Aula 22 (16 / Mar)

Na aula de hoje:

* Resolução de exercícios Folha 5
  - Ex. 1 (normalização, densidade de probabilidade e valor esperado).
  - Ex. 3 (duas partículas não interagentes).
  - Ex. 6 (equação do movimento clássica).

Folha de Problemas 5

Postulados da Mecânica Quântica

① Normalização, densidade de probabilidade e valor esperado

$$\langle x | \psi \rangle = \psi(x) = N \frac{e^{i p_0 x/\hbar}}{\sqrt{x^2 + a^2}}$$

(a) $\langle \psi \overset{\hat{1}}{|} \psi \rangle = 1$

$$\iff \int_{-\infty}^{+\infty} dx \, \langle \psi | x \rangle \langle x | \psi \rangle = 1$$

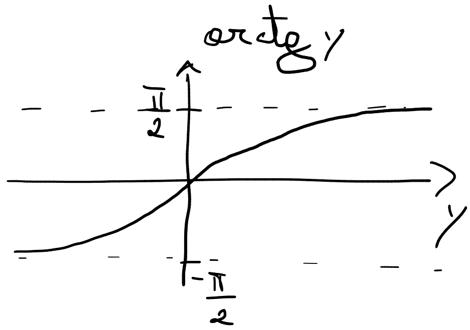
$$\iff \int_{-\infty}^{+\infty} N^2 \cdot \frac{1}{x^2 + a^2} \cdot dx = 1$$

$$\iff N^2 \cdot \underbrace{\int_{-\infty}^{+\infty} \frac{dx}{x^2+a^2}}_{= I} = 1$$

$$y \equiv \frac{x}{a} \Rightarrow dx = a \cdot dy$$

$$I = \int_{-\infty}^{+\infty} \frac{1}{\left(\frac{x}{a}\right)^2 + 1} \frac{dx}{a^2} = \frac{1}{a} \int_{-\infty}^{+\infty} \frac{1}{y^2+1} dy$$

$$= \frac{1}{a} \Big[\operatorname{arctg} y \Big]_{-\infty}^{+\infty}$$



$$= \frac{1}{a} \left(\frac{\pi}{2} - \left(-\frac{\pi}{2} \right) \right) = \frac{\pi}{a}$$

$$\Rightarrow N^2 \cdot \frac{\pi}{a} = 1 \iff N = \sqrt{\frac{a}{\pi}}$$

(b) $P_{[-\frac{a}{\sqrt{3}}, \frac{a}{\sqrt{3}}]} = \,?\, = \int_{-a/\sqrt{3}}^{a/\sqrt{3}} |\langle x|\psi\rangle|^2 \cdot dx$

$$= \int_{-a/\sqrt{3}}^{a/\sqrt{3}} \frac{a}{\pi} \cdot \frac{1}{x^2 + a^2} \, dx$$

$$= \frac{a}{\pi} \cdot \frac{1}{a^2} \int_{-a/\sqrt{3}}^{a/\sqrt{3}} \frac{1}{\left(\frac{x}{a}\right)^2 + 1} \, dx$$

$\frac{x}{a} = y \Rightarrow dx = a\,dy$

$$= \frac{1}{\cancel{a}\cdot\pi} \int_{-1/\sqrt{3}}^{1/\sqrt{3}} \cancel{a} \cdot dy \cdot \frac{1}{y^2+1}$$

$$= \frac{1}{\pi} \Big[\operatorname{arctg} y \Big]_{-1/\sqrt{3}}^{1/\sqrt{3}}$$

$$= \frac{1}{\pi} \Big[\underbrace{\operatorname{arctg}\left(\frac{1}{\sqrt{3}}\right)}_{\pi/6} - \underbrace{\operatorname{arctg}\left(-\frac{1}{\sqrt{3}}\right)}_{-\pi/6} \Big]$$

$$= \frac{2\cancel{\pi}}{\cancel{\pi}\cdot 6} = \frac{1}{3}$$

(c) Valor esperado de $\hat{X}$ e $\hat{P}$

$$\langle \hat{X} \rangle = \langle \psi | \overset{\hat{\mathbb{1}}}{\hat{X}} | \psi \rangle = \int_{-\infty}^{+\infty} dx \, \langle \psi | \underbrace{\hat{X} | x \rangle}_{= x | x \rangle} \langle x | \psi \rangle$$

$$= \int_{-\infty}^{+\infty} dx \; x \, \langle \psi | x \rangle \langle x | \psi \rangle$$

$$N = \sqrt{a/\pi}$$

$$= \int_{-\infty}^{+\infty} dx \; \underbrace{\frac{x}{x^2 + a^2}}_{\to \text{ função ímpar}} \cdot \frac{a}{\pi} = 0$$

$$\langle \hat{P} \rangle = \int_{-\infty}^{+\infty} dx \; \langle \psi | \overbrace{\hat{P} | x \rangle}^{= -i\hbar \frac{\partial}{\partial x} | x \rangle} \langle x | \psi \rangle$$

$$= \int_{-\infty}^{+\infty} dx \; \frac{a}{\pi} \cdot \frac{e^{-ip_0 x/\hbar}}{\sqrt{x^2 + a^2}} \left(-i\hbar \frac{\partial}{\partial x} \right) \frac{e^{ip_0 x/\hbar}}{\sqrt{x^2 + a^2}}$$

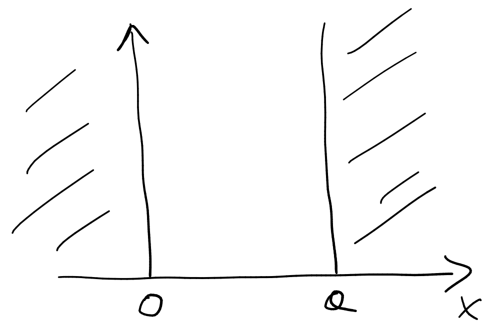
$$= -\frac{i\hbar a}{\pi} \int_{-\infty}^{+\infty} dx \; \frac{e^{-i\cdots}}{\sqrt{x^2+a^2}} \left(\frac{ip_0}{\hbar} \frac{e^{i\cdots}}{\sqrt{x^2+a^2}^{\,2}} - \frac{1}{2} \underbrace{\frac{e^{i\cdots} \, 2x}{\sqrt{x^2+a^2}^{\,3}}}_{\to 0 \text{ ímpar}} \right)$$

$$= \frac{\cancel{\hbar} a}{\pi} \frac{p_0}{\cancel{\hbar}} \underbrace{\int_{-\infty}^{+\infty} \frac{dx}{\sqrt{x^2+a^2}^{\,2}}}_{= \pi/a}$$

$$= p_0 \; //$$

③ Duas partículas não interagentes

$$V(x) = \begin{cases} 0 & , x \in [0,a] \\ +\infty & , x \notin [0,a] \end{cases}$$



$$\hat{H} = \hat{H}_1 + \hat{H}_2$$

$$= \left[\frac{\hat{P}_1^2}{2m} + \hat{V}(\hat{x}_1) \right] + \left[\frac{\hat{P}_2^2}{2m} + V(\hat{X}_2) \right]$$

(a) Partícula 1 : $\psi(x_1) \longrightarrow \mathcal{F}_1 \longrightarrow \mathcal{E}_1$

Partícula 2 : $\psi(x_2) \longrightarrow \mathcal{F}_2 \longrightarrow \mathcal{E}_2$

$\mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_2$ será o espaço de estados do sistema de duas partículas

$$\hat{H}_1 |\phi_m^1\rangle = E_m^1 |\phi_m^1\rangle$$

$$\hat{H}_2 |\phi_m^2\rangle = E_m^2 |\phi_m^2\rangle$$

Sabemos que $\{|\phi_n^1\rangle\}$ será base de $\mathcal{E}_1$,
e $\{|\phi_m^2\rangle\}$ será base $\mathcal{E}_2$.

↳ O conjunto $\{|\phi_n^1\rangle \otimes |\phi_m^2\rangle\}$ é base de $\mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_2$.

O estado mais geral em $\mathcal{E}$

$$|\psi\rangle = \sum_{n,m} c_{n,m} |\phi_n^1\rangle |\phi_m^2\rangle .$$

(b) Nós sabemos que $\{|\phi_n^1\rangle\}$ e $\{|\phi_m^2\rangle\}$

$$\hat{H}_1 |\phi_n^1\rangle = E_n^1 |\phi_n^1\rangle$$

$$\hat{H}_2 |\phi_m^2\rangle = E_m^2 |\phi_m^2\rangle$$

ou seja são soluções de

$$i\hbar \frac{d}{dt} |\phi_n^1\rangle = \hat{H}_1 |\phi_n^1\rangle$$

$$i\hbar \frac{d}{dt} |\phi_m^2\rangle = \hat{H}_2 |\phi_m^2\rangle$$

então é trivial que

$$i\hbar \frac{d}{dt} |\phi_n^1\rangle \otimes |\phi_m^2\rangle = \hat{H} |\phi_n^1\rangle \otimes |\phi_m^2\rangle$$

$$\Rightarrow i\hbar \left[\underbrace{\frac{d|\phi_n^1\rangle}{dt}}_{= \frac{\hat{H}_1 |\phi_n^1\rangle}{i\hbar}} \otimes |\phi_m^2\rangle + |\phi_n^1\rangle \otimes \underbrace{\frac{d}{dt}|\phi_m^2\rangle}_{= \frac{1}{i\hbar}\hat{H}_2 |\phi_m^2\rangle} \right] =$$

$$= \left(\hat{H}_1 + \hat{H}_2\right) |\phi_n^1\rangle \otimes |\phi_m^2\rangle$$

$$\Leftrightarrow \left(\hat{H}_1 + \hat{H}_2\right) |\phi_n^1\rangle \otimes |\phi_m^2\rangle = \left(\hat{H}_1 + \hat{H}_2\right) |\phi_n^1\rangle \otimes |\phi_m^2\rangle$$

$\square$

(e) As auto-energias de $\hat{H} = \hat{H}_1 + \hat{H}_2$ serão

$E_{(n,m)} = E_n^1 + E_m^2$ para auto-estado $|\phi_n^1\rangle \otimes |\phi_m^2\rangle$

$$= \frac{\hbar^2 \pi^2}{2ma^2}\left(n^2 + m^2\right)$$

$\hookrightarrow n, m = 1, 2, 3, \ldots$

Os três estados de menor energia,

$E_{(1,1)} = \frac{\hbar^2 \pi^2}{2ma^2} \cdot 2 \longrightarrow \deg = 1$

$E_{(1,2)} = E_{(2,1)} = \frac{\hbar^2 \pi^2}{2ma^2} 5 \longrightarrow \deg = 2$

$E_{(2,2)} = \frac{\hbar^2 \pi^2}{2ma^2} 8 \longrightarrow \deg = 1.$

(d) $t = t_0$ $\quad |\psi(t_0)\rangle = \frac{1}{\sqrt{6}}\left[|\phi_1^1 \phi_2^2\rangle + \sqrt{2}\, |\phi_3^1 \phi_2^2\rangle + \sqrt{3}\, |\phi_1^1 \phi_4^2\rangle \right]$

Em $t = t_a$

$$|\psi(t_a)\rangle = \frac{1}{\sqrt{6}}\left[e^{-i E_{(1,2)} \frac{t_a - t_0}{\hbar}} |\phi_1^1 \phi_2^2\rangle + \sqrt{2}\,.\, e^{-i E_{(3,2)} \frac{t_a - t_0}{\hbar}} |\phi_3^1 \phi_2^2\rangle + \sqrt{3}\, e^{-i E_{(1,4)} \frac{t_a - t_0}{\hbar}} |\phi_1^1 \phi_4^2\rangle \right]$$

Medição da energia partícula 1 em t

$$E_1^{(1)} = \frac{\hbar^2 \pi^2}{2ma^2} \longrightarrow P_{E_1} = \frac{1}{6} + \frac{3}{6} = \frac{2}{3}$$

$$E_3^{(1)} = \frac{\hbar^2 \pi^2}{2ma^2}.9 \longrightarrow P_{E_3} = \frac{2}{6} = \frac{1}{3}$$

(e) Se medirmos $E_1^{(1)} = \frac{\hbar^2 \pi^2}{2ma^2}$ em $t = t_a$ para a energia da partícula 1, então $t > t_a$

$$|\psi(t_a)\rangle = \frac{1}{2}\left[e^{-i E_{(1,2)} \frac{t_a - t_0}{\hbar}} |\phi_1^1 \phi_2^2\rangle + \sqrt{3}\, e^{-i E_{(1,4)} \frac{t_a - t_0}{\hbar}} |\phi_1^1 \phi_4^2\rangle \right]$$

Os valores possíveis numa medição de E_m^2 energia da partícula 2 em $t > t_a$ serão

$$E_2^{(2)} = \cdots \longrightarrow P_{E_2} = \frac{1}{4}$$

$$E_4^{(2)} = \cdots \longrightarrow P_{E_4} = \frac{3}{4}.$$

(5) $\hat{V}(|\hat{X}_1 - \hat{X}_2|)$

(1) $\hat{H} = \hat{H}_1 + \hat{H}_2 \longrightarrow \hat{H} = \hat{H}_1(\hat{X}_1, \hat{P}_1) + \hat{H}_2(\hat{X}_2, \hat{P}_2) + \hat{V}(|\hat{X}_1 - \hat{X}_2|)$

(2) Sim, $\mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_2$.

(3) Sim, $\{|\phi_n^1\rangle \otimes |\phi_m^2\rangle\}$ será base, mas já não é base onde $\hat{H}$ é diagonal pois já não são auto-estados de $\hat{H}$.

(4) Não.

6 Equação do movimento clássica

$$\hat{H} = \frac{\hat{\vec{P}}^2}{2m} + \hat{V}(\hat{\vec{R}}) \text{ é assumido}$$

$$\hat{\vec{R}} = (\hat{X}, \hat{Y}, \hat{Z}) \quad e \quad \hat{\vec{P}} = (\hat{P}_x, \hat{P}_y, \hat{P}_z)$$

(a) $$\frac{d}{dt}\langle \hat{\vec{R}} \cdot \hat{\vec{P}} \rangle = \underset{0}{?} = \frac{d}{dt}\langle \psi(t) | \hat{\vec{R}} \cdot \hat{\vec{P}} | \psi(t) \rangle$$

$$= \Big\langle \underbrace{\cancel{\frac{\partial}{\partial t} \hat{\vec{R}} \cdot \hat{\vec{P}}}}_{0} \Big\rangle + \frac{1}{i\hbar}\langle [\hat{\vec{R}} \cdot \hat{\vec{P}}, \hat{H}] \rangle$$

$$= \frac{1}{i\hbar}\langle [\underbrace{\hat{\vec{R}} \cdot \hat{\vec{P}}}_{\hat{X}\hat{P}_x + \hat{Y}\hat{P}_y + \hat{Z}\hat{P}_x}, \underbrace{\hat{H}}_{\frac{P_x^2 + P_y^2 + P_z^2}{2m} + \hat{V}(\hat{X}, \hat{Y}, \hat{Z})}] \rangle$$

Temos que calcular o comutador

$$[\hat{X}\hat{P}_x, \hat{P}_x^2] = \hat{X}\hat{P}_x^3 - \hat{P}_x^2\hat{X}\hat{P}_x + \hat{P}_x\hat{X}\hat{P}_x^2 - \hat{P}_x\hat{X}\hat{P}_x^2$$

$$= \underbrace{[\hat{X}, \hat{P}_x]}_{i\hbar\hat{1}}\hat{P}_x^2 + \hat{P}_x\underbrace{[\hat{X}, \hat{P}_x]}_{i\hbar\hat{1}}\hat{P}_x$$

$$= 2i\hbar\hat{P}_x^2$$

$$[\hat{X}\hat{P}_x, \hat{P}_y^2] = 0$$

$$[\hat{X}\hat{P}_x, \hat{V}(\hat{\vec{R}})] = \hat{X}\overbrace{[\hat{P}_x, \hat{V}(\hat{\vec{R}})]}^{-i\hbar\frac{\partial \hat{V}}{\partial \hat{X}}} = -i\hbar\hat{X}\frac{\partial \hat{V}}{\partial \hat{X}}$$

sendo os outros comutadores análogos a estes. Podemos então escrever,

$$[\hat{\vec{R}}\cdot\hat{\vec{P}}, \hat{H}] = \sum_{i,j} \underbrace{\left[\hat{R}_i\hat{P}_i, \frac{\hat{P}_j^2}{2m}\right]}_{= \frac{2i\hbar}{2m}\hat{P}_j^2 \cdot \delta_{ij}} + \sum_i \underbrace{\left[\hat{R}_i\hat{P}_i, \hat{V}(\hat{\vec{R}})\right]}_{= -i\hbar \hat{R}_i \frac{\partial \hat{V}}{\partial \hat{R}_i}}$$

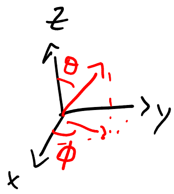
$$= \sum_i \left[i\hbar \frac{\hat{P}_i^2}{m} - i\hbar \hat{R}_i \frac{\partial \hat{V}}{\partial \hat{R}_i} \right]$$

$$= i\hbar \left(\frac{\hat{\vec{P}}^2}{m} - \hat{\vec{R}}\cdot\vec{\nabla}\hat{V} \right)$$

e assim podemos finalmente escrever

$$\frac{d}{dt}\langle \hat{\vec{R}}\cdot\hat{\vec{P}} \rangle = \frac{1}{\cancel{i\hbar}} \cancel{i\hbar} \left\langle \frac{\hat{\vec{P}}^2}{m} - \hat{\vec{R}}\cdot\vec{\nabla}\hat{V} \right\rangle$$

$\square$



coord. esféricas

(b) $$\hat{V}(\hat{\vec{R}}) = \frac{e^2}{\hat{R}} \Rightarrow \vec{\nabla}\hat{V} = \left(\frac{\partial}{\partial \hat{R}}, \frac{1}{\hat{R}}\frac{\partial}{\partial \hat{\theta}}, \frac{1}{\hat{R}\,\mathrm{sen}\hat{\theta}}\frac{\partial}{\partial \hat{\phi}} \right)\hat{V}$$

$(\hat{R}, \hat{\theta}, \hat{\phi})$

$$= \left(-\frac{e^2}{\hat{R}^2}, 0, 0 \right)$$

e assim $\hat{\vec{R}}\cdot\vec{\nabla}V = -\frac{e^2}{\hat{R}}$, logo, como temos estado estacionário, para o qual sabemos que

$$\frac{d}{dt}\langle\phi|\hat{\vec{R}}\cdot\hat{\vec{P}}|\phi\rangle = 0$$

$\to H|\phi\rangle = E|\phi\rangle$, ou seja $|\phi\rangle$ é estado estacionário,

$$\frac{d}{dt}\langle\hat{A}\rangle = \langle\cancel{\frac{\partial\hat{A}}{\partial t}}\rangle + \frac{1}{i\hbar}\langle\underbrace{[\hat{A},\hat{H}]}\rangle$$

0

$$\langle\phi|\hat{A}\hat{H}-\hat{H}\hat{A}|\phi\rangle = \langle\phi|\hat{A}E-E\hat{A}|\phi\rangle$$
$$= E\langle\phi|\hat{A}-\hat{A}|\phi\rangle = 0$$

$$\Rightarrow \frac{d}{dt}\langle\phi|A|\phi\rangle = 0$$

e então teremos

$$\left\langle\frac{\hat{\vec{P}}^2}{m} - \hat{\vec{R}}\cdot\vec{\nabla}\hat{V}\right\rangle = 0$$

$$\Leftrightarrow \left\langle\frac{\hat{\vec{P}}^2}{m}\right\rangle = \langle\hat{\vec{R}}\cdot\vec{\nabla}\hat{V}\rangle$$

$$\Leftrightarrow 2\langle E_c\rangle = -\langle E_p\rangle$$

$$\Leftrightarrow \langle E_p\rangle = -2\langle E_c\rangle$$

$\square$