi_m\rangle\}$

Probabilidade

$p_i = [0, 1]$

$\boxed{0 \leq p_i \leq 1}$

$\hat{\rho} = p_1|\Psi_1\rangle\langle\Psi_1| + p_2|\Psi_2\rangle\langle\Psi_2| + \dots p_m|\Psi_m\rangle\langle\Psi_m| \dots$

$\sum p_i = 1$ (normalização)

Resposta:

$$\hat{\rho} = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| = \frac{1}{2}(|+\rangle\langle +| + |-\rangle\langle -|)$$

⇒ Estado puro: $\hat{\rho} = \sum_i |\Psi_i\rangle\langle\Psi_i|$

$$\begin{cases} \hat{\rho}_+ = |+\rangle\langle +| \\ \hat{\rho}_- = |-\rangle\langle -| \end{cases}$$

$$\boxed{\Psi = \alpha|+\rangle + \beta|-\rangle}$$

estado puro

$|\alpha|^2 + |\beta|^2 = 1$

$\rho_\Psi = |\Psi\rangle\langle\Psi|$

$= (\alpha|+\rangle + \beta|-\rangle)(\alpha^*\langle +| + \beta^\dagger\langle -|)$

$$\boxed{\hat{\rho} \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|}$$

$P_i \in \mathbb{R} : [0,1]$

$\sum P_i = 1$

$$= p_1 |\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2| + \dots + p_n|\psi_n\rangle\langle\psi_n|$$

* Propiedades $\hat{\rho}$:

1) Hermitiano: $\hat{\rho} = \hat{\rho}^\dagger \longrightarrow \hat{\rho} = |\psi\rangle\langle\psi| \rightsquigarrow \hat{\rho}^\dagger = |\psi\rangle\langle\psi|$

2) Autovalores $0 \leq \lambda_i \leq 1$

3) traço unitário: $\boxed{Tr(\hat{\rho}) = 1}$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & \cdots & & a_{2n} \\ \vdots & & & \\ a_{n1} & \cdots & & a_{nn} \end{pmatrix} = M$$

$\hookrightarrow \sum_i a_{ii} \equiv Tr(M)$

$\hat{M} = \sum_{ij} M_{ij} |u_i\rangle\langle u_j|$

$\hookrightarrow Tr(\hat{M}) = \sum_i M_{ii}$

4) p/ estados puros $\hat{\rho} = |\psi\rangle\langle\psi|$

$\hookrightarrow Tr(\hat{\rho}^2) = Tr(\hat{\rho}\hat{\rho}) = 1$

$\rightsquigarrow \hat{\rho} = |\psi\rangle\langle\psi| \rightsquigarrow \hat{\rho}\cdot\hat{\rho} = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|)$

$= |\psi\rangle \underbrace{\langle\psi|\psi\rangle}_{1} \langle\psi|$

$\hat{\rho}^2 = |\psi\rangle\langle\psi| = \underline{\underline{\hat{\rho}}}$

5) p/ estado de mistura: $\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

$\hookrightarrow \underline{Tr(\hat{\rho}^2) < 1}$

$\hat{\rho}_M = p_1 |1\rangle\langle 1| + p_2 |2\rangle\langle 2|$

$\hat{\rho}_M^2 = \hat{\rho}_M \cdot \hat{\rho}_M = (p_1 |1\rangle\langle 1| + p_2|2\rangle\langle 2|)(p_1|1\rangle\langle 1| + p_2|2\rangle\langle 2|)$

$= p_1^2 |1\rangle\underbrace{\langle 1|1\rangle}_{1}\langle 1| + p_1 p_2 |1\rangle\underbrace{\langle 1|2\rangle}_{0}\langle 2| + \cancel{p_2 p_1 |2\rangle\langle 2|1\rangle\langle 1|} +$

$+ p_2^2 |2\rangle\langle 2| \Rightarrow \boxed{\hat{\rho}_M^2 = p_1^2 |1\rangle\langle 1| + p_2^2 |2\rangle\langle 2|}$

$\hookrightarrow Tr(\hat{\rho}_M^2) = p_1^2 + p_2^2 \leq 1$

p/ $P_1, P_2 < 1 \Rightarrow \boxed{P_1^2 + P_2^2 < 1}$

6) $\langle \hat{A} \rangle_\psi = \langle\psi|\hat{A}|\psi\rangle$

$\hookrightarrow \hat{\rho}_\psi = |\psi\rangle\langle\psi|$

$$\boxed{\langle \hat{A} \rangle_\psi = Tr(\hat{\rho}_\psi \cdot \hat{A}) = Tr(\hat{A}\hat{\rho})}$$

$\hookrightarrow Tr(\hat{A}\hat{B}) = Tr(\hat{B}\hat{A}) = Tr(AB) = Tr(BA)$

$$|\psi\rangle = \sum_i^n c_i |i\rangle = c_1|1\rangle + c_2|2\rangle + \cdots + c_n|n\rangle$$ estado puro

$$c_i = \langle i|\psi\rangle \quad ; \quad \langle i|j\rangle = \delta_{ij}$$

$$\sum |c_i|^2 = 1 \leftarrow \langle\psi|\psi\rangle = 1$$

$|1\rangle\langle 1|$

$$\hat{\rho} = |\psi\rangle\langle\psi| = (c_1|1\rangle + c_2|2\rangle + \cdots c_n|n\rangle)(c_1^*\langle 1| + c_2^*\langle 2| + \cdots c_n^*\langle n|)$$

$$= \left(\sum_i^n c_i|i\rangle\right)\cdot\left(\sum_j c_j^*\langle j|\right) = \underbrace{\sum_i^n |c_i|^2 |i\rangle\langle i|}_{\text{populações}} + \underbrace{\sum_{i\neq j} c_i c_j^* |i\rangle\langle j|}_{\text{coerência}}$$

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1n} \\ \rho_{21} & \rho_{22} & \cdots & \rho_{2n} \\ \vdots & & & \\ \rho_{n1} & \rho_{n2} & \cdots & \rho_{nn} \end{pmatrix}$$

Coerências $\rho_{ij} = \rho_{ji}^*$

Populações $|c_i|^2 = \rho_{ii}$

$$Tr(\rho) = \rho_{11} + \rho_{22} + \cdots \rho_{nn} = 1$$
$$= |c_1|^2 + |c_2|^2 + \cdots |c_n|^2$$

$c_j \in \mathbb{C}$ $\quad (i)^2 = -1$

$c_j = |c_j| e^{i\theta}$; $z = r\cdot e^{i\theta}$, $r = |z|$

forma polar

$\Delta\theta = \Delta_{ij}$

$$c_i c_j^* = |c_i| e^{i\theta_i} \cdot |c_j| e^{-i\theta_j} = |c_i||c_j| e^{i(\theta_i - \theta_j)}$$

· Exemplo

$$\hat{\rho} \rightarrow \rho = \begin{pmatrix} 3/4 & (1+i)/4 \\ \frac{(1-i)}{4} & 1/4 \end{pmatrix}$$

a) $\hat{\rho}$ representa um op. densidade $\Rightarrow$ Sim

b) estado puro? $\Rightarrow$ Misto

c) seja $\hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$; $\langle\hat{Z}\rangle = ?$ $\quad \langle\hat{Z}\rangle = \frac{1}{2}$

$$(a+ib)(a-ib) = a^2 - abi + abi - (ib)^2 = a^2 + b^2$$

$1/16 + 1/16$ $\quad a = \frac{1}{4}$, $b = \frac{1}{4}$ $= \frac{1}{16}$

$\hookrightarrow Tr(\rho) = 1$ ✓

$$Tr(\rho^2) \Rightarrow \rho\cdot\rho = \begin{pmatrix} 3/4 & (1+i)/4 \\ \frac{(1-i)}{4} & 1/4 \end{pmatrix}\begin{pmatrix} 3/4 & \frac{1+i}{4} \\ \frac{1-i}{4} & 1/4 \end{pmatrix} = \begin{pmatrix} \left[(3/4)^2 + \left(\frac{1+i}{4}\right)\cdot\left(\frac{1-i}{4}\right)\right] & \left[\quad \left(\frac{1+i}{4}\right)\right] \\ \left[\frac{3}{4}\left(\frac{1-i}{4}\right) + \frac{1}{4}\left(\frac{1-i}{4}\right)\right] & \left[\frac{1}{8} + \left(\frac{1}{4}\right)^2\right] \end{pmatrix} = \begin{pmatrix} (3/4)^2 + 1/8 & \frac{1+i}{4} \\ \frac{1-i}{4} & \left(\left(\frac{1}{4}\right)^2 + 1/8\right) \end{pmatrix}$$

$$= \begin{pmatrix} \frac{9}{16} + \frac{2}{16} & \frac{1+i}{4} \\ \frac{1-i}{4} & \left(\frac{1}{16} + \frac{2}{16}\right) \end{pmatrix} = \begin{pmatrix} \frac{11}{16} & \frac{1+i}{4} \\ \frac{1-i}{4} & \frac{3}{16} \end{pmatrix}$$

$$\hookrightarrow Tr(\rho^2) = \frac{11+3}{16} = \frac{14}{16} < 1$$

$$\hat{\rho} = \begin{pmatrix} 3/4 & \frac{1+i}{4} \\ \frac{1-i}{4} & 1/4 \end{pmatrix} \quad ; \quad \hat{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\langle \hat{z} \rangle_\rho = \langle \hat{z} \rangle = Tr(\hat{\rho}\hat{z}) \; ; \quad \Rightarrow \rho \cdot z = \begin{pmatrix} 3/4 & \frac{1+i}{4} \\ \frac{1-i}{4} & 1/4 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} 3/4 & -\frac{(1+i)}{4} \\ \frac{1-i}{4} & -1/4 \end{pmatrix} \Rightarrow Tr(\hat{\rho}\hat{A}) = \frac{3}{4} - \frac{1}{4} = \frac{2}{4} = \frac{1}{2}$$

$$\boxed{\langle \hat{z} \rangle = \frac{1}{2}}$$

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* observação importante sobre representações

↳ Representação matricial de $\hat{\rho} \to \rho = \begin{pmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1n} \\ \rho_{21} & \rho_{22} & \cdots & \rho_{2n} \\ \vdots & \vdots & \ddots & \\ \rho_{n1} & \cdots & & \rho_{nn} \end{pmatrix}$ depende da BASE usada na representação

↳ P/ ter certeza sobre a pureza do estado deve-se usar $\boxed{Tr(\hat{\rho}^2)}$

Possível ter:

- Estados puros
- Estados de Mistura parcial
- Estados de Mistura total (mistura completa)

↳ Exemplo 1: $\left\{ \begin{array}{l} \text{Caso de} \\ \text{de qbit} \\ \{|0\rangle, |1\rangle\} \end{array} \right. \Rightarrow \left\{ \begin{array}{l} 50\% \text{ no estado } |0\rangle \\ 50\% \text{ no estado } |1\rangle \end{array} \right. \Rightarrow \hat{\rho}_M = ?$

$$\Rightarrow \hat{\rho}_M = \sum_{k=1}^{2} p_k |\psi_k\rangle\langle\psi_k| = p_1 |0\rangle\langle 0| + p_2 |1\rangle\langle 1|$$
$$= \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right)$$

↳ $$\boxed{\rho_M = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}}$$

↳ Exemplo 2:

⇒ Estados de superposição (estados puros)

$$\left. \begin{array}{l} |+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \\ |-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}} \end{array} \right\} \Rightarrow \begin{array}{l} \hat{\rho}_+ = |+\rangle\langle +| \\ \hat{\rho}_- = |-\rangle\langle -| \end{array}$$

Em geral:

$$\underbrace{\frac{1}{n}}_{\text{dimensão do espaço; Máxima Mistura}} \leq Tr(\hat{\rho}^2) \leq \underbrace{1}_{\text{Estado puro}}$$

Evolução temporal (dinâmica quântica)

$$\frac{\partial}{\partial t}\hat{\rho}(\vec{r},t) \rightsquigarrow \frac{\partial \hat{\rho}}{\partial t} = \partial_t \hat{\rho} = \frac{\partial}{\partial t}\left(\sum_k p_k |\psi_k\rangle\langle\psi_k|\right)$$

$$\Downarrow$$

$$\{|\psi_k\rangle\}$$

$$\downarrow$$

$$\sum p_k \left\{\left(\boxed{\frac{\partial|\psi_k\rangle}{\partial t}}\langle\psi_k|\right) + |\psi_k\rangle\boxed{\frac{\partial\langle\psi_k|}{\partial t}}\right\}$$

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle \qquad \hat{H} = \hat{H}^{+}$$

$$\downarrow$$

$$-i\hbar\frac{\partial\langle\psi|}{\partial t} = \langle\psi|\hat{H}^{+} = \langle\psi|\hat{H}$$

$$\frac{\partial\hat{\rho}}{\partial t} = \sum_k \frac{p_k}{i\hbar}\left\{\hat{H}|\psi_k\rangle\langle\psi_k| - |\psi_k\rangle\langle\psi_k|\hat{H}\right\}$$

$$\hookrightarrow [\hat{H}, |\psi_k\rangle\langle\psi_k|]$$

$$\frac{\partial\hat{\rho}}{\partial t} = \frac{1}{i\hbar}[\hat{H},\hat{\rho}] = \frac{i}{\hbar}[\hat{\rho},\hat{H}]$$

$$\boxed{\hat{\rho}(t) = \mathcal{U}(t,t_0)\,\hat{\rho}(t_0)\,\mathcal{U}^{+}(t,t_0)}$$

(qdo $\hat{H}$ ñ depende do tempo)

$$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} = \mathbb{1} - \frac{i}{\hbar}\hat{H}(t-t_0) + \cdots$$

Vetor de Bloch

Em um espaço de Hilbert de dimensão $n=2$, i.e. sistema de 2-níveis é sempre possível escrever $\hat{\rho}$

$$\longrightarrow \boxed{\hat{\rho} = \frac{1}{2}\left(\mathbb{1} + \vec{r}\cdot\vec{\sigma}\right)} \quad ; \quad \begin{cases} \vec{r} : \text{vetor de Bloch} \\ \vec{r} = (r_x, r_y, r_z) \\ \vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \end{cases}$$

Matrizes de Pauli

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$a\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}$$

$$\begin{pmatrix} 0 & -ib \\ ib & 0 \end{pmatrix}$$

$$M = a\mathbb{1} + \sum_i b_i \sigma_i = a\mathbb{1} + b\sigma_x + c\sigma_y + d\sigma_z = \begin{pmatrix} \alpha & z \\ z^* & \beta \end{pmatrix}$$

$$M = \sum_{i=0}^{3} a_i \sigma_i$$

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\hat{S}_x = \frac{\hbar}{2}\hat{\sigma}_x$$
$$\hookrightarrow \hat{S}_i = \frac{\hbar}{2}\hat{\sigma}_i$$

$\vec{r}$: representa o "estado" do sistema físico.

$\rightarrow \|\vec{r}\| \leq 1$ $\begin{cases} \|\vec{r}\| = 1 \rightarrow \text{estado puro} \\ \|\vec{r}\| < 1 \rightarrow \text{" misto (mistura)} \end{cases}$

$$r_x = Tr(\hat{\rho}\,\hat{\sigma}_x) \; ; \quad r_y = Tr(\hat{\rho}\,\hat{\sigma}_y) \; ; \quad r_z = Tr(\hat{\rho}\,\hat{\sigma}_z)$$

Exemplo

$$\hat{\rho} \Rightarrow \rho = \begin{pmatrix} 2/3 & \frac{1}{6} - \frac{1}{3}i \\ \frac{1}{6} + \frac{i}{3} & 1/3 \end{pmatrix} \quad ; \quad \vec{S} = (S_x, S_y, S_z)$$

a) encontrar o vetor de Bloch $(\vec{r})$

b) Esse é um estado puro ou mistura?

c) Se medir $\hat{S}_z$, qual a prob de $|\uparrow\rangle$ e $|\downarrow\rangle$?

:

Resolução

a) $\vec{r} = (r_x, r_y, r_z)$; $r_x = Tr(\hat{\rho}\cdot\hat{\sigma}_x) = Tr(\rho\,\sigma_x) = Tr\left(\begin{pmatrix} 2/3 & \frac{1}{6}-\frac{i}{3} \\ \frac{1}{6}+i/3 & 1/3 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right) = Tr\begin{pmatrix} \frac{1}{6}-\frac{i}{3} & 2/3 \\ 1/3 & 1/6+\frac{i}{3} \end{pmatrix} = 1/3$

$$r_y = Tr(\rho\,\sigma_y) = \ldots = 2/3$$
$$r_z = Tr(\rho\,\sigma_z) = \ldots = 1/3 \quad \Rightarrow \boxed{\vec{r} = (1/3, 2/3, 1/3)}$$

b) $\|\vec{r}\| = \sqrt{r_x^2 + r_y^2 + r_z^2} = \sqrt{1/9 + 4/9 + 1/9} = \sqrt{\frac{6}{9}} = \sqrt{\frac{2}{3}} \Rightarrow \|\vec{r}\| < 1 \rightarrow$ Mistura!

c) $\langle \hat{S}_z \rangle = Tr(\hat{\rho}\,\hat{S}_z) \Rightarrow$ $\langle \hat{\sigma}_z \rangle = Tr(\hat{\rho}\,\hat{\sigma}_z) = r_z$

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

$$\hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z$$

Prob. medir $|\uparrow\rangle = |0\rangle \Rightarrow \hat{P}_0 = |0\rangle\langle 0| = \hat{M}_0$

$\uparrow P_\uparrow$ $\langle \hat{M}_0 \rangle = Tr(\hat{\rho}\,\hat{M}_0) = 2/3$