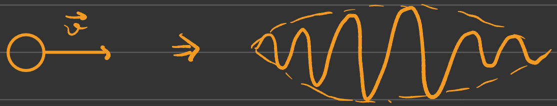
21/06/23

Eq. de Schrödinger

* De Broglie → ondas de matéria

* Equação para descrever evolução das ondas?



* Classicamente:

→ Lei de Newton:

$$\rightarrow m\frac{d^2x}{dt^2} = F(x) \Rightarrow m\ddot{x} = -kx \Rightarrow \ddot{x} + \frac{k}{m}x = 0$$

$$\rightarrow x(t) = e^{\alpha t} \Rightarrow \ddot{x} + \frac{k}{m}x = \left(\alpha^2 + \frac{k}{m}\right)e^{\alpha t} = 0$$

$$\alpha^2 = -\frac{k}{m} \Rightarrow \alpha = \pm i\sqrt{\frac{k}{m}} = \pm i\omega \Rightarrow x(t) = Ae^{i\omega t} + Be^{-i\omega t}$$

$$\rightarrow x(t) = A[\cos(\omega t) + i\,\mathrm{sen}(\omega t)] + B[\cos(\omega t) - i\,\mathrm{sen}(\omega t)]$$

$$x(t) = (A+B)\cos(\omega t) + (A-B)\,i\,\mathrm{sen}(\omega t)$$

$$\therefore x(t) = C\cos(\omega t) + D\,\mathrm{sen}(\omega t)$$

$$\rightarrow \left.\begin{array}{l} x(0) = x_0 \\ \dot{x}(0) = 0 \end{array}\right\} \quad \boxed{x(t) = x_0\cos(\omega t)}$$

* Sistemas quânticos:

→ O que sabemos?

1) $\lambda = \frac{h}{p}$, $E = h\nu$

2) $E = K + U = \frac{p^2}{2m} + V(x,t)$

3) a solução da nova equação que vai reger a dinâmica da partícula/onda, $\psi(x,t)$, deve ser linear:

$\psi_1(x,t)$ e $\psi_2(x,t)$ são soluções

$$\therefore \psi(x,t) = A\psi_1(x,t) + B\psi_2(x,t)$$

* Essa nova equação deve ser compatível com os pontos 1, 2 e 3:

→ $E = h\nu = \frac{h}{2\pi} 2\pi\nu = \hbar\omega$ (4)

→ $p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k$ (5)

→ Substituindo (4) e (5) na equação (2):

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V(x,t) \qquad (6)$$

→ Suponha $V(x,t) = V_0$. Logo, $F = -\frac{\partial V}{\partial x} = 0 \Rightarrow v = cte$

$\therefore\ p = cte \Rightarrow k = cte \Rightarrow \omega = cte \Rightarrow E = cte$

→ k, ω não constantes: $\psi_{ansatz}(x,t) = \text{sen}(kx - \omega t) \qquad (7)$

↳ $\frac{\partial \psi_a}{\partial x} = k\cos(kx-\omega t)$, $\frac{\partial^2 \psi_a}{\partial x^2} = -k^2 \text{sen}(kx-\omega t)$, $\frac{\partial \psi_a}{\partial t} = -\omega\cos(kx-\omega t)$

→ Proposta de equação: $A\frac{\partial^2 \psi}{\partial x^2} + V(x,t)\psi = B\frac{\partial \psi}{\partial t} \quad (8)$ → equação da onda

→ Substituindo (7) em (8):

$$-k^2 A\,\text{sen}(kx-\omega t) + V_0\,\text{sen}(kx-\omega t) = -B\omega\cos(kx-\omega t)$$

$$(V_0 - k^2 A)\,\text{sen}(kx-\omega t) = -B\omega\cos(kx-\omega t)$$

$$\text{tg}(kx-\omega t) = \frac{B\omega}{k^2 A - V_0}$$

→ x e t não podem ser quaisquer!

→ Nova proposta de solução: $\Psi_{ansatz} = C\,\text{sen}(kx - \omega t) + \cos(kx - \omega t)$ (9)

↳ $\dfrac{\partial \Psi_a}{\partial x} = kC\cos(kx-\omega t) - k\,\text{sen}(kx-\omega t)$

↳ $\dfrac{\partial^2 \Psi_a}{\partial x^2} = -k^2 C\,\text{sen}(kx-\omega t) - k^2\cos(kx-\omega t)$

↳ $\dfrac{\partial \Psi_a}{\partial t} = -\omega C\cos(kx-\omega t) + \omega\,\text{sen}(kx-\omega t)$

→ Substituindo (9) em (8):

$$B\left[-\omega C\cos(kx-\omega t) + \omega\,\text{sen}(kx-\omega t)\right] =$$
$$= A\left[-k^2 C\,\text{sen}(kx-\omega t) - k^2\cos(kx-\omega t)\right] + V_0\left[C\,\text{sen}(kx-\omega t) + \cos(kx-\omega t)\right]$$

$$-BC\omega\cos(kx-\omega t) + B\omega\,\text{sen}(kx-\omega t) =$$
$$= -k^2AC\,\text{sen}(kx-\omega t) - k^2A\cos(kx-\omega t) + V_0C\,\text{sen}(kx-\omega t) + V_0\cos(kx-\omega t)$$

$$\left.\begin{aligned} &\rightarrow V_0 - k^2A = -BC\omega \\ &\rightarrow V_0 - k^2A = \frac{B\omega}{C} \end{aligned}\right\} \quad -BC\omega = \frac{B\omega}{C} \Rightarrow C^2 = -1$$

$$C = \pm i$$

$$\left.\begin{aligned} &\rightarrow V_0 - k^2A = \pm iB\omega \\ &\rightarrow V_0 + \frac{\hbar^2 k^2}{2m} = \hbar\omega \end{aligned}\right\} \quad \pm iB = \hbar \Rightarrow B = \pm i\hbar$$

$$A = -\frac{\hbar^2}{2m}$$

→ Escolha: $B = i\hbar$

→ Voltando para (6):

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

Equação de Schrödinger

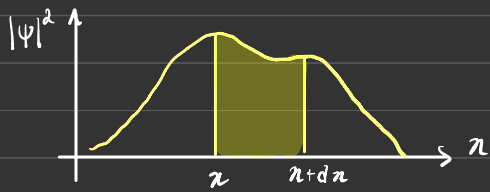
→ Dado um potencial $V(x,t)$, obtemos $\Psi(x,t)$

Max Born e a interpretação probabilística

→ as soluções da eq. Schrödinger são complexas, mas

$$|\psi(x,t)|^2 = \psi^*(x,t)\,\psi(x,t)$$

é um número real.



→ Interpretação: $|\psi(x,t)|^2 dx$ é a probabilidade de que a partícula se encontre entre x e $x+dx$ no instante t.

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$$

→ $\dfrac{d}{dt}\left[\int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx\right] = (*) = ?$

→ $(*) = \displaystyle\int_{-\infty}^{+\infty} \frac{\partial}{\partial t}\left[\psi^*(x,t)\,\psi(x,t)\right] dx$

$= \displaystyle\int_{-\infty}^{+\infty} \left[\psi^*(x,t)\frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi(x,t)\right] dx$

→ Pela eq. Schrödinger,

→ $\dfrac{\partial \psi}{\partial t} = \dfrac{-\hbar^2}{2mi\hbar}\dfrac{\partial^2 \psi}{\partial x^2} + \dfrac{V(x,t)}{i\hbar}\psi = \dfrac{i\hbar}{2m}\dfrac{\partial^2 \psi}{\partial x^2} - \dfrac{i}{\hbar}V(x,t)\psi$

→ $\dfrac{\partial \psi^*}{\partial t} = \dfrac{-i\hbar}{2m}\dfrac{\partial^2 \psi}{\partial x^2} + \dfrac{i}{\hbar}V(x,t)\psi^*$

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Consequências da Eq. Schrödinger

→ $P_{ab} = \int_a^b |\Psi(x,t)|^2 dx$ = probabilidade da partícula estar entre a e b

→ $\frac{dP_{ab}}{dt} = -\frac{\hbar}{2m} i \left[J(b,t) - J(a,t) \right]$ → espécie de equação mestra

* Obs.: $\boxed{J(x,t) = \Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x}}$: corrente de probabilidade

Se P_{ab} aumenta, significa que está "fluindo" mais probabilidade para dentro de uma região por uma extremidade do que saindo pela outra

$\therefore \boxed{\frac{d}{dt} \int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 0}$, portanto $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = cte$
⇒ normalizável

→ Uma vez que interpretamos $\rho(x) = |\Psi(x,t)|^2$ como uma função densidade de probabilidade,

* $\langle x \rangle = \int_{-\infty}^{+\infty} x \rho(x) dx = \int_{-\infty}^{+\infty} x \Psi^*(x,t) \Psi(x,t) dx$
↳ onde a partícula está, em média

* $\langle v \rangle = \frac{d\langle x \rangle}{dt} = \int_{-\infty}^{+\infty} \frac{\partial}{\partial t} \left[x \Psi^*(x,t) \Psi(x,t) \right]$
↳ valor esperado da probabilidade

$$\rightarrow \langle v \rangle = \int_{-\infty}^{+\infty} x \frac{\partial}{\partial t}\left[\psi^*(x,t)\,\psi(x,t)\right] dx$$

$$= \int_{-\infty}^{+\infty} x \left[\frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t}\right] dx \quad (1)$$

→ Pela Eq. Schrödinger,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x,y)\psi = i\hbar \frac{\partial \psi}{\partial t} \Rightarrow \begin{cases} \dfrac{\partial \psi}{\partial t} = \dfrac{\hbar i}{2m}\dfrac{\partial^2 \psi}{\partial t^2} - i\dfrac{V(x,t)}{\hbar}\psi \\[2ex] \dfrac{\partial \psi^*}{\partial t} = -\dfrac{\hbar i}{2m}\dfrac{\partial^2 \psi^*}{\partial t^2} + i\dfrac{V(x,t)}{\hbar}\psi^* \end{cases} \quad (2)$$

→ Substituindo (2) em (1):

$$\langle v \rangle = \int_{-\infty}^{+\infty} x \left\{\left[-\frac{\hbar}{2m} i \frac{\partial^2 \psi^*}{\partial x^2} + i\frac{V(x,t)}{\hbar}\psi^*\right]\psi + \psi^*\left[\frac{\hbar}{2m} i \frac{\partial^2 \psi}{\partial x^2} - i\frac{V(x,t)}{\hbar}\psi\right]\right\} dx$$

$$= \int_{-\infty}^{+\infty} x \left[-\frac{\hbar}{2m} i \frac{\partial^2 \psi^*}{\partial x^2} + \frac{\hbar}{2m} i\, \psi^* \frac{\partial^2 \psi}{\partial x^2}\right] dx$$

$$= -\frac{\hbar}{2m} i \int_{-\infty}^{+\infty} x \left[\frac{\partial^2 \psi^*}{\partial x^2}\psi - \psi^* \frac{\partial^2 \psi}{\partial x^2}\right] dx$$

$$\hookrightarrow \frac{\partial}{\partial x}\left[\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right] = \frac{\partial^2 \psi^*}{\partial x^2}\psi + \frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x} - \psi^*\frac{\partial^2 \psi}{\partial x^2}\Big]$$

$$= \frac{\partial^2 \psi}{\partial x^2}\psi^* - \psi^* \frac{\partial^2 \psi}{\partial x^2}$$

→ Logo,

$$\langle v \rangle = -\frac{\hbar}{2m} i \underbrace{\int_{-\infty}^{+\infty} x \frac{\partial}{\partial x}\left[\frac{\partial \psi^*}{\partial x}\psi - \psi^* \frac{\partial \psi}{\partial x}\right] dx}_{I}$$

→ Integrando I por partes:

$$I = x\left[\underbrace{\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}}_{=0}\right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty}\left[\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right] dx$$

↳ $\psi, \psi^*, \psi_x, \psi^*_x$ se anulam em $x \to \pm\infty$

→ $$I = -\underbrace{\int_{-\infty}^{+\infty} \frac{\partial \psi^*}{\partial x}\psi \, dx}_{II} + \int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

→ Integrando II por partes:

$$II = \underbrace{\psi^*\psi \Big|_{-\infty}^{+\infty}}_{=0} - \int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x} dx \Rightarrow II = -\int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

$$\therefore I = 2\int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

$\Rightarrow \langle v \rangle = -\frac{\hbar i}{m} \int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x} \, dx$

$\rightarrow \langle p \rangle = m \langle v \rangle \Rightarrow \langle p \rangle = -\hbar i \int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x} \, dx$

→ Poderíamos escrever assim:

$$\begin{cases} \langle x \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t) \, x \, \psi(x,t) \, dx \\ \langle p \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x,t) \, dx \end{cases}$$

→ Denotamos x como o operador posição e $p = -i\hbar \, \partial/\partial x$ como o operador momentum da partícula

$$\left.\begin{aligned} &\rightarrow \frac{p^2}{2m} + V(x,t) = E \\ &\rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x,t)\,\psi(x,t) = i\hbar \frac{\partial \psi}{\partial t} \end{aligned}\right\} \quad p^2 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Rightarrow p = i\hbar \frac{\partial}{\partial x}$$

*Obs.: Operador energia: $E = i\hbar \frac{\partial}{\partial t}$

→ Dado um operador $O(x,p) = O\left(x, i\hbar \frac{\partial}{\partial x}\right)$, podemos definir genericamente

$$\boxed{\langle O \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t) \, \hat{O} \, \psi(x,t) \, dx}$$

$$\rightarrow \langle p\rangle = m\langle v\rangle \Rightarrow \frac{d\langle p\rangle}{dt} = m\frac{d}{dt}\langle v\rangle = m\langle a\rangle$$

$$\frac{d\langle p\rangle}{dt} = -i\hbar\int_{-\infty}^{+\infty} \underbrace{\frac{\partial}{\partial t}\left(\psi^*\frac{\partial\psi}{\partial x}\right)}_{(*)} dx$$

$$\rightarrow (*) = \frac{\partial\psi^*}{\partial t}\frac{\partial\psi}{\partial x} + \psi^*\frac{\partial}{\partial t}\frac{\partial\psi}{\partial x}$$

$$\begin{cases} \dfrac{\partial\psi}{\partial t} = \dfrac{\hbar i}{2m}\dfrac{\partial^2\psi}{\partial x^2} - i\dfrac{V}{\hbar}\psi \\ \dfrac{\partial\psi^*}{\partial t} = -\dfrac{\hbar i}{2m}\dfrac{\partial^2\psi^*}{\partial x^2} + i\dfrac{V}{\hbar}\psi^* \end{cases}$$

$$\Rightarrow (*) = \frac{\partial\psi^*}{\partial t}\frac{\partial\psi}{\partial x} + \psi^*\frac{\partial}{\partial x}\frac{\partial\psi}{\partial t}$$

$$= \left(-\frac{\hbar i}{2m}\frac{\partial^2\psi^*}{\partial x^2} + i\frac{V}{\hbar}\psi^*\right)\frac{\partial\psi}{\partial x} + \psi^*\frac{\partial}{\partial x}\left(\frac{\hbar i}{2m}\frac{\partial^2\psi}{\partial x^2} - i\frac{V}{\hbar}\psi\right)$$

$$= -\frac{\hbar i}{2m}\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x} + i\frac{V}{\hbar}\psi^*\frac{\partial\psi}{\partial x} + \frac{\hbar i}{2m}\psi^*\frac{\partial^3\psi}{\partial x^3} - \frac{i}{\hbar}\psi^*\left(\frac{\partial V}{\partial x}\psi + V\frac{\partial\psi}{\partial x}\right)$$

$$= -\frac{\hbar i}{2m}\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x} + \cancel{i\frac{V}{\hbar}\psi^*\frac{\partial\psi}{\partial x}} + i\frac{\hbar}{2m}\psi^*\frac{\partial^3\psi}{\partial x^3} - \frac{i}{\hbar}\psi^*\frac{\partial V}{\partial x}\psi - \cancel{i\frac{V}{\hbar}\psi^*\frac{\partial\psi}{\partial x}}$$

$$= -\frac{\hbar i}{2m}\left(\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x} - \psi^*\frac{\partial^3\psi}{\partial x^3}\right) - \frac{i}{\hbar}\psi^*\frac{\partial V}{\partial x}\psi$$

$$\Rightarrow \frac{d\langle p\rangle}{dt} = -\frac{\hbar^2}{2m}\underbrace{\int_{-\infty}^{+\infty}\left(\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x} - \psi^*\frac{\partial^3\psi}{\partial x^3}\right)dx}_{I} - \int_{-\infty}^{+\infty}\psi^*\frac{\partial V}{\partial x}\psi\, dx$$

$$\Rightarrow I = \int_{-\infty}^{+\infty}\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x}dx - \overset{\text{por partes}}{\int_{-\infty}^{+\infty}\psi^*\frac{\partial^3\psi}{\partial x^3}dx}$$

$$= \int_{-\infty}^{+\infty}\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x}dx - \underbrace{\psi^*\frac{\partial^2\psi}{\partial x^2}\Big|_{-\infty}^{+\infty}}_{=0} + \int_{-\infty}^{+\infty}\frac{\partial\psi^*}{\partial x}\frac{\partial^2\psi}{\partial x^2}dx$$

$$= \int_{-\infty}^{+\infty}\left(\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x} + \underbrace{\frac{\partial\psi^*}{\partial x}\frac{\partial^2\psi}{\partial x^2}}_{\text{por partes}}\right)dx$$

$$= \int_{-\infty}^{+\infty}\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x}dx + \underbrace{\frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x}\Big|_{-\infty}^{+\infty}}_{=0} - \int_{-\infty}^{+\infty}\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x}dx$$

$$= \int_{-\infty}^{+\infty}\left(\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x} - \frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x}\right)dx$$

$$= 0 \;//$$

$$\Rightarrow \frac{d\langle p\rangle}{dt} = -i\hbar\int_{-\infty}^{+\infty} -\frac{i}{\hbar}\psi^*\frac{\partial V}{\partial x}\psi\, dx$$

$$= -\int_{-\infty}^{+\infty}\psi^*(x,t)\frac{\partial V}{\partial x}\psi(x,t)\,dx$$

$$= -\left\langle\frac{\partial V}{\partial x}\right\rangle$$

$$\therefore \boxed{\frac{d\langle p\rangle}{dt} = -\left\langle\frac{\partial V}{\partial x}\right\rangle}$$ Teorema de Ehrenfest

03/07/23

Solução da Eq. Schrödinger para $V(x,t) = V(x)$

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

$$\rightarrow \frac{p^2}{2m} + V = E \Rightarrow \frac{p^2}{2m}\psi + V\psi = E\psi$$

$$\rightarrow p = -i\hbar\frac{\partial}{\partial x} \Rightarrow p^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

$$\boxed{\hat{E} = i\hbar\frac{\partial}{\partial t}}$$

→ Pelo fato de $V(x,t) = V(x)$, posso tentar soluções que são separáveis na posição e no tempo.

* Ansatz: $\psi(x,t) = \varphi(x)\phi(t)$

$$\rightarrow -\frac{\hbar^2}{2m}\phi(t)\frac{d^2\varphi}{dt^2} + V(x)\varphi(x)\phi(t) = i\hbar\varphi(x)\frac{d\phi}{dt} \qquad (\div\varphi\phi)$$

$$\rightarrow \underbrace{-\frac{\hbar^2}{2m}\frac{1}{\varphi}\frac{d^2\varphi}{dx^2} + V(x)}_{\text{só depende de } x} = \underbrace{i\hbar\frac{1}{\phi}\frac{d\phi}{dt}}_{\text{só depende de } t} = E$$

→ A parte temporal nos dará:

$$\hookrightarrow i\hbar\frac{1}{\phi}\frac{d\phi}{dt} = E \Rightarrow \frac{d\phi}{dt} = \frac{E}{i\hbar}\phi = -i\frac{E}{\hbar}\phi$$

$$\hookrightarrow \phi = e^{\alpha t} \Rightarrow \alpha e^{\alpha t} = -i\frac{E}{\hbar}e^{\alpha t} \Rightarrow \alpha = -i\frac{E}{\hbar} \Rightarrow \boxed{\phi(t) = e^{-i\frac{E}{\hbar}t}}$$

→ a parte espacial nos dará:

↳ $-\frac{\hbar^2}{2m}\frac{1}{\varphi}\frac{d^2\varphi}{dx^2} + V(x) = E \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + V(x)\varphi = E\varphi$

↳ Denoto $\mathcal{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$: operador Hamiltoniano

$$\boxed{\mathcal{H}\varphi = E\varphi}$$

→ Uma solução procurada é da forma $\boxed{\Psi(x,t) = \varphi(x)\, e^{-i\frac{E}{\hbar}t}}$

→ $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{+\infty} \Psi^*(x,t)\Psi(x,t)\, dx$
$= \int_{-\infty}^{+\infty} \varphi^*(x)\, e^{i\frac{E}{\hbar}t}\, \varphi(x)\, e^{-i\frac{E}{\hbar}t}\, dx$
$= \int_{-\infty}^{+\infty} \varphi^*(x)\,\varphi(x)\, dx$
$= \int_{-\infty}^{+\infty} |\varphi(x)|^2 dx$
$= 1$

$\therefore \int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{+\infty} |\varphi(x)|^2 dx = 1$

*Obs.: $\langle \mathcal{H} \rangle = \int_{-\infty}^{+\infty} \Psi^* \mathcal{H} \Psi\, dx$
$= \int_{-\infty}^{+\infty} \varphi^*(x)\, e^{i\frac{E}{\hbar}t}\, \mathcal{H}\, e^{-i\frac{E}{\hbar}t}\, \varphi(x)\, dx$
$= \int_{-\infty}^{+\infty} \varphi^*(x)\, \mathcal{H}\varphi(x)\, dx$
$= \int_{-\infty}^{+\infty} \varphi^*(x)\, E\varphi\, dx$
$= E\int_{-\infty}^{+\infty} \varphi^*(x)\,\varphi(x)\, dx$
$= E$

$\therefore \langle \mathcal{H} \rangle = E$

$$\rightarrow \langle H^2 \rangle = \int_{-\infty}^{+\infty} \psi^* H^2 \psi \, dx$$
$$= \int_{-\infty}^{+\infty} \psi^*(x) H^2 \psi(x) \, dx$$
$$= \int_{-\infty}^{+\infty} \psi^*(x) H (H\psi) \, dx$$
$$= E \int_{-\infty}^{+\infty} \psi^*(x) E \psi \, dx$$
$$= E^2 \int_{-\infty}^{+\infty} \psi^*(x) \psi(x) \, dx$$
$$= E^2$$
$$\therefore \langle H^2 \rangle = E^2$$

→ Definimos: $\sigma_H = \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$
$$= \sqrt{E^2 - E^2}$$
$$= 0$$
$$\therefore \sigma_H = 0$$

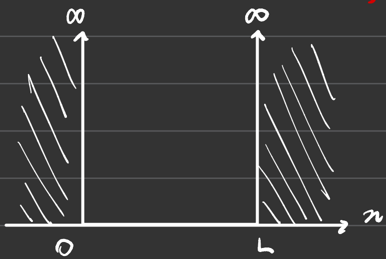
↳ Se fizermos uma média de H não espero outro resultado que não seja E

* Obs.: Se ψ_1 e ψ_2 são soluções de $H\psi = E\psi$, com respectivos valores de E E_1 e E_2 ($H\psi_1 = E\psi_1$, $H\psi_2 = E\psi_2$), então a solução mais geral do problema é:

$$\boxed{\Psi(x,t) = c_1 \psi_1(x) e^{-iE_1 t/\hbar} + c_2 \psi_2(x) e^{-iE_2 t/\hbar}}$$

05/07/23

Poço de potencial infinito



$$V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{caso contrário} \end{cases}$$

→ Eq. de Schrödinger independente do tempo:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dt^2} + V(x)\varphi(x) = E\varphi(x)$$

→ No interior da caixa:

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = E\varphi(x) \Rightarrow \frac{d^2\varphi}{dx^2} + \frac{2mE}{\hbar^2}\varphi = 0$$

$$\varphi(0) = \varphi(L) = 0 \Rightarrow \varphi(x) = \sqrt{\frac{2}{L}}\,\text{sen}\left(\frac{n\pi x}{L}\right)$$

$$\rightarrow K_n = \frac{n\pi}{L} = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow \frac{n^2\pi^2}{L^2} = \frac{2m}{\hbar^2}E \Rightarrow E_n = \frac{n^2\pi^2}{2mL^2}\hbar^2, \quad n = 1, 2, \dots$$

→ A parte temporal é dada por $\phi(t) = e^{-i\frac{E}{\hbar}t}$

→ Solução geral: $\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \varphi_n(x) e^{-i\frac{E}{\hbar}t}}$

→ Observamos que

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Psi(x,t)\,dx = 1 \Rightarrow \int_{-\infty}^{\infty} \left(\sum_{n=0}^{\infty} c_n^* \varphi_n^*(x)\, e^{i\frac{E}{\hbar}t}\right)\left(\sum_{n=0}^{\infty} c_n \varphi_n(x)\, e^{-i\frac{E}{\hbar}t}\right) dx$$

$$\sum_{n=0}^{\infty} |c_n|^2 \int_{-\infty}^{\infty} |\varphi_n(x)|^2 dx + \sum_{n\neq m} c_n^* c_m \left(\int_{-\infty}^{\infty} \varphi_n^*(x)\,\varphi_m(x)\,dx\right) e^{i\frac{(E_n-E_m)}{\hbar}t}$$

→ Para o poço:

$$\int_{-\infty}^{\infty} \varphi_n^*(x)\,\varphi_m(x)\,dx = \frac{2}{L}\int_0^L \operatorname{sen}\left(\frac{n\pi x}{L}\right) \operatorname{sen}\left(\frac{m\pi x}{L}\right) dx = \delta_{n,m}$$

$$\therefore \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \sum_{n=0}^{\infty} |c_n|^2 = 1$$

→ É natural interpretarmos que em uma medida de algum observável físico $p_n = |c_n|^2 = c_n^* c_n$ o sistema esteja no estado φ_n

10/08/23

Princípio da Incerteza no poço de potencial

→ $V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{senão} \end{cases}$

→ Eq. Schrödinger independente do tempo: $-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi}{\partial x^2} + V(x)\varphi = E\varphi$

$$H\varphi = E\varphi$$

→ $\varphi(0) = \varphi(L) = 0 \Rightarrow E_n = \frac{\pi^2\hbar^2}{2mL} n^2$ | $\varphi_n(x) = \sqrt{\frac{2}{L}}\,\text{sen}\left(\frac{n\pi x}{L}\right)$

autoenergia | autofunções

→ Solução geral: $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \varphi_n(x) e^{-i\frac{E_n}{\hbar}t}$

→ Vimos que $\begin{cases} \int_0^L \varphi_n^*(x)\varphi_m(x)\,dx = \delta_{n,m} \rightarrow \text{ortonormais} \\ c_n = \int_0^L \varphi_n^* \Psi(x,t)\,dx \end{cases}$

→ Operador hamiltoniano: $\langle \mathcal{H} \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\,\mathcal{H}\,\Psi(x,t)\,dx$

$$= \int_{-\infty}^{+\infty} \left(\sum_{n=1}^{\infty} c_n \varphi_n(x) e^{-i\frac{E_n}{\hbar}t}\right)^* \mathcal{H} \left(\sum_{m=1}^{\infty} c_m \varphi_m(x) e^{-i\frac{E_m}{\hbar}t}\right) dx$$

$$= \sum_{n=1}^{\infty} E_n c_n^* c_n \int_{-\infty}^{+\infty} \varphi_n^* \varphi_m\,dx\; e^{\frac{i}{\hbar}(E_n-E_m)t} +$$

$$+ \sum_{n\neq m} E_n c_n^* c_m \left(\cancel{\int_{-\infty}^{+\infty} \varphi_n^* \varphi_m\,dx}^{\,0}\right) e^{\frac{i}{\hbar}(E_n-E_m)t}$$

$$\therefore \langle \mathcal{H} \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

Formalismo da MQ

$\rightarrow \int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{+\infty} \Psi^*(x,t)\,\Psi(x,t)\, dx = 1$

↳ Conjunto de funções de módulo quadrado integrável: $\int_a^b |f(x)|^2 dx < \infty$

$L_2(a,b)$

→ Espaço de Hilbert: espaço de funções munido de produto interno

→ Produto interno interessante para a MQ: $\langle f|g\rangle = \int_a^b f^*(x)\, g(x)\, dx$

a) $\langle c_1 f_1 + c_2 f_2 | f_3\rangle = c_1^* \langle f_1|f_3\rangle + c_2^* \langle f_2|f_3\rangle$

$$\begin{aligned}\langle c_1 f_1 + c_2 f_2 | f_3\rangle &= \int_a^b (c_1 f_1 + c_2 f_2)^* f_3\, dx \\ &= \int_a^b (c_1^* f_1^* + c_2^* f_2^*) f_3\, dx \\ &= c_1^* \int_a^b f_1^* f_3\, dx + c_2^* \int_a^b f_2^* f_3\, dx \\ &= c_1^* \langle f_1|f_3\rangle + c_2^* \langle f_2|f_3\rangle\end{aligned}$$

b) $\langle f_1 | c_2 f_2 + c_3 f_3\rangle = c_2 \langle f_1|f_2\rangle + c_3 \langle f_1|f_3\rangle$

c) $\langle f|g\rangle^* = \langle g|f\rangle$

$$\begin{aligned}\langle f|g\rangle^* &= \left[\int_a^b f^*(x)\, g(x)\, dx\right]^* \\ &= \int_a^b [f^*(x) g(x)]^* dx \\ &= \int_a^b f(x)\, g^*(x)\, dx \\ &= \int_a^b g^*(x)\, f(x)\, dx \\ &= \langle g|f\rangle\end{aligned}$$

d) $\langle f|f\rangle = \|f\|^2 \geq 0$

$$\begin{aligned}\langle f|f\rangle &= \int_a^b f^*(x)\, f(x)\, dx \\ &= \int_a^b |f(x)|^2 dx \\ &= \|f\|^2 \geq 0\end{aligned}$$

• **Obs.:** O espaço L_2 é um particular espaço de Hilbert muito interessante p/ MQ:

$$\left| \int_a^b f^*(x)\, g(x)\, dx \right| \leq \sqrt{\int_a^b |f(x)|^2 dx \int_a^b |g(x)|^2 dx}$$

$$|\langle f|g\rangle| \leq \sqrt{\langle f|f\rangle \langle g|g\rangle} \rightarrow \text{Desigualdade de Cauchy-Schwartz}$$

$$\rightarrow 0 \leq \|f - \lambda g\|^2 = \langle f-\lambda g | f - \lambda g\rangle$$
$$= \int_a^b (f-\lambda g)^* (f - \lambda g)\, dx$$
$$= \int_a^b (f^* - \lambda^* g^*)(f - \lambda g)\, dx$$
$$= \int_a^b f^* f\, dx - \lambda \int_a^b f^* g\, dx - \lambda^* \int_a^b g^* f\, dx + \lambda^* \lambda \int_a^b g^* g\, dx$$

$$\Rightarrow \langle f|f\rangle - \lambda \langle f|g\rangle - \lambda^* \langle g|f\rangle + |\lambda|^2 \langle g|g\rangle \geq 0$$

$\rightarrow$ Escolho um λ que satisfaça $\lambda = \dfrac{\langle g|f\rangle}{\langle g|g\rangle}$, $\lambda^* = \dfrac{\langle f|g\rangle}{\langle g|g\rangle}$

$$\rightarrow \langle f|f\rangle - \frac{\langle g|f\rangle}{\cancel{\langle g|g\rangle}} \langle f|g\rangle - \frac{\langle f|g\rangle}{\cancel{\langle g|g\rangle}} \langle g|f\rangle + \frac{\langle g|f\rangle \langle f|g\rangle}{\langle g|g\rangle^{\cancel{2}}} \cancel{\langle g|g\rangle} \geq 0$$

$$\Rightarrow \langle f|f\rangle - \frac{2|\langle f|g\rangle|^2}{\langle g|g\rangle} + \frac{|\langle f|g\rangle|^2}{\langle g|g\rangle} \geq 0$$

$$\langle f|f\rangle - \frac{|\langle f|g\rangle|^2}{\langle g|g\rangle} \geq 0$$

$$\therefore \boxed{|\langle f|g\rangle|^2 \leq \langle f|f\rangle \langle g|g\rangle}$$

* Observáveis físicos $\rightarrow \mathbb{R} \rightarrow$ operadores hermitianos

12/07/23

→ Um fato que observamos no caso do poço de potencial infinito:

$$\langle \varphi_n | \varphi_m \rangle = \delta_{n,m} = \begin{cases} 1, & n = m \\ 0, & n \neq m \end{cases}$$

→ Independente do tempo: $H\varphi = E\varphi$

$$H = -\frac{\hbar^2}{2m} + V(x) \qquad V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{senão} \end{cases}$$

$$\varphi_n(x) = \sqrt{\frac{2}{L}}\,\text{sen}\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, \ldots$$

$$E_n = \frac{\pi^2 \hbar^2}{2mL^2} n^2, \quad n = 1, 2, \ldots$$

→ As nossas autofunções formam um conjunto ortonormal

→ Espaço de Hilbert da MQ: $\langle \varphi | \psi \rangle = \int_{-\infty}^{+\infty} \varphi^*(x)\,\psi(x)\,dx$

$$\langle \varphi | \varphi \rangle = \int_{-\infty}^{+\infty} \varphi^*(x)\,\varphi(x)\,dx = \int_{-\infty}^{+\infty} |\varphi(x)|^2\,dx < \infty$$

→ $\psi(x,t) = \sum_{n=1}^{\infty} c_n \varphi_n(x) e^{-i\frac{E_n}{\hbar}t}$ → evolução temporal

⇒ $\psi(x,0) = \sum_{n=1}^{\infty} c_n \varphi_n(x)$ → estamos dizendo que $\{\varphi_n(x)\}_{n=1}^{\infty}$ forma um conjunto completo: qualquer função de onda será uma combinação linear somente das funções do espaço

→ Por que conjuntos ortonormais?

$$\langle \hat{O} \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t)\, \hat{O}\, \psi(x,t)\, dx = \langle \psi | \hat{O} \psi \rangle$$

$$\langle \hat{O} \rangle^* = \left(\int_{-\infty}^{+\infty} \psi^*(x,t)\, \overbrace{\hat{O}\, \psi(x,t)}^{\psi'}\, dx \right)^* = \int_{-\infty}^{+\infty} \psi(x,t) \left(\hat{O}\psi(x,t)\right)^* dx$$

$$= \int_{-\infty}^{+\infty} (\hat{O}\psi)^* \psi\, dx$$

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

hipótese

→ Definição: $\left.\begin{array}{l} \langle \psi | \hat{O}\psi \rangle = \langle \hat{O}\psi | \psi \rangle \\ \langle \hat{O} \rangle^* = \langle O \rangle \end{array}\right\}$ se isso é verdade, então $\hat{O}$ é chamado de hermitiano ou autoadjunto

→ No caso geral, se $\langle \varphi | \hat{O} \psi \rangle = \langle \hat{O}\varphi | \psi \rangle$, dizemos que o operador $\hat{O}$ é hermitiano (as funções de onda podem ser diferentes)

$$\int \varphi^* \hat{O} \psi\, dx = \int (\hat{O}\varphi)^* \psi\, dx$$

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

→ Obs.: Chamamos de conjugado hermitiano do operador $\hat{O}$ o operador $\hat{O}^\dagger$ que faz a seguinte operação:

$$\langle \psi_1 | \hat{O} \psi_2 \rangle = \langle \hat{O}^\dagger \psi_1 | \psi_2 \rangle$$ → adjunta

se $\hat{O} = \hat{O}^\dagger$ então $\hat{O}$ é hermitiano → autoadjunta

$\rightarrow (\hat{O}^\dagger)^\dagger = ?$

$$\langle (\hat{O}^\dagger)^\dagger \psi_1 | \psi_2 \rangle = \langle \psi_1 | \hat{O}^\dagger \psi_2 \rangle$$
$$= \langle \hat{O}^\dagger \psi_2 | \psi_1 \rangle^*$$
$$= \langle \psi_2 | \hat{O} \psi_1 \rangle^*$$
$$= \left(\int \psi_2^* \hat{O} \psi_1 \, dx \right)^*$$
$$= \int \psi_2 \hat{O} \psi_1^* \, dx$$
$$= \langle \hat{O} \psi_1 | \psi_2 \rangle$$

$\therefore \boxed{(\hat{O}^\dagger)^\dagger = \hat{O}}$

Mostramos na aula anterior:

$$\langle \varphi | \psi \rangle^* = \left(\int \varphi^* \psi \, dx \right)^*$$
$$= \int \varphi \psi^* dx$$
$$= \int \psi^* \varphi \, dx$$
$$= \langle \psi | \varphi \rangle$$

{ Operador conjugado hermitiano $\leftrightarrow$ operador adjunto
Operador hermitiano $\leftrightarrow$ operador autoadjunto

$\rightarrow$ Obs.: $\hat{p} = -i\hbar \frac{\partial}{\partial x}$ é hermitiano?

$$\langle \psi_1 | \hat{p} \psi_2 \rangle = \int_{-\infty}^{+\infty} \psi_1^* \left(-i\hbar \frac{\partial \psi_2}{\partial x} \right) dx$$
$$= -i\hbar \int_{-\infty}^{+\infty} \psi_1^* \frac{\partial \psi_2}{\partial x} dx$$
$$= -i\hbar \left[\psi_1^* \psi_2 \Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \psi_2 \frac{\partial \psi_1^*}{\partial x} dx \right]$$
$$= i\hbar \int_{-\infty}^{+\infty} \psi_2 \frac{\partial \psi_1^*}{\partial x} dx$$
$$= \int_{-\infty}^{+\infty} \left(-i\hbar \frac{\partial \psi_1}{\partial x} \right)^* \psi_2 \, dx$$
$$= \int_{-\infty}^{+\infty} (\hat{p} \psi_1)^* \psi_2 \, dx$$
$$= \langle \hat{p} \psi_1 | \psi_2 \rangle$$

$\therefore \langle \psi_1 | \hat{p} \psi_2 \rangle = \langle \hat{p} \psi_1 | \psi_2 \rangle \rightarrow \hat{p}$ é hermitiano

→ Autovalores de operadores hermitianos:

→ Seja A um operador hermitiano: $\langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle$, $A\psi = a\psi$

$$\begin{cases} \langle A\psi|\psi\rangle = \int (A\psi)^* \psi \, dx = \int (a\psi)^* \psi \, dx = a^* \int \psi^* \psi \, dx \\ \langle \psi|A\psi\rangle = \int \psi^* A\psi \, dx = a \int \psi^* \psi \, dx \end{cases}$$

→ Se A é hermitiano, então $a = a^*$; logo, $a \in \mathbb{R}$

→ Autofunções associadas a autovalores distintos:

→ Se A é hermitiano e $A\psi_1 = \lambda_1 \psi_1$, $A\psi_2 = \lambda_2 \psi_2$,

$$\langle A\psi_1|\psi_2\rangle = \int (\lambda_1 \psi_1)^* \psi_2 \, dx = \lambda_1^* \int \psi_1^* \psi_2 \, dx = \lambda_1^* \langle \psi_1|\psi_2\rangle$$
$$\langle \psi_1|A\psi_2\rangle = \int \psi_1^* A\psi_2 \, dx = \lambda_2 \int \psi_1^* \psi_2 \, dx = \lambda_2 \langle \psi_1|\psi_2\rangle$$

→ $\langle A\psi_1|\psi_2\rangle = \langle \psi_1|A\psi_2\rangle \Rightarrow \lambda_1^* \langle \psi_1|\psi_2\rangle = \lambda_2 \langle \psi_1|\psi_2\rangle$

$$(\lambda_1^* - \lambda_2)\langle \psi_1|\psi_2\rangle = 0$$

Se $\lambda_1 \neq \lambda_2 \Rightarrow \lambda_1^* - \lambda_2 \neq 0$

$\therefore \langle \psi_1|\psi_2\rangle = 0$ → autofunções são ortogonais

→ Aplicando a Desigualdade de Cauchy:

$\rightarrow \langle O \rangle = \int \psi^* \hat{O} \psi \, dx = \langle \psi | \hat{O} \psi \rangle$

→ Desvio padrão de um operador:

$$\sigma_{\hat{O}}^2 = \langle (\hat{O} - \langle O \rangle)^2 \rangle$$
$$= \langle \psi | (\hat{O} - \langle O \rangle)^2 \psi \rangle$$
$$= \langle \psi | (\hat{O}^2 - 2\langle O \rangle \hat{O} + \langle O \rangle^2) \psi \rangle$$
$$= \langle \psi | \hat{O}^2 \psi \rangle - 2\langle O \rangle \langle \psi | \hat{O} \psi \rangle + \langle O \rangle^2 \langle \psi | \psi \rangle$$
$$= \langle O^2 \rangle - 2\langle O \rangle \langle O \rangle + \langle O \rangle^2$$
$$= \langle O^2 \rangle - \langle O \rangle^2 \;//$$

→ Obs: Se $\hat{O}$ é hermitiano, $\hat{O} - \underbrace{\langle O \rangle}_{\text{operador constante}}$ é hermitiano também

$$\Rightarrow \sigma_{\hat{O}}^2 = \langle \psi | (O - \langle O \rangle)^2 \psi \rangle = \langle (O - \langle O \rangle) \psi | (O - \langle O \rangle) \psi \rangle$$

→ Para quaisquer dois operadores:

$$\sigma_{\hat{A}}^2 = \langle (A - \langle A \rangle) \psi | (A - \langle A \rangle) \psi \rangle$$
$$\sigma_{\hat{B}}^2 = \langle (B - \langle B \rangle) \psi | (B - \langle B \rangle) \psi \rangle$$

$$\rightarrow \left.\begin{aligned} \varphi &= (A - \langle A \rangle)\psi \\ \phi &= (B - \langle B \rangle)\psi \end{aligned}\right\} \quad \sigma_{\hat{A}}^2 \sigma_{\hat{B}}^2 = \langle \varphi | \varphi \rangle \langle \phi | \phi \rangle \geq |\langle \varphi | \phi \rangle|^2$$

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

$\rightarrow |\langle\varphi|\phi\rangle|^2 \geq \left(\dfrac{\langle\varphi|\phi\rangle - \langle\varphi|\phi\rangle^*}{2i}\right)^2$

A e A-⟨A⟩ são hermitianos

$\rightarrow \langle\varphi|\phi\rangle = \langle(A-\langle A\rangle)\psi|(B-\langle B\rangle)\psi\rangle$

$= \langle\psi|[(A-\langle A\rangle)(B-\langle B\rangle)]\psi\rangle$

$= \langle\psi|(AB)\psi\rangle - \langle B\rangle\langle\psi|A\psi\rangle - \langle A\rangle\langle\psi|B\psi\rangle + \langle A\rangle\langle B\rangle\overbrace{\langle\psi|\psi\rangle}^{1}$

$= \langle AB\rangle - \langle B\rangle\langle A\rangle - \cancel{\langle A\rangle\langle B\rangle} + \cancel{\langle A\rangle\langle B\rangle}$

$= \langle AB\rangle - \langle A\rangle\langle B\rangle$

$\rightarrow \langle\phi|\psi\rangle = \langle BA\rangle - \langle B\rangle\langle A\rangle$

$\Rightarrow \sigma_A^2\sigma_B^2 \geq \left(\dfrac{\langle AB\rangle - \langle A\rangle\langle B\rangle - \langle BA\rangle + \langle B\rangle\langle A\rangle}{2i}\right)^2$

$= \left(\dfrac{\langle AB\rangle - \langle BA\rangle}{2i}\right)^2$

$= \left(\dfrac{\langle AB - BA\rangle}{2i}\right)^2$

→ Definimos $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ como o comutador entre os operadores $\hat{A}$ e $\hat{B}$.

↳ se $[\hat{A},\hat{B}] = 0 \rightarrow \hat{A}$ e $\hat{B}$ comutam

→ Logo, $\sigma_A^2\sigma_B^2 \geq \left(\dfrac{\langle[\hat{A},\hat{B}]\rangle}{2i}\right)^2$

→ Ex.: $\hat{A} = \hat{x}$

$\hat{B} = \hat{p} = -i\hbar\, \partial/\partial x$

$$\langle \psi | [\hat{x}, \hat{p}] \psi \rangle = \int \psi^* \hat{x}\hat{p}\,\psi\, dx - \int \psi^* \hat{p}\hat{x}\,\psi\, dx$$
$$= -i\hbar \int \psi^* x \frac{\partial \psi}{\partial x} dx + i\hbar \int \psi^* \frac{\partial}{\partial x}(x\psi)\, dx$$
$$= -i\hbar \int \psi^* x \frac{\partial \psi}{\partial x} dx + i\hbar \int \psi^* \left(\psi + x \frac{\partial \psi}{\partial x}\right) dx$$
$$= \cancel{-i\hbar \int \psi^* x \frac{\partial \psi}{\partial x} dx} + i\hbar \int \psi^* \psi\, dx \cancel{+ i\hbar \int \psi^* x \frac{\partial \psi}{\partial x} dx}$$
$$= \int \psi^* (i\hbar) \psi\, dx$$

$$\langle \psi | [\hat{x}, \hat{p}] \psi \rangle = \langle \psi | i\hbar \psi \rangle$$

$$\therefore \boxed{[\hat{x}, \hat{p}] = i\hbar}$$

→ Regra prática: $\hat{x}\hat{p}\psi = -i\hbar\, x \frac{\partial}{\partial x}\psi$

$\hat{p}\hat{x}\psi = -i\hbar \frac{\partial}{\partial x}(x\psi) = -i\hbar\psi - i\hbar\, x \frac{\partial \psi}{\partial x}$

$\Rightarrow (\hat{x}\hat{p} - \hat{p}\hat{x})\psi = i\hbar\psi$

$[\hat{x}, \hat{p}] = i\hbar$

→ Princípio da incerteza: $\sigma_x^2 \sigma_p^2 \geq \left(\frac{i\hbar}{2i}\right)^2$

$$\boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}}$$

14/07/23

Partícula livre

→ $V(x) = 0, \quad -\infty < x < \infty$

→ A equação de Schrödinger independente do tempo:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial x^2} = E\varphi \Rightarrow \frac{\partial^2\varphi}{\partial x^2} + \frac{2mE}{\hbar^2} = 0 \Rightarrow \frac{\partial^2\varphi}{\partial x^2} + k^2\varphi = 0$$

$$\therefore \varphi(x) = Ae^{ikx} + Be^{-ikx}, \quad E_k = \frac{\hbar^2}{2m}k^2$$

→ Sabemos que a parte temporal agrega $e^{-i\frac{E}{\hbar}t}$. Logo, a solução geral é

$$\Psi_k(x,t) = Ae^{i(kx - \frac{E_k}{\hbar}t)} + Be^{-i(kx + \frac{E_k}{\hbar}t)}$$
$$= Ae^{ik(x - \underbrace{\frac{\hbar k}{2m}}_{v}t)} + Be^{-ik(x + \underbrace{\frac{\hbar k}{2m}}_{v}t)}$$
$$\therefore \Psi_k(x,t) = Ae^{ik(x-vt)} + Be^{-ik(x+vt)}$$

→ Ou, de maneira mais geral, com $k = \pm\sqrt{\frac{2mE}{\hbar^2}}$,

$$\boxed{\Psi_k(x,t) = A_k e^{ik(x - \frac{\hbar k}{2m}t)}}$$

→ Normalizando: $\int_{-\infty}^{+\infty} \Psi_k^*(x,t)\,\Psi_k(x,t)\,dx = 1$

$$A_k^* A_k \int_{-\infty}^{+\infty} dx = 1$$
$$|A_k|^2\,\infty = 1\ ?$$

↳ Estado físico não normalizável porque k é livre.
Devemos considerar uma superposição de ks

→ Suponha $\psi(x,t) \approx \sum_{j=1}^{\infty} c_{k_j} \psi_k(x,t)$, $k_j = j\Delta k$

$$\Rightarrow \psi(x,t) \approx \sum_{j=1}^{\infty} \frac{c_{k_j}}{\Delta k} \psi_{k_j}(x,t)\, \Delta k$$

→ No limite $\Delta k \to 0$:

$$\lim_{\Delta k \to 0} \frac{c_{k_j}}{\Delta k} = \frac{1}{\sqrt{2\pi}} \phi(k)$$

$$\lim_{\Delta k \to 0} \psi(x,t) = \lim_{\Delta k \to 0} \sum_{j=1}^{\infty} \frac{c_{k_j}}{\Delta k} \psi_{k_j}(x,t)\, \Delta k = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \phi(k)\, \psi_k(x,t)\, dk$$

→ Logo: $\boxed{\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, \psi_k(x,t)\, dk}$ } Pacote de onda

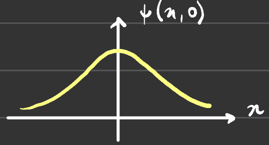
→ No caso discreto: $\psi(x,t) = \sum_{n=1}^{\infty} c_n \varphi_n(x)\, e^{-i\frac{E_n}{\hbar}t}$

→ Se temos uma condição inicial:

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, \psi_k(x,0)\, dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, dx$$

→ Logo, $\psi(x,0) = \mathcal{F}^{-1}[\phi(k)] \Rightarrow \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x,0)\, e^{-ikx}\, dx = \mathcal{F}[\psi(x,0)]$

→ Exemplo: $\psi(x,0) = Ae^{-\alpha x^2}$, $-\infty < x < \infty$ → pacote gaussiano



Normalização: $\int_{-\infty}^{+\infty} \psi^*(x,0)\,\psi(x,0)\,dx = \int_{-\infty}^{+\infty} A^* e^{-\alpha x^2} A e^{-\alpha x^2} dx = |A|^2 \int_{-\infty}^{+\infty} e^{-2\alpha x^2} dx = 1$

$$\int_{-\infty}^{+\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{a}} \Rightarrow \int_{-\infty}^{+\infty} e^{-2\alpha x^2} dx = \sqrt{\frac{\pi}{2a}}$$

$$\Rightarrow |A|^2 \sqrt{\frac{\pi}{2a}} = 1 \Rightarrow A = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}}$$

$$\rightarrow \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2} e^{-ikx} dx$$

$$= \frac{1}{\sqrt{2\pi}} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \int_{-\infty}^{+\infty} e^{-ax^2} e^{-ikx} dx$$

$$\hookrightarrow \int_{-\infty}^{+\infty} e^{-(\sqrt{\alpha}\,x + b)^2} dx = \sqrt{\frac{\pi}{\alpha}}$$

$$\hookrightarrow -ax^2 - ikx + c = -(\sqrt{\alpha}\,x + b)^2$$

$$-\cancel{\alpha x^2} \underline{-ikx} = -\cancel{\alpha x^2} \underline{-2b\sqrt{\alpha}\,x} \underbrace{-b^2 - c}_{=0}$$

$$\begin{cases} -ik = -2b\sqrt{\alpha} \Rightarrow b = \dfrac{ik}{2\sqrt{a}} \\ -b^2 - c = 0 \Rightarrow -c = b^2 \Rightarrow -c = -\dfrac{k^2}{4\alpha} \end{cases}$$

$$\hookrightarrow \text{Truque: } \int_{-\infty}^{+\infty} e^{-\alpha x^2 + \beta x} dx = \int_{-\infty}^{+\infty} e^{-(\sqrt{\alpha}\,x + b)^2 - c} dx = e^{-c} \int_{-\infty}^{+\infty} e^{-(\sqrt{\alpha}\,x + b)^2} dx = e^{-c}\sqrt{\frac{\pi}{\alpha}}$$

↳ escrever b e c em função de α e β

$$\Rightarrow \int_{-\infty}^{+\infty} e^{-\alpha x^2 - ikx}\, dx = \sqrt{\frac{\pi}{\alpha}}\, e^{-\frac{k^2}{4\alpha}}$$

$$\Rightarrow \phi(k) = \frac{1}{\sqrt{2\pi}} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{\pi}{\alpha}}\, e^{-\frac{k^2}{4\alpha}} = \frac{2^{\frac{1}{4}}\alpha^{\frac{1}{4}}}{2^{\frac{1}{2}}\pi^{\frac{1}{4}}\alpha^{\frac{1}{2}}}\, e^{-\frac{k^2}{4\alpha}} = \frac{1}{2^{\frac{1}{4}}\alpha^{\frac{1}{4}}\pi^{\frac{1}{4}}}\, e^{-\frac{k^2}{4\alpha}}$$

$$\therefore \boxed{\phi(k) = \frac{1}{(2\pi\alpha)^{\frac{1}{4}}}\, e^{-\frac{k^2}{4\alpha}}}$$

→ O pacote de onda: $\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{e^{-k^2/4\alpha}}{(2\pi\alpha)^{\frac{1}{4}}}\, e^{ikx - i\frac{\hbar k^2}{2m}t}\, dk$

↳ $\psi_k(x,t) = e^{ik\left(x - \frac{\hbar k}{2m}t\right)}$

$$\rightarrow \psi(x,t) = \frac{1}{\sqrt{2\pi}\,(2\pi\alpha)^{\frac{1}{4}}} \int_{-\infty}^{+\infty} e^{-\underbrace{\left(\frac{1}{4\alpha} + \frac{i\hbar}{2m}t\right)}_{\beta} k^2 + ikx}\, dk$$

$$= \frac{1}{(2\pi)^{\frac{3}{4}}\alpha^{\frac{1}{4}}} \int_{-\infty}^{+\infty} e^{-\beta k^2 + ikx}\, dk, \quad \text{onde } \beta = \frac{1}{4\alpha} + \frac{i\hbar}{2m}t$$

$$\rightarrow -(\sqrt{\beta}k + b)^2 + C = -\beta k^2 + ikx$$

$$\cancel{-\beta k^2} \underbrace{-2\sqrt{\beta}bk} \underbrace{-b^2 + C} = \cancel{-\beta k^2} + \underbrace{ik}x$$

$$\begin{cases} -2\sqrt{\beta}b = ix \Rightarrow b = -\frac{ix}{2\sqrt{\beta}} \\ c = b^2 = \frac{-x^2}{4\beta} \end{cases}$$

$$\Rightarrow I = \int_{-\infty}^{+\infty} e^{-(\sqrt{\beta}k+b)^2 + c}\, dk = e^c \int_{-\infty}^{+\infty} e^{-(\sqrt{\beta}k+b)^2}\, dk = e^c\sqrt{\frac{\pi}{\beta}} = \sqrt{\frac{\pi}{\beta}}\, e^{-\frac{x^2}{4\beta}}$$

→ Assim,

$$\psi(x,t) = \frac{1}{(2\pi)^{\frac{3}{4}}\alpha^{\frac{1}{4}}} e^{-\frac{x^2}{4\beta}} \frac{\sqrt{\pi}}{\sqrt{\beta}} = \frac{1}{(8\pi\alpha)^{\frac{1}{4}}} \frac{1}{\sqrt{\beta}} e^{-\frac{x^2}{4\beta}}$$

$$= \frac{1}{(8\pi\alpha)^{\frac{1}{4}}} \frac{1}{\sqrt{\frac{1}{4\alpha} + \frac{i\hbar}{2m}t}} \exp\left(\frac{-x^2}{4\left(\frac{1}{4\alpha} + \frac{i\hbar}{2m}t\right)}\right)$$

$$= \frac{1}{(8\pi\alpha)^{\frac{1}{4}}} \frac{2\sqrt{\alpha}}{\sqrt{1+\frac{2\alpha i\hbar}{m}t}} \exp\left(\frac{-x^2}{\frac{1}{\alpha} + \frac{2i\hbar}{m}t}\right)$$

→ Logo, o pacote gaussiano é $\boxed{\psi(x,t) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{1+\frac{2\alpha i\hbar}{m}t}} \exp\left(\frac{-\alpha x^2}{1+\frac{2i\hbar}{m}\alpha t}\right)}$

↳ Condição inicial gaussiana ⟶ pacote gaussiano

17/07/23

→ $-\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial x^2} = E\varphi$

→ $\varphi(x) = Ae^{ikx}$, $\quad k = \pm\sqrt{\frac{2mE}{\hbar^2}}$, $\quad E = \frac{\hbar^2 k^2}{2m}$

→ Juntando a evolução temporal: $\Psi_k(x,t) = Ae^{ikx}e^{-i\frac{E}{\hbar}t}$

$$\Psi_k(x,t) = Ae^{ikx - i\frac{\hbar k^2}{2m}t}$$

$$\Psi_k(x,t) = Ae^{ik\left(x - \frac{\hbar k}{2m}t\right)}$$

(separadamente não é interessante)

→ Se olharmos para uma "superposição":

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)\,\Psi_k(x,t)\,dk$$

pacote de onda

↳ Obs.: $\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)\,e^{ikx}\,dk = \mathcal{F}^{-1}[\phi(k)]$

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(x,0)\,e^{-ikx}\,dx = \mathcal{F}[\Psi(x,0)]$$

Distribuição dos ks: $\rho(k)\,dk = |\phi(k)|^2\,dk$ é a probabilidade de encontrar a partícula com momento entre $p = \hbar k$ e $p + dp = \hbar(k + dk)$

* Exemplo: $\psi(x,0) = Ae^{-\alpha x^2}, \quad -\infty < x < \infty$

- Normalizamos a função
- Calculamos o $\phi(k)$: $\phi(k) = \dfrac{1}{(2\pi\alpha)^{\frac{1}{4}}} e^{-k^2/4\alpha}$
- Calculamos: $\psi(x,t) = \dfrac{1}{\sqrt{2\pi}} \displaystyle\int_{-\infty}^{+\infty} \dfrac{1}{(2\pi\alpha)^{\frac{1}{4}}} e^{\frac{-k^2}{4\alpha}} e^{ik\left(x - \frac{\hbar k}{2m}t\right)} dk$

$$\psi(x,t) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \frac{e^{-\alpha x^2/\left(1+\frac{2\alpha\hbar}{m}it\right)}}{\sqrt{1+\frac{2\alpha\hbar}{m}it}}$$

$$\hookrightarrow \gamma = 1 + \frac{2\alpha\hbar}{m} t\, i = |\gamma| e^{i\varphi} = \sqrt{1 + \frac{4\alpha^2\hbar^2}{m^2} t^2}\, e^{i\varphi}, \quad \varphi = \arctan\left(\frac{2\alpha\hbar}{m} t\right)$$

$$\gamma^{\frac{1}{2}} = \left(1 + \frac{4\alpha^2\hbar^2}{m^2} t^2\right)^{\frac{1}{4}} e^{i\varphi/2}$$

$$\left(\gamma^{\frac{1}{2}}\right)^* = \left(1 + \frac{4\alpha^2\hbar^2}{m^2} t^2\right)^{\frac{1}{4}} e^{-i\varphi/2}$$

$$\gamma^{\frac{1}{2}}\left(\gamma^{\frac{1}{2}}\right)^* = w = \sqrt{1 + \frac{4\alpha^2\hbar^2}{m^2} t^2}$$

$$\rightarrow \exp\left(\frac{-\alpha x^2}{1+\frac{2\alpha\hbar}{m}it}\right) = \exp\left[-\alpha x^2 \frac{\left(1-\frac{2\alpha\hbar}{m}it\right)}{\underbrace{\left(1+\frac{4\alpha^2\hbar^2}{m^2}t^2\right)}_{w^2}}\right] = \exp\left(-\frac{\alpha x^2}{w^2}\right) \exp\left(\frac{\overbrace{\frac{2\alpha^2\hbar}{m} x^2 t}^{\theta}}{w^2} i\right)$$

$$= e^{-\frac{\alpha}{w^2}x^2 + i\theta}$$

$$\rightarrow |\psi|^2 = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}} \frac{\exp\left(-\frac{\alpha x^2}{w^2} - i\theta\right)}{(\gamma^{\frac{1}{2}})^*} \frac{\exp\left(-\frac{\alpha x^2}{w^2} + i\theta\right)}{\gamma^{\frac{1}{2}}} = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}} \frac{e^{-\frac{2\alpha}{w^2}x^2}}{w}$$

$$|\psi|^2 = \left(\frac{2\alpha}{\pi w^2}\right)^{\frac{1}{2}} e^{-\frac{2\alpha}{w^2}x^2} = \frac{1}{\sqrt{2\pi\sigma_x^2}} e^{-\frac{x^2}{2\sigma_x^2}}$$ } gaussiana de média $\mu = 0$ e variância σ_x^2

$$\rightarrow \frac{1}{2\sigma_x^2} = \frac{2\alpha}{w^2} \Rightarrow \sigma_x^2 = \frac{w^2}{4\alpha}$$

$$\frac{1}{\sqrt{2\pi\sigma_x^2}} = \frac{1}{\sqrt{2\pi\frac{w^2}{4\alpha}}} = \sqrt{\frac{2\alpha}{\pi w^2}}$$

$$\rightarrow \int_{-\infty}^{+\infty} |\psi|^2 dx = 1, \text{ pois } p(x) = \frac{1}{\sqrt{2\pi\sigma_x^2}} e^{-\frac{x^2}{2\sigma_x^2}} = N(0, \sigma_x^2)$$

$$\rightarrow \langle x \rangle = \int_{-\infty}^{+\infty} x \frac{1}{\sqrt{2\pi\sigma_x^2}} e^{-\frac{x^2}{2\sigma_x^2}} dx = \frac{1}{\sqrt{2\pi\sigma_x^2}} \int_{-\infty}^{+\infty} x e^{-\frac{x^2}{2\sigma_x^2}} dx = 0 //$$

$$\rightarrow \langle x^2 \rangle = \int_{-\infty}^{+\infty} \psi^* x^2 \psi dx = \int_{-\infty}^{+\infty} x^2 |\psi|^2 dx = \int_{-\infty}^{+\infty} x^2 p(x) dx = \frac{1}{\sqrt{2\pi\sigma_x^2}} \int_{-\infty}^{+\infty} x^2 e^{-\frac{x^2}{2\sigma_x^2}} dx$$

$$= \frac{1}{\sqrt{2\pi\sigma_x^2}} \left\{ -\frac{d}{da} \left[\underbrace{\int_{-\infty}^{+\infty} e^{-ax^2} dx}_{\sqrt{\frac{\pi}{a}},\ a = \frac{1}{2\sigma_x^2}} \right] \right\}$$

$$= \frac{1}{\sqrt{2\pi\sigma_x^2}} \frac{\sqrt{\pi}}{2a^{\frac{3}{2}}} = \frac{1}{\sqrt{2\pi\sigma_x^2}} \frac{\sqrt{\pi}}{2} (2\sigma_x^2)^{\frac{3}{2}} = \sigma_x^2$$

$$\Rightarrow \Delta x = \sigma_x$$

$$\rightarrow p(z) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(z-\mu)^2}{2\sigma^2}}$$

μ → valor esperado

σ^2 → variância

$$\rightarrow \langle z \rangle = \int_{-\infty}^{+\infty} z\, p(z)\, dz = \mu$$
$$\rightarrow \langle z^2 \rangle = \int_{-\infty}^{+\infty} z^2 p(z)\, dz = \sigma^2 + \mu^2$$

$$\left.\begin{matrix} \langle z \rangle = \mu \\ \langle z^2 \rangle = \sigma^2+\mu^2 \end{matrix}\right\} \langle z^2 \rangle - \langle z \rangle^2 = \sigma^2 + \mu^2 - \mu^2 = \sigma^2$$

→ Calculamos que $\langle x^2 \rangle - \langle x \rangle^2 = (\Delta x)^2 = \sigma_x^2 = \frac{w^2}{4a}$

$$\sigma_x^2 = \frac{1 + \frac{4a^2\hbar^2}{m}t^2}{4a} \Rightarrow \Delta x = \frac{1}{2\sqrt{a}}\left(1 + \frac{4a^2\hbar^2}{m^2}t^2\right)^{\frac{1}{2}}$$

↳ obs.: Não faça

$$\left\{\begin{matrix} \langle p \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x}\right) \psi(x,t)\, dx = 0 \\ \langle p^2 \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x}\right)^2 \psi(x,t)\, dx = \dots \end{matrix}\right\}$$

quando se tem $\phi(k)$:

$$\rightarrow p = \frac{h}{\lambda} = \frac{h}{2\pi}\,\frac{2\pi}{\lambda} = \hbar k$$

→ espaço k: $\phi(k)$ é a função de onda

$$\rightarrow \langle p \rangle = \int_{-\infty}^{+\infty} \phi^*(k)(\hbar k)\phi(k)\, dk = \frac{\hbar}{(2\pi a)^{\frac{1}{2}}} \int_{-\infty}^{+\infty} e^{-\frac{k^2}{4a}}\, k\, e^{-\frac{k^2}{4a}}\, dk = \frac{\hbar}{(2\pi a)^{\frac{1}{2}}} \int_{-\infty}^{+\infty} k e^{-\frac{k^2}{2a}}\, dk = 0$$

$$\rightarrow \langle p^2 \rangle = \int_{-\infty}^{+\infty} \phi^*(k)(\hbar k)^2 \phi(k)\, dk = \frac{\hbar^2}{(2\pi a)^{\frac{1}{2}}} \int_{-\infty}^{+\infty} k^2 e^{-\frac{k^2}{2a}}\, dk = \frac{\hbar^2}{(2\pi a)^{\frac{1}{2}}} \cdot \frac{1}{2} \frac{\sqrt{\pi}}{\left(\frac{1}{2a}\right)^{\frac{3}{2}}} = a\hbar^2$$

$$\Rightarrow \Delta p = \sqrt{a}\,\hbar$$

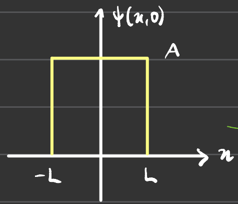
$$\to \Delta x \, \Delta p = \frac{1}{2\sqrt{\alpha}} \left(1 + \frac{4\alpha^2 \hbar^2}{m^2} t^2 \right) \sqrt{\alpha}\, \hbar$$

$$\Delta x \, \Delta p = \left(1 + \frac{4\alpha^2 \hbar^2}{m^2} t \right)^{\frac{1}{2}} \frac{\hbar}{2} \geq \frac{\hbar}{2}$$

↳ $\Delta x \, \Delta p = \hbar/2$ para $t = 0$

↳ Gaussiana se alarga com o tempo ($\Delta x \propto t \to$ "difusão")

* Ex. 2:



$$\psi(x,0) = \begin{cases} A, & -L < x < L \\ 0, & \text{senão} \end{cases} \to \text{partícula livre}$$

↳ pacote "constante"

• Normalização: $\int_{-\infty}^{+\infty} |\psi(x,0)|^2 dx = 1 \Rightarrow \int_{-L}^{+L} |A|^2 dx = 1 \Rightarrow |A|^2 \int_{-L}^{L} dx \Rightarrow A = \frac{1}{\sqrt{2L}}$

• Calculando $\phi(k)$: $\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x,0)\, e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{-L}^{L} \frac{1}{\sqrt{2L}} e^{-ikx} dx$

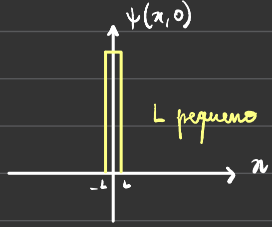
$$= \frac{1}{\sqrt{4\pi L}} \int_{-L}^{L} e^{-ikx} dx = \frac{1}{\sqrt{4\pi L}} \left. \frac{e^{-ikx}}{-ik} \right|_{-L}^{L} = \frac{1}{\sqrt{\pi L}} \frac{e^{-ikL} - e^{ikL}}{-2ik}$$

↳ $\text{sen}(kL) = \frac{e^{ikL} - e^{-ikL}}{2i} \Rightarrow \phi(k) = \frac{1}{\sqrt{\pi L}} \frac{\text{sen}(kL)}{k}$

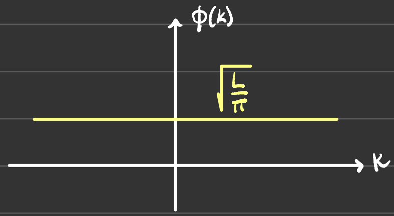
→ O pacote de onda: $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i\left(kx - \frac{k^2\hbar}{2m} t\right)} dk$

→ $|\Psi(x,t)|^2$: só numericamente

↳ Obs.: $L \ll 1$, $\operatorname{sen} kL \approx kL \Rightarrow \phi(k) = \frac{1}{\sqrt{\pi L}} \frac{kL}{k} = \sqrt{\frac{L}{\pi}}$.



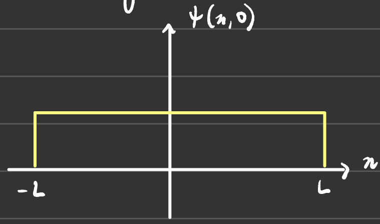
→



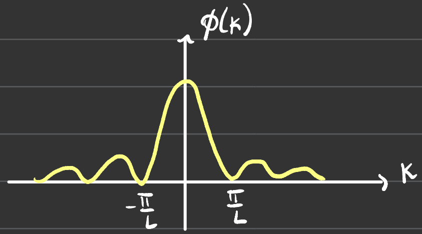
Localizado

Deslocalizado

L grande:



→



Deslocalizado

Localizado

19/07/23

→ O pacote de onda: $\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i\left(kx - \frac{k^2\hbar}{2m}t\right)}\, dk$ (1)

→ $\psi_k = A e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}$
$\psi_k = A e^{ik(x - vt)}$
$\Big\}\ v_{MQ} = \frac{\hbar k}{2m}$

→ Classicamente: $E = \frac{1}{2} m v_{MC}^2 \Rightarrow v_{MC} = \sqrt{\frac{2E}{m}}$

→ $v_{MQ} = \frac{\hbar}{2m} \cdot \frac{\sqrt{2mE}}{\hbar} = \sqrt{\frac{E}{2m}} \Rightarrow v_{MC} = 2 v_{MQ}$

→ a equação (1) pode ser escrita como:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i(kx - \omega t)}\, dk$$

{ hipótese não necessária, apenas para estudar esse caso

→ Vamos supor que o pacote esteja em torno de um k_0:

→ $\omega_k = \frac{\hbar k^2}{2m}$ → relação de dispersão

→ $\omega_k = \omega_k(k_0) + \left.\frac{d\omega_k}{dk}\right|_{k=k_0} (k-k_0) + \frac{1}{2} \left.\frac{d^2\omega_k}{dk^2}\right|_{k=k_0} (k-k_0)^2 + \dots$

$\Rightarrow \omega_k \approx \omega_0 + \omega_0' (k-k_0)$ (2)

→ Substituindo (2) em (1):

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i(kx - w_0 t - w_0'(k-k_0)t)}\, dk$$

→ Fazendo $k - k_0 = s$:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i[(k_0+s)x - w_0 t - w_0' s t \underset{+k_0 w_0' t - k_0 w_0' t}{}]}\, ds$$

$$= \frac{1}{\sqrt{2\pi}} e^{i(k_0 w_0' t - w_0 t)} \int_{-\infty}^{+\infty} \phi(s+k_0)\, e^{i[(k_0+s)x - (k_0+s) w_0' t]}\, ds$$

$$= \frac{1}{\sqrt{2\pi}} e^{i(k_0 w_0' t - w_0 t)} \int_{-\infty}^{+\infty} \phi(s+k_0)\, e^{i(k_0+s)(x - w_0' t)}\, ds$$

"shift" na posição

$$\therefore \psi(x,t) = \underbrace{e^{i(k_0 w_0' - w_0)t}}_{\text{"fase"}}\, \psi(x - w_0' t, 0)$$

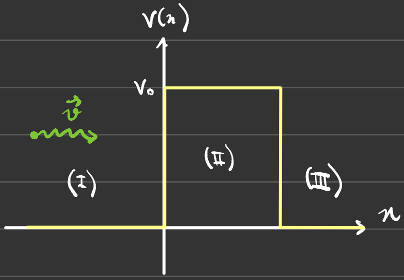
→ Observe: $\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx}\, dk$

→ $|\psi(x,t)|^2 = |\psi(x - w_0' t)|^2$

→ w_0' é a velocidade do pacote: $w_0' = \frac{dw_k}{dk} = \frac{d}{dk}\left(\frac{\hbar k^2}{2m}\right) = \frac{\hbar k}{m} = \frac{\hbar}{m} \frac{\sqrt{2mE}}{\hbar}$

$$\therefore w_0' = \sqrt{\frac{2E}{m}} = v_{MC} \quad //$$

Barreira de potencial e tunelamento



$$V_0 = \begin{cases} 0, & x < 0 \\ V_0, & 0 \leq x < L \\ 0, & x \geq L \end{cases}$$

* $E > V_0$:

Classicamente:

↳ $x < 0$: $\frac{p^2}{2m} + 0 = E \Rightarrow p = \sqrt{2mE} \Rightarrow v_1 = \sqrt{\frac{2E}{m}}$

↳ $0 \leq x < L$: $\frac{p^2}{2m} + V_0 = E \Rightarrow p^2 = 2m(E - V_0) \Rightarrow p = \sqrt{2m(E-V_0)} \Rightarrow v_2 = \sqrt{\frac{2(E-V_0)}{m}}$

↳ $x \geq L$: $v_3 = v_1$

Quanticamente:

↳ $x < 0$: $-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = E\varphi \Rightarrow \frac{d^2\varphi}{dx^2} + \frac{2mE}{\hbar^2}\varphi = 0 \Rightarrow \varphi_1(x) = Ae^{ikx} + Be^{-ikx}$, $k = \sqrt{\frac{2mE}{\hbar^2}}$

↳ $0 \leq x < L$: $-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + V_0\varphi = E\varphi \Rightarrow \frac{d^2\varphi}{dx^2} + \frac{2m(E-V_0)}{\hbar^2} = 0 \Rightarrow \varphi_2(x) = Ce^{iqx} + De^{-iqx}$

$q = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

↳ $x \geq L$: $\varphi_3(x) = Ee^{ikx} + Fe^{-ikx}$

* $E < V_0$:

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

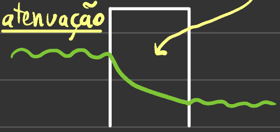
↳ $x < 0$: $-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = E\varphi \Rightarrow \frac{d^2\varphi}{dx^2} + \frac{2mE}{\hbar^2}\varphi = 0 \Rightarrow \varphi_1(x) = A_1 e^{ikx} + B_1 e^{-ikx} = \psi_I^{inc} \; \psi_I^{ref}$

↳ $0 \leq x \leq L$: $-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + V_0\varphi = E\varphi \Rightarrow \frac{d^2\varphi}{dx^2} + \frac{2m(E-V_0)}{\hbar^2}\varphi = 0$

$$q = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$\Rightarrow \frac{d^2\varphi}{dx^2} - \frac{2m}{\hbar^2}(V_0-E)\varphi = 0 \Rightarrow \frac{d^2\varphi}{dx^2} - q^2\varphi = 0 \Rightarrow \varphi_2(x) = A_2 e^{qx} + B_2 \underbrace{e^{-qx}}$

atenuação



↳ $x \geq L$: $\varphi_3(x) = A_3 e^{ikx} + \underbrace{B_3}_{=0} e^{-ikx}$

$=0 \rightarrow$ não há reflexão na região III

21/07/23

→ Para obter os coeficientes A_i e B_i, exigimos a continuidade da função de onda e da sua derivada

→ Continuidade em $x=0$:

↳ $\varphi_1(0) = \varphi_2(0) \Rightarrow A_1 + B_1 = A_2 + B_2 \quad (1)$

↳ $\dfrac{d\varphi_1}{dx} = ikA_1 e^{ikx} - ikB_1 e^{-ikx}$

$\dfrac{d\varphi_2}{dx} = qA_2 e^{qx} - qB_2 e^{-qx}$

$$\left.\frac{d\varphi_1}{dx}\right|_{x=0} = \left.\frac{d\varphi_2}{dx}\right|_{x=0}$$

$$ik(A_1 - B_1) = q(A_2 - B_2) \quad (2)$$

→ Continuidade em $x=L$:

↳ $\varphi_2(L) = \varphi_3(L) \Rightarrow A_2 e^{qL} + B_2 e^{-qL} = A_3 e^{ikL} \quad (3)$

↳ $\dfrac{d\varphi_3}{dx} = ikA_3 e^{ikL} \rightarrow \left.\dfrac{d\varphi_2}{dx}\right|_{x=L} = \left.\dfrac{d\varphi_3}{dx}\right|_{x=L}$

$$q(A_2 e^{qL} - B_2 e^{-qL}) = ikA_3 e^{ikL} \quad (4)$$

→ Denotamos $\alpha = \dfrac{q}{k} > 0$ e $\gamma = A_3 e^{ikL} > 0$

$\rightarrow$ De (3) e (4):

$$A_2 e^{qL} + B_2 e^{-qL} = \sigma$$
$$A_2 e^{qL} - B_2 e^{-qL} = i\alpha^{-1}\sigma$$

$$2A_2 e^{qL} = (1+\alpha^{-1}i)\,\sigma \qquad\qquad 2B_2 e^{-qL}\,(1-\alpha^{-1}i)\,\sigma$$

$$A_2 = \frac{(1+\alpha^{-1}i)}{2}\sigma e^{-qL} \quad (5) \qquad\qquad B_2 = \frac{(1-\alpha^{-1}i)}{2}\sigma e^{qL} \quad (6)$$

$\rightarrow$ De (1), (5) e (6):

$$A_1 + B_1 = A_2 + B_2$$
$$= \frac{(1+\alpha^{-1}i)}{2}\sigma e^{-qL} + \frac{(1-\alpha^{-1}i)}{2}\sigma e^{qL}$$
$$= \frac{\sigma}{2}e^{-qL} + \frac{\alpha^{-1}\sigma e^{-qL}}{2}i + \frac{\sigma}{2}e^{qL} - \frac{\alpha^{-1}\sigma e^{qL}}{2}i$$
$$= \sigma\cosh(qL) - i\alpha^{-1}\sigma\,\text{senh}(qL)$$
$$\therefore A_1 + B_1 = \sigma\left[\cosh(qL) - i\alpha^{-1}\,\text{senh}(qL)\right] \quad (7)$$

$\rightarrow$ De (2), (5) e (6):

$$A_1 - B_1 = \frac{q}{ik}A_2 - \frac{q}{ik}B_2$$
$$= -i\alpha A_2 + i\alpha B_2$$
$$= -\alpha i\left(\frac{1+\alpha^{-1}i}{2}\sigma e^{-qL}\right) + \alpha i\left(\frac{1-\alpha^{-1}i}{2}\sigma e^{qL}\right)$$
$$= \frac{(1-\alpha i)}{2}\sigma e^{-qL} + \frac{(1+\alpha i)}{2}\sigma e^{qL}$$
$$= \sigma\frac{e^{qL}+e^{-qL}}{2} + \sigma\alpha i\,\frac{e^{qL}-e^{-qL}}{2}$$
$$= \sigma\cosh(qL) + \sigma\alpha i\,\text{senh}(qL)$$
$$\therefore A_1 - B_1 = \sigma\left[\cosh(qL) + \alpha i\,\text{senh}(qL)\right] \quad (8)$$

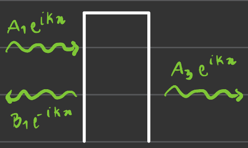
→ De (7) e (8):

$$A_1 + B_1 = \gamma\left[\cosh(qL) - i\alpha^{-1}\,\text{senh}(qL)\right]$$
$$A_1 - B_1 = \gamma\left[\cosh(qL) + i\alpha\,\text{senh}(qL)\right]$$
$$2A_1 = \gamma\left[2\cosh(qL) + i(\alpha - \alpha^{-1})\,\text{senh}(qL)\right]$$
$$\therefore A_1 = \gamma\left[\cosh(qL) + i\,\frac{(\alpha-\alpha^{-1})}{2}\,\text{senh}(qL)\right] \qquad (9)$$

e também,

$$2B_1 = -\gamma i(\alpha + \alpha^{-1})\,\text{senh}(qL)$$
$$\therefore B_1 = -i\gamma\,\frac{(\alpha+\alpha^{-1})}{2}\,\text{senh}(qL) \qquad (10)$$

→ Probabilidade → $|\psi|^2$



Definimos uma "probabilidade relativa":

$$T = \frac{|A_3 e^{ikx}|^2}{|A_1 e^{-ikx}|^2}$$

o que chamamos de coeficiente de transmissão:

$$T = \frac{|A_3|^2}{|A_1|^2}$$

→ De uma maneira mais geral, $T = \dfrac{|\psi_{trans}|^2}{|\psi_{inc}|^2}$

$$\hookrightarrow T = \frac{|\gamma|^2}{|\gamma|^2\left[\cosh^2(qL) + \frac{(\alpha-\alpha^{-1})^2}{4}\,\text{senh}^2(qL)\right]} \Rightarrow T = \frac{1}{\cosh^2(qL) + \frac{1}{4}(\alpha-\alpha^{-1})^2\,\text{senh}^2(qL)}$$

→ Analogamente, $R = \dfrac{|\psi_{ref}|^2}{|\psi_{inc}|^2}$

↳ $$R = \frac{|B_1 e^{-ikx}|^2}{|A_1 e^{ikx}|^2} = \frac{|B_1|^2}{|A_1|^2} = \frac{\frac{1}{4}|\sigma|^2(\alpha^{-1}+\alpha)^2 \operatorname{senh}^2(qL)}{|\sigma|^2\left[\cosh^2(qL) + \frac{1}{4}(\alpha-\alpha^{-1})^2\operatorname{senh}^2(qL)\right]}$$

$$R = \frac{\frac{1}{4}(\alpha+\alpha^{-1})^2\operatorname{senh}^2(qL)}{\cosh^2(qL) + \frac{1}{4}(\alpha-\alpha^{-1})^2\operatorname{senh}^2(qL)}$$

→ $\cosh^2(qL) - \operatorname{senh}^2(qL) = 1 \Rightarrow \operatorname{senh}^2(qL) = 1 + \cosh^2(qL)$

→ $z \equiv \cosh^2(qL) + \frac{1}{4}(\alpha-\alpha^{-1})^2\operatorname{senh}^2(qL)$

$$\begin{aligned}
z &= 1 + \operatorname{senh}^2(qL) + \tfrac{1}{4}(\alpha-\alpha^{-1})^2\operatorname{senh}^2(qL) \\
&= 1 + \left[1 + \tfrac{1}{4}(\alpha-\alpha^{-1})^2\right]\operatorname{senh}^2(qL) \\
&= 1 + \left[1 + \tfrac{1}{4}(\alpha^2 - 2 + \alpha^{-2})\right]\operatorname{senh}^2(qL) \\
&= 1 + \left[\tfrac{1}{4}(\alpha^2 + 2 + \alpha^{-2})\right]\operatorname{senh}^2(qL) \\
&= 1 + \tfrac{1}{4}(\alpha+\alpha^{-1})^2\operatorname{senh}^2(qL)
\end{aligned}$$

→ Reescrevendo: $$\left.\begin{aligned} T &= \frac{1}{z} \\ R &= \frac{z-1}{z} \end{aligned}\right\} \quad \boxed{T + R = 1}$$

→ $T = \dfrac{1}{1 + \frac{1}{4}\left(\frac{q}{k} + \frac{k}{q}\right)^2 \operatorname{senh}^2(qL)}$, $k = \sqrt{\dfrac{2mE}{\hbar^2}}$, $q = \sqrt{\dfrac{2m(V_0-E)}{\hbar^2}}$

→ $$\frac{q}{k} + \frac{k}{q} = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}\sqrt{\frac{\hbar^2}{2mE}} + \sqrt{\frac{2mE}{\hbar^2}}\sqrt{\frac{\hbar^2}{2m(V_0-E)}}$$

$$= \sqrt{\frac{V_0-E}{E}} + \sqrt{\frac{E}{V_0-E}}$$

$$\rightarrow \left(\frac{q}{k}+\frac{k}{q}\right)^2 = \frac{V_0-E}{E} + \frac{E}{V_0-E} + 2$$

$$= \frac{(V_0-E)^2+E^2}{E(V_0-E)} + \frac{2E(V_0-E)}{E(V_0-E)}$$

$$= \frac{V_0^2 - \cancel{2EV_0} + \cancel{E^2} + E^2 + \cancel{2EV_0} - \cancel{2E^2}}{E(V_0-E)}$$

$$\therefore \left(\frac{q}{k}+\frac{k}{q}\right)^2 = \frac{V_0^2}{E(V_0-E)}$$

→ Logo, em função dos parâmetros do problema,

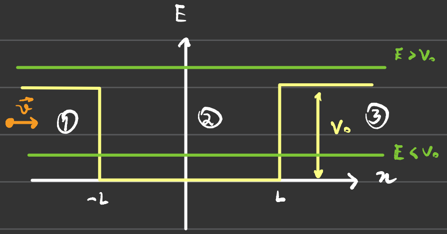
$$T = \frac{1}{1+\frac{V_0^2}{4E(V_0-E)}\,\mathrm{senh}^2\left(\sqrt{\frac{2m(V_0-E)}{\hbar^2}}\,L\right)}$$

→ Para $qL \gg 1$, $\mathrm{senh}^2(qL) = \frac{e^{qL}-e^{-qL}}{2} \approx \frac{e^{qL}}{2} \Rightarrow T \approx \frac{1}{1+\frac{V_0^2 e^{2qL}}{16E(V_0-E)}}$ $\gg 1$

$$\boxed{T \approx \frac{16E(V_0-E)}{V_0^2}\exp\left[-2\sqrt{\frac{2m}{\hbar^2}(V_0-E)}\,L\right]}$$

24/07/23

Poço finito



$$V(x) = \begin{cases} V_0, & x \leq -L \\ 0, & -L < x < L \\ V_0, & x \geq L \end{cases}$$

$*$ $E > V_0$:

↓

espalhamento

① $-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi}{\partial x^2} + V_0 \varphi = E\varphi \Rightarrow \varphi_1(x) = A_1 e^{ikx} + B_1 e^{-ikx}, \quad k = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

② $-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi}{\partial x^2} = E\varphi \Rightarrow \varphi_2(x) = A_2 e^{iqx} + B_2 e^{-iqx}, \quad q = \sqrt{\frac{2mE}{\hbar^2}}$

③ $-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi}{\partial x^2} + V_0 \varphi = E\varphi \Rightarrow \varphi_3(x) = A_3 e^{ikx}$

→ Continuidade de φ e $d\varphi/dx$ em $x = -L$:

$\varphi_1(-L) = \varphi_2(-L) \Rightarrow A_1 e^{-ikL} + B_1 e^{ikL} = A_2 e^{-iqL} + B_2 e^{iqL}$ (1)

$$\left.\begin{aligned} \frac{d\varphi_1}{dx} &= ik A_1 e^{ikx} - ik B_1 e^{-ikx} \\ \frac{d\varphi_2}{dx} &= iq A_2 e^{iqx} - iq B_2 e^{-iqx} \end{aligned}\right\}$$

$\varphi_1'(-L) = \varphi_2'(-L)$

$ik\left(A_1 e^{-ikL} - B_1 e^{ikL}\right) = iq\left(A_2 e^{-iqL} - B_2 e^{iqL}\right)$ (2)

→ Denotemos $\alpha = \frac{q}{k}$

$$\rightarrow \quad A_1 e^{-ikL} + B_1 e^{ikL} = A_2 e^{-iqL} + B_2 e^{iqL}$$

$$+ \quad A_1 e^{-ikL} - B_1 e^{ikL} = \alpha A_2 e^{-iqL} - \alpha B_2 e^{iqL}$$

$$2 A_1 e^{-ikL} = (1+\alpha) A_2 e^{-iqL} + (1-\alpha) B_2 e^{iqL}$$

$$A_1 e^{-ikL} = \frac{(1+\alpha)}{2} A_2 e^{-iqL} + \frac{(1-\alpha)}{2} B_2 e^{iqL} \quad (3)$$

→ subtraindo: $2 B_1 e^{ikL} = (1-\alpha) A_2 e^{-iqL} + (1+\alpha) B_2 e^{iqL}$

$$B_1 e^{ikL} = \frac{(1-\alpha)}{2} A_2 e^{-iqL} + \frac{(1+\alpha)}{2} B_2 e^{iqL} \quad (4)$$

→ Obs.:

$$\left.\begin{aligned} \psi_{inc} &= A_1 e^{ikx} \\ \psi_{ref} &= B_1 e^{-ikx} \\ \psi_{trans} &= A_3 e^{ikx} \end{aligned}\right\} \quad \begin{aligned} T &= \frac{|\psi_{trans}|^2}{|\psi_{inc}|^2} = \frac{|A_3|^2}{|A_1|^2} \\ R &= \frac{|\psi_{ref}|^2}{|\psi_{inc}|^2} = \frac{|B_1|^2}{|A_1|^2} \end{aligned}$$

→ continuidade de φ e φ' em $x = L$:

$$\varphi_2(L) = \varphi_3(L) \Rightarrow A_2 e^{iqL} + B_2 e^{-iqL} = \overbrace{A_3 e^{ikL}}^{\equiv \gamma}$$

$$\frac{d\varphi_3}{dx} = ik A_3 e^{ikx} \Rightarrow iq A_2 e^{iqL} - iq B_2 e^{-iqL} = ik A_3 e^{ikL}$$

$$A_2 e^{iqL} + B_2 e^{-iqL} = \gamma$$

$$+ \quad A_2 e^{iqL} - B_2 e^{-iqL} = \alpha^{-1} \gamma$$

$$2 A_2 e^{iqL} = (1+\alpha^{-1}) \gamma \qquad 2 B_2 e^{-iqL} = (1-\alpha^{-1}) \gamma$$

$$A_2 = \frac{(1+\alpha^{-1})}{2} \gamma e^{-iqL} \quad (5) \qquad B_2 = \frac{(1-\alpha^{-1})}{2} \gamma e^{iqL} \quad (6)$$

→ substituindo (5) e (6) em (3):

$$A_1 e^{-ikL} = \frac{(1+\alpha)}{2}\frac{(1+\alpha^{-1})}{2}\tau e^{-2iqL} + \frac{(1-\alpha)}{2}\frac{(1-\alpha^{-1})}{2}\tau e^{2iqL}$$

$$= \frac{(2+\alpha+\alpha^{-1})}{4}\tau e^{-2iqL} + \frac{(2-\alpha-\alpha^{-1})}{4}\tau e^{2iqL}$$

$$= \frac{1}{2}\tau\left(e^{-2iqL}+e^{2iqL}\right) + \frac{(\alpha+\alpha^{-1})}{4}\tau\left(e^{-2iqL}-e^{2iqL}\right)$$

$$= \tau\cos(2qL) + i\frac{(\alpha+\alpha^{-1})}{2}\tau \,\mathrm{sen}(2qL)$$

$$= \tau\left[\cos(2qL) - i\frac{(\alpha+\alpha^{-1})}{2}\mathrm{sen}(2qL)\right]$$

$$|A_2 e^{-ikL}|^2 = |A_1|^2 = |\tau|^2\left[\cos^2(2qL) + \frac{(\alpha+\alpha^{-1})^2}{4}\mathrm{sen}^2(2qL)\right]$$

$$= |\tau|^2\left[\cos^2(2qL) + \mathrm{sen}^2(2qL) - \mathrm{sen}^2(2qL) + \frac{(\alpha+\alpha^{-1})}{4}\mathrm{sen}^2(2qL)\right]$$

$$= |\tau^2|\left\{1+\left[\frac{(\alpha+\alpha^{-1})^2}{4}-1\right]\mathrm{sen}^2(2qL)\right\}$$

→ Definimos $\tau = A_3 e^{ikx}$

$|\tau| = |A_3||e^{ikx}| = |A_3|$

$$\Rightarrow |A_1|^2 = |A_3|^2\left\{1+\left[\frac{(\alpha+\alpha^{-1})^2}{4}-1\right]\mathrm{sen}^2(2qL)\right\} \quad (7)$$

$$\rightarrow T = \frac{|A_3|^2}{|A_1|^2} = \frac{1}{1 + \underbrace{\left[\frac{(\alpha+\alpha^{-1})^2}{4} - 1\right]}_{(*)} \operatorname{sen}^2(2qL)}$$

$$\rightarrow \alpha = \frac{q}{K}, \quad q = \sqrt{\frac{2mE}{\hbar^2}}, \quad k = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

$$\rightarrow (*) = \frac{\alpha^2 + \alpha^{-2} + 2}{4} - \frac{4}{4} = \frac{\alpha^2 + \alpha^{-2} - 2}{4} = \frac{1}{4}\left[\frac{E}{E-V_0} + \frac{E-V_0}{E} - 2\right]$$

$$= \frac{1}{4}\left[\frac{E^2}{E(E-V_0)} + \frac{(E-V_0)^2}{E(E-V_0)} - \frac{2E(E-V_0)}{E(E-V_0)}\right]$$

$$= \frac{1}{4}\left[\frac{\cancel{E^2} + \cancel{E^2} - \cancel{2EV_0} + V_0^2 - \cancel{2E^2} + \cancel{2EV_0}}{E(E-V_0)}\right]$$

$$= \frac{V_0^2}{4E(E-V_0)}$$

$$\Rightarrow T = \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)} \operatorname{sen}^2\left(\sqrt{\frac{8mE}{\hbar^2}}\, L\right)}$$

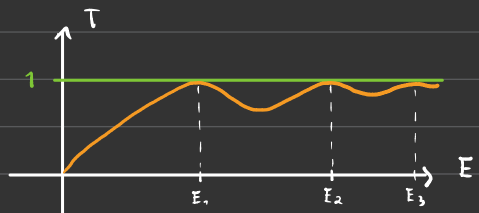
↳ Quando $T = 1$?

$$T = 1 \Rightarrow \operatorname{sen}^2\left(\sqrt{\frac{8mE}{\hbar^2}}\, L\right) = 0 \Rightarrow \sqrt{\frac{8mE}{\hbar^2}}\, L = n\pi, \quad n = 1, 2, 3, \dots$$

$$\frac{8mE}{\hbar^2} L^2 = n^2\pi^2$$

$$\therefore \boxed{E_n = \frac{\hbar^2\pi^2}{8mL^2} n^2}$$

→ energias do poço de potencial infinito $-L < x < L$



$\ast$ $E < V_0$: estados ligados

① $$-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi}{\partial x^2} + V_0\varphi = E\varphi$$

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\varphi = 0 \Rightarrow \frac{\partial^2 \varphi}{\partial x^2} - \overbrace{\frac{2m}{\hbar^2}(V_0 - E)}^{k>0}\varphi = 0$$

$$\varphi_1(x) = A_1 e^{kx} + \overbrace{B_1 e^{-kx}}^{\text{não é fisicamente aceitável}}$$

$$\varphi_1(x) = A_1 e^{kx}$$

② $$\varphi_2(x) = A_2 \operatorname{sen}(qx) + B_2\cos(qx), \quad q = \sqrt{\frac{2mE}{\hbar^2}}$$

Por simetria, $A_2 = 0 \Rightarrow \varphi_2(x) = B_2\cos(qx)$

③ $$\varphi_3(x) = \overbrace{A_3 e^{kx}}^{\text{não é fisicamente aceitável}} + B_3 e^{-kx} \Rightarrow \varphi_3(x) = B_3 e^{-kx}$$

$$\Rightarrow \begin{cases} \varphi_1(x) = A_1 e^{kx}, & x < -L \\ \varphi_2(x) = B_2\cos(qx), & -L < x < L \\ \varphi_3(x) = B_3 e^{-kx}, & x > L \end{cases}$$

→ Continuidade de φ e φ' em $x = L$:

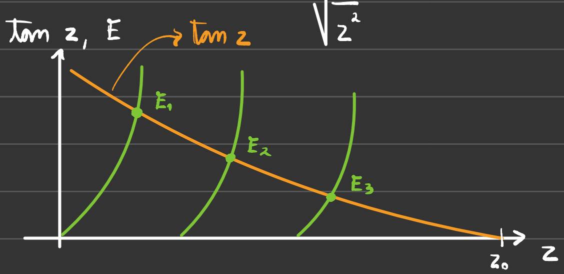
$$\varphi_2(L) = \varphi_3(L) \Rightarrow B_2 \cos(qL) = B_3 e^{-KL} \quad (8)$$

$$\left.\begin{aligned} \frac{d\varphi_2}{dx} &= -qB_2 \,\text{sen}(qx) \\ \frac{d\varphi_3}{dx} &= -KB_3 e^{-Kx} \end{aligned}\right\} \begin{aligned} -qB_2 \,\text{sen}(qL) &= -KB_3 e^{-KL} \\ qB_2 \,\text{sen}(qL) &= KB_3 e^{-KL} \quad (9) \end{aligned}$$

→ Dividindo (9) por (8):

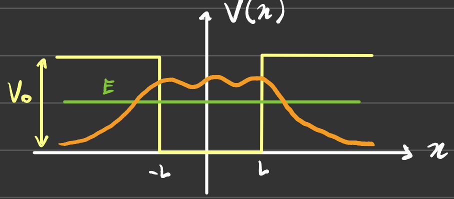
$$\left.\begin{aligned} &q \tan(qL) = K \Rightarrow \tan(qL) = \frac{K}{q} \\ &q = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow z \equiv qL = \sqrt{\frac{2mE}{\hbar^2}}\, L \end{aligned}\right\} \begin{aligned} \frac{K}{q} &= \frac{\sqrt{\frac{2m}{\hbar^2}(V_0 - E)}\, L}{\sqrt{\frac{2m}{\hbar^2} E}\, L}, \quad z_0 \equiv \sqrt{\frac{2mV_0}{\hbar^2}}\, L \\ &= \sqrt{\frac{z_0^2 - z^2}{z^2}} \\ &= \sqrt{\frac{z_0^2}{z^2} - 1} \end{aligned}$$

$$\therefore \tan z = \sqrt{\frac{z_0^2}{z^2} - 1} \quad (10)$$



26/07/23

Poço de potencial finito



$$V(x) = \begin{cases} V_0, & x < -L \\ 0, & -L < x < L \\ V_0, & x > L \end{cases}$$

* $E > V_0$: estados de espalhamento

* $E < V_0$: $-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi}{\partial x^2} + V_0\varphi = E\varphi$

↳ $x < -L$: $\frac{\partial^2\varphi}{\partial x^2} + \frac{2m(E-V_0)}{\hbar^2}\varphi = 0$

$\frac{\partial^2\varphi}{\partial x^2} - \frac{2m}{\hbar}(V_0 - E)\varphi = 0$

$\varphi_1(x) = Ae^{kx} + \cancel{Be^{-kx}}$, $k = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$

Solução fisicamente aceitável: $\varphi_1(x) = Ae^{kx}$

↳ $-L < x < L$: $\varphi_2(x) = \cancel{C\,\mathrm{sen}}(qx) + D\cos(qx)$, $q = \sqrt{\frac{2mE}{\hbar^2}}$

Por simetria: $\varphi_2(x) = D\cos(qx)$

↳ $x > L$: $\varphi_3(x) = \cancel{Ee^{kx}} + Fe^{-kx}$

Solução fisicamente aceitável: $\varphi_3(x) = Fe^{-kx}$

* Qual a probabilidade $\bar{P}$ da partícula estar na região proibida $x < -L$ ou $x > L$?

→ Pela continuidade de φ em $x = -L$ e $x = L$:

↳ $\varphi_1(-L) = \varphi_2(-L) \Rightarrow Ae^{-KL} = D\cos(qL) \quad (1)$

↳ $\varphi_2(L) = \varphi_3(L) \Rightarrow D\cos(qL) = Fe^{-KL} \quad (2)$

→ De (1) e (2): $A = De^{KL}\cos(qL) = F$

→ Assim, $\varphi(x) = \begin{cases} De^{KL}\cos(qL)\,e^{Kx}, & x < -L \\ D\cos(qx), & -L < x < L \\ De^{KL}\cos(qL)\,e^{-Kx}, & x > L \end{cases}$

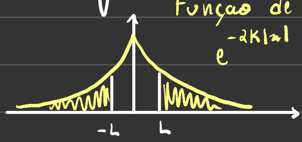
→ Normalizando: $\int_{-\infty}^{+\infty} \varphi^*(x)\varphi(x)\,dx = \int_{-\infty}^{-L} |D|^2 e^{2KL}\cos^2(qL)\,e^{2Kx}\,dx +$

$+ \int_{-L}^{L} |D|^2\cos^2(qx)\,dx + \int_{L}^{\infty} |D|^2 e^{2KL}\cos^2(qL)\,e^{-2Kx}\,dx$

$= |D|^2 \left[\underbrace{e^{2KL}\cos^2(qL)\int_{-\infty}^{-L} e^{2Kx}\,dx}_{} + \underbrace{\int_{-L}^{+L}\cos^2(qL)\,dx}_{\text{II}} + \underbrace{e^{2KL}\cos^2(qL)\int_{L}^{\infty} e^{-2Kx}\,dx}_{\text{I}} \right]$

Função de Laplace

$e^{-2K|x|}$



↳ $\text{I} = 2e^{2KL}\cos^2(qL)\int_{L}^{\infty} e^{-2Kx}\,dx = 2e^{2KL}\cos^2(qL)\left.\dfrac{e^{-2Kx}}{-2K}\right|_{L}^{\infty} = \dfrac{\cos^2(qL)}{K}$

↳ $\text{II} = \int_{-L}^{L}\cos^2(qL)\,dx = \int_{-L}^{L}\dfrac{1+\cos(2qx)}{2}\,dx = L + \dfrac{1}{4q}\,\text{sen}(2qx)\Big|_{-L}^{L} = L + \dfrac{1}{2q}\,\text{sen}(2qL)$

$\Rightarrow \int_{-\infty}^{+\infty}\varphi^*(x)\varphi(x)\,dx = |D^2|\left[L + \dfrac{\text{sen}(2qL)}{2q} + \dfrac{\cos^2(qL)}{K}\right] = 1$

→ Assim, a função de onda normalizada seria

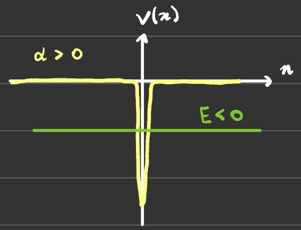
$$\varphi(x) = \frac{1}{\sqrt{L + \frac{1}{2q}\,\mathrm{sen}(2qL) + \frac{1}{K}\cos^2(qL)}} \cdot \begin{cases} e^{KL}\cos(qL)\,e^{Kx}, & x < -L \\ \cos(qx), & -L < x < L \\ e^{KL}\cos(qL)\,e^{-Kx}, & x > L \end{cases}$$

$$\rightarrow \bar{P} = \int_{-\infty}^{-L} |\varphi|^2 dx + \int_{L}^{\infty} |\varphi|^2 dx = \frac{1}{L + \frac{1}{2q}\,\mathrm{sen}(2qL) + \frac{1}{K}\cos^2(qL)} \left[2e^{2KL}\cos^2(qL) \int_{L}^{\infty} e^{-2Kx}\, dx \right]$$

$$\boxed{\bar{P} = \frac{\frac{1}{K}\cos^2(qL)}{L + \frac{1}{2q}\,\mathrm{sen}(2qL) + \frac{1}{K}\cos^2(qL)}}$$

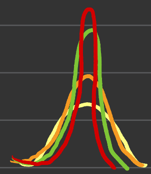
$$\hookrightarrow \lim_{V_0 \to \infty} \bar{P} = 0$$

Poço de potencial Delta



$$V(x) = -\alpha\,\delta(x), \qquad \delta(x) = \begin{cases} \infty, & x = 0 \\ 0, & \text{senão} \end{cases}$$

→ $\delta(x)$: sequência de distribuições: e^{-nx^2}



* $E > 0$: estados de espalhamento

* $E < 0$: estados ligados

↳ $x < 0$: $-\dfrac{\hbar^2}{2m}\dfrac{\partial^2\varphi}{\partial x^2} = E\varphi$

↳ $x > 0$: $-\dfrac{\hbar^2}{2m}\dfrac{\partial^2\varphi}{\partial x^2} = E\varphi$

$$\frac{\partial^2\varphi}{\partial x^2} + \frac{2mE}{\hbar^2}\varphi = 0 \Rightarrow \frac{\partial^2\varphi}{\partial x^2} - \frac{2m}{\hbar^2}(-E)\varphi = 0$$

$$\frac{\partial^2\varphi}{\partial x^2} - k^2\varphi = 0, \quad k = \sqrt{\frac{2m}{\hbar^2}(-E)}$$

$$\Rightarrow \begin{array}{l} \varphi_1(x) = Ae^{kx} + \cancel{Be^{-kx}}, \quad x < 0 \\ \varphi_2(x) = \cancel{Ce^{kx}} + De^{-kx}, \quad x > 0 \end{array} \quad \varphi(x) = \begin{cases} Ae^{kx}, & x < 0 \\ De^{-kx}, & x > 0 \end{cases}$$

→ Continuidade da função de onda em $x = 0$: $Ae^{k0} = De^{-k0}$

$$A = D$$

$$\therefore \varphi(x) = \begin{cases} Ae^{kx}, & x < 0 \\ Ae^{-kx}, & x > 0 \end{cases}$$

$$\rightarrow -\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + V(x)\varphi = E\varphi$$

$$\rightarrow \int_{-\varepsilon}^{\varepsilon} -\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2}\,dx + \int_{-\varepsilon}^{\varepsilon} V(x)\varphi(x)\,dx = E\int_{-\varepsilon}^{\varepsilon}\varphi(x)\,dx$$

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2\varphi}{dx^2}\,dx - \alpha\int_{-\varepsilon}^{\varepsilon}\delta(x)\varphi(x)\,dx = E\int_{-\varepsilon}^{\varepsilon}\varphi(x)\,dx$$

$$-\frac{\hbar^2}{2m}\left[\frac{d\varphi}{dx}(\varepsilon) - \frac{d\varphi}{dx}(-\varepsilon)\right] - \alpha\varphi(0) = E\int_{-\varepsilon}^{\varepsilon}\varphi(x)\,dx$$

$$\rightarrow \frac{d\varphi}{dx}(\varepsilon) = -AKe^{-K\varepsilon},\quad \frac{d\varphi}{dx}(-\varepsilon) = -AKe^{-K\varepsilon},\quad \varphi(0) = A$$

$$\Rightarrow -\frac{\hbar^2}{2m}(-2)AKe^{K\varepsilon} - \alpha A = E\int_{-\varepsilon}^{\varepsilon}\varphi(x)\,dx$$

$\rightarrow$ No limite $\varepsilon \rightarrow 0$: $\quad \frac{\hbar^2}{\cancel{2}m}\cdot\cancel{2}AK - \alpha A = 0 \Rightarrow \frac{\hbar^2}{m}\cancel{A}K - \alpha\cancel{A} = 0$

$$\therefore \alpha = \frac{\hbar^2}{m}K,\quad K = \frac{m\alpha}{\hbar^2}$$

$$\rightarrow \alpha = \frac{\hbar^2}{m}\sqrt{\frac{2m(-E)}{\hbar^2}} \Rightarrow \alpha^2 = \frac{\hbar^4}{m^{\cancel{2}}}\cdot\frac{2\cancel{m}(-E)}{\cancel{\hbar^2}} \Rightarrow \alpha^2 = -\frac{2\hbar^2 E}{m} \Rightarrow \boxed{E = -\frac{m\alpha^2}{2\hbar^2}}$$

Apenas 1 estado ligado

→ Normalizando: $\int_{-\infty}^{\infty} |\varphi(x)|^2 dx = |A|^2 \int_{-\infty}^{0} e^{2kx} dx + |A|^2 \int_{0}^{\infty} e^{-2kx} dx$

$$= 2|A|^2 \int_0^\infty e^{-2kx} dx$$

$$= 2|A|^2 \left. \frac{e^{-2kx}}{-2k} \right|_0^\infty$$

$$= \frac{|A|^2}{k} = 1$$

$$\therefore |A| = \sqrt{k} = \sqrt{\frac{m\alpha}{\hbar^2}}$$

→ Logo, $\boxed{\varphi(x) = \sqrt{\frac{m\alpha}{\hbar^2}}\, e^{-\frac{m\alpha}{\hbar^2}|x|}}$, $-\infty < x < \infty$