

Numerical integration of the S. eqn

Caso simple: $V(x) = V(x)$ (1)

$$\psi'' = \frac{2m}{\hbar^2} (V(x) - E) \psi(x) \quad (2)$$

Método primitivo:

$$\psi(x + \Delta x) \approx \psi(x) + \Delta x \psi'(x) + O(\Delta x)^2 \quad (3)$$

$$\Rightarrow \psi'(x + \Delta x) \approx \psi'(x) + \Delta x \psi''(x) + O(\Delta x)^2 \quad (4)$$

$$x_1 = x_0 + \Delta x, \quad x_2 = x_1 + \Delta x = x_0 + 2\Delta x.$$

$$\psi(x_1) \approx \psi(x_0) + \Delta x \psi'(x_0)$$

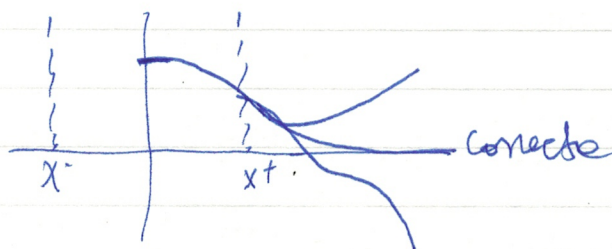
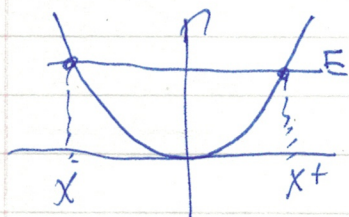
$$\psi'(x_1) \approx \psi'(x_0) + \Delta x \psi''(x_0)$$

$$\stackrel{(4)}{=} \psi'(x_0) + \frac{2m}{\hbar^2} \Delta x (V(x_0) - E) \psi(x_0) \quad (5)$$

$x_0 = 0$, y $\psi(0)$ dados, integra desde $x_0 = 0$ hasta x_f .
 $\psi'(0)$ " " Por E dado

También usar Taylor de orden superior.

$$\psi(x+h) + \psi(x-h) = 2\psi(x) + h^2 \psi''(x)$$



Autofunciones & Autovalores

→ tiene el aspecto $\frac{\check{P}^2}{2m}$ con $\check{P} = -i\hbar \frac{\partial}{\partial x}$

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

tiene la forma:

Operador x función = número x función

$$\boxed{H \psi = E \psi}$$

operador autofunción autovalor

ej. ∴ El operador $\check{P}_x = -i\hbar \frac{\partial}{\partial x}$ tiene como autofn. a $\psi = e^{ikx}$ ya que

$$\check{P}_x \psi = -i\hbar \frac{\partial}{\partial x} e^{ikx} = \hbar k e^{ikx} = \hbar k \psi$$

• Sea el autovalor de $\check{P}_x$ es $\hbar k$.

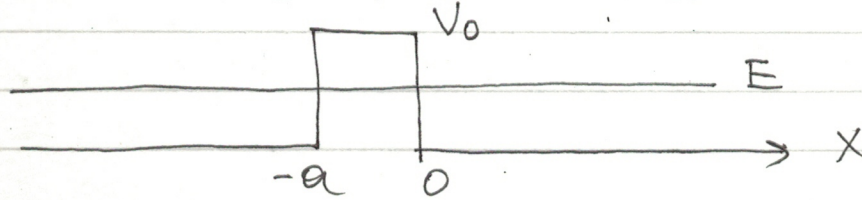
Consideremos $\check{L}_z = x p_y - y p_x = x (-i\hbar) \frac{\partial}{\partial y} - y (-i\hbar) \frac{\partial}{\partial x}$

op. de momento angular = $i\hbar [y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y}]$

Postulato 1: Cualq. variable dinámica que describe el movimiento de una partícula puede ser representada por un operador. Las cantidades observables son representadas por operadores hermíticos (autovalores reales)

Postulato 2: El único resultado posible de la medición de una variable dinámica es uno de los autovalores del correspondiente operador. Después de la medición, el sist. queda en el estado que corresponde al autovalor medido.

Penetración de barrera

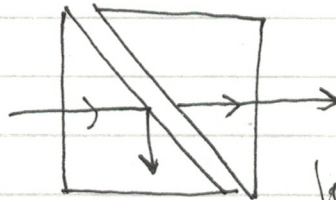
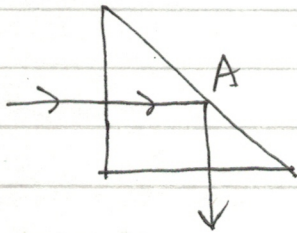


clásico: la partícula NO puede pasar si $E < V_0$.

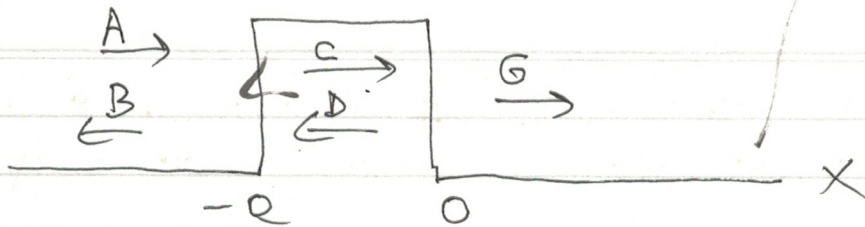
$$E = \frac{p^2}{2m} + V \Rightarrow \frac{p^2}{2m} = E - V < 0 \text{ dentro de la barrera} \Rightarrow \text{momento imaginario!} \rightarrow t$$

cuánticamente: 

óptico: reflexión total interna.



los prismas se acoplan
por los campos evanescentes



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

$$u = A e^{ikx} + B e^{-ikx} \quad x < -a$$

$$u = C e^{\alpha x} + D e^{-\alpha x} \quad -a < x < 0$$

$$u = G e^{ikx} \quad x > 0$$

$$\alpha = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

Cont. en $x=0$

cont. en $x=-a$

$$u' : \quad C + D = G$$

$$u' : \quad \alpha(C - D) = i k G$$

$$A e^{-ika} + B e^{ika} = C e^{-\alpha a} + D e^{\alpha a}$$

$$i k (A e^{-ika} - B e^{ika}) = \alpha (C e^{-\alpha a} - D e^{\alpha a})$$

$$\begin{cases} \alpha C + \alpha D = \alpha G \\ \alpha C - \alpha D = i k G \end{cases}$$

$$2\alpha D = (\alpha - i k) G$$

$$\Rightarrow \begin{cases} 2\alpha C = (\alpha + i k) G \\ C = \frac{(\alpha + i k) G}{2\alpha} \end{cases}$$

$$D = \frac{(\alpha - i k) G}{2\alpha}$$

$$\Rightarrow C e^{-\alpha a} + D e^{\alpha a} = \left[\frac{(\alpha + i k)}{2\alpha} e^{-\alpha a} + \frac{(\alpha - i k)}{2\alpha} e^{\alpha a} \right] G = \left[\cosh(\alpha a) - \frac{i k}{\alpha} \sinh(\alpha a) \right] G$$

$$\hookrightarrow C e^{-\alpha a} - D e^{\alpha a} = \left[\frac{(\alpha + i k)}{2\alpha} e^{-\alpha a} - \frac{(\alpha - i k)}{2\alpha} e^{\alpha a} \right] G = \left[\frac{i k}{\alpha} \cosh(\alpha a) - \sinh(\alpha a) \right] G$$

$$A e^{-ika} + B e^{ika} = G \left[\cosh(\alpha a) - \frac{i k}{\alpha} \sinh(\alpha a) \right]$$

$$A e^{-ika} - B e^{ika} = G \frac{\alpha}{i k} \left[\frac{i k}{\alpha} \cosh(\alpha a) - \sinh(\alpha a) \right]$$

$$= G \left[\cosh(\alpha a) - \frac{\alpha}{i k} \sinh(\alpha a) \right]$$

next: Despejar B/A (relac con el coefic de reflexion)

$$\frac{A e^{-i k a} + B e^{i k a}}{A e^{-i k a} - B e^{i k a}} = \frac{\cosh(\alpha a) - \frac{i k}{\alpha} \sinh(\alpha a)}{\cosh(\alpha a) - \frac{\alpha}{i k} \sinh(\alpha a)}$$

$$\frac{(1 + (B/A) e^{2 i k a}) (\cosh(\alpha a) - \frac{\alpha}{i k} \sinh(\alpha a))}{(1 - (B/A) e^{2 i k a}) (\cosh(\alpha a) - \frac{i k}{\alpha} \sinh(\alpha a))} = 1$$

$$\cosh(\alpha a) - \frac{\alpha}{i k} \sinh(\alpha a) + \left(\frac{B}{A}\right) e^{2 i k a} (\cosh(\alpha a) - \frac{\alpha}{i k} \sinh(\alpha a)) =$$

$$(\cosh(\alpha a) - \frac{i k}{\alpha} \sinh(\alpha a)) - (B/A) e^{2 i k a} (\cosh(\alpha a) - \frac{i k}{\alpha} \sinh(\alpha a))$$

$$\left(\frac{B}{A}\right) e^{2 i k a} \left[\cosh(\alpha a) - \frac{\alpha}{i k} \sinh(\alpha a) + \cosh(\alpha a) - \frac{i k}{\alpha} \sinh(\alpha a) \right] =$$

$$\cosh(\alpha a) - \frac{i k}{\alpha} \sinh(\alpha a) - \cosh(\alpha a) + \frac{\alpha}{i k} \sinh(\alpha a)$$

$$e^{2 i k a} (B/A) \left[2 \cosh(\alpha a) - \left(\frac{\alpha}{i k} + \frac{i k}{\alpha}\right) \sinh(\alpha a) \right] = \left(\frac{\alpha}{i k} - \frac{i k}{\alpha}\right) \sinh(\alpha a)$$

$$\frac{B}{A} = e^{-2 i k a} \frac{\left(\frac{\alpha}{i k} - \frac{i k}{\alpha}\right) \sinh(\alpha a)}{\left[2 \cosh(\alpha a) - \left(\frac{\alpha}{i k} + \frac{i k}{\alpha}\right) \sinh(\alpha a) \right]}$$

$$= e^{-2 i k a} \frac{(\alpha^2 + k^2) \sinh(\alpha a)}{[2 i k \alpha \cosh(\alpha a) + (k^2 - \alpha^2) \sinh(\alpha a)]}$$

$$\Rightarrow R = \frac{|B|^2}{|A|^2} = \left[1 + \frac{4(k\alpha)^2}{(k^2 + \alpha^2)^2 \sinh^2(\alpha a)} \right]^{-1}$$

pero $k^2 = 2mE/\hbar^2$, $\alpha^2 = 2m(V_0 - E)/\hbar^2$

resonancias

$$R = \left[1 + \frac{4 \left(\frac{2m}{\hbar^2} \right) E \cdot \frac{2m}{\hbar^2} (V_0 - E)}{\left(\frac{2m}{\hbar^2} \right) V_0^2 \sinh^2(\alpha a)} \right] = \left(1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2(\alpha a)} \right)$$

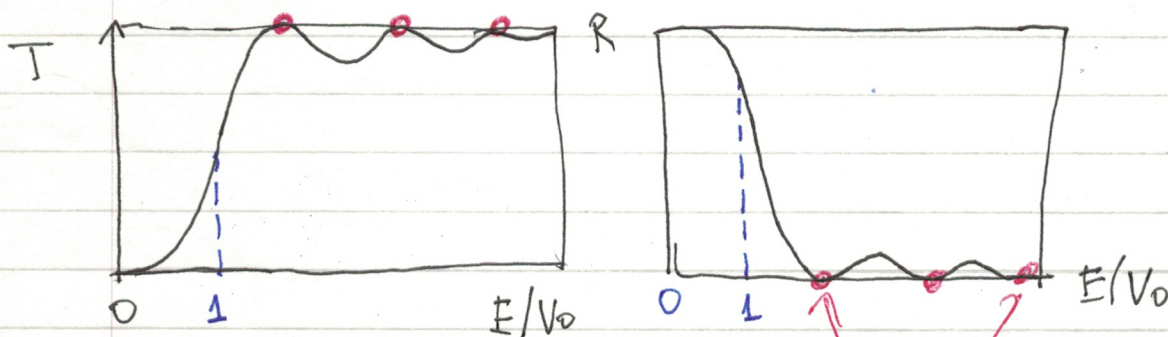
$$R = \left[1 + \frac{4(E/V_0)(1 - (E/V_0))}{\sinh^2 \left[\sqrt{\frac{2mV_0 a^2}{\hbar^2} \left(1 - \frac{E}{V_0} \right)} \right]} \right]^{-1}$$

Definir al par $V_0 = 8\hbar^2/mea^2 \Rightarrow R = \left[1 + \frac{4(E/V_0)(1 - E/V_0)}{\sinh^2 \left[4\sqrt{1 - \frac{E}{V_0}} \right]} \right]^{-1}$

Por su parte, $T = 1 - R$ (verdad?)

$$= \left[1 + \frac{\sinh^2 \left[\sqrt{\frac{2mV_0 a^2}{\hbar^2} \left(1 - \frac{E}{V_0} \right)} \right]}{4(E/V_0)(1 - (E/V_0))} \right]^{-1}$$

También sirve para $E > V_0$: ($\sinh(i\alpha) = i \sin(\alpha)$) o $\sinh(i\alpha) = -i \sin(\alpha)$



resonancias

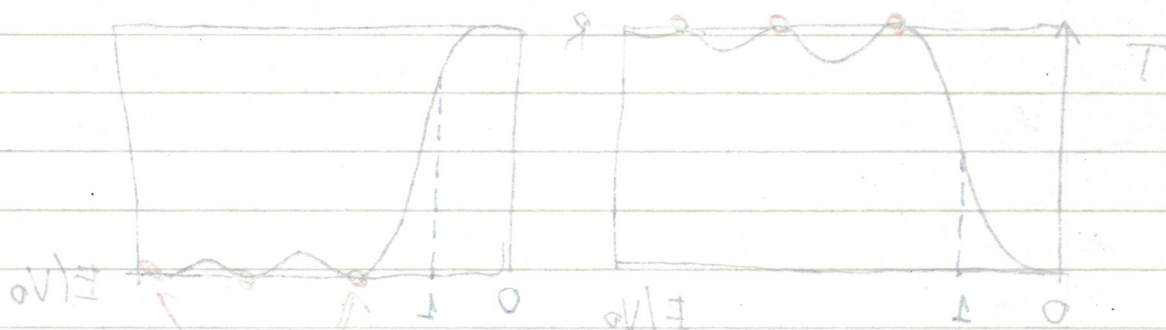
Resonancias cuando $T=1$
 $R=0$

$$E > V_0: T = \frac{1}{1 + \sin^2 \left(\sqrt{\frac{2m\alpha^2 V_0}{\hbar^2} \left(\frac{E}{V_0} - 1 \right)} \right)} = 1$$

$$T=1 \Rightarrow \sqrt{\frac{2m\alpha^2 V_0}{\hbar^2} \left(\frac{E}{V_0} - 1 \right)} = n\pi$$

$$\Rightarrow \boxed{E_n = V_0 + \frac{\pi^2 \hbar^2}{2m\alpha^2} n^2} \quad n=0, 1, 2, \dots$$

ojo: No es cuantización de energía y son energías resonantes.



Resonancias

Valores esperados

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x)\psi = E\psi(x) \quad | \psi^* \int$$

$$\int_{-\infty}^{\infty} \psi^*(x) \left(-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} \right) dx + \int_{-\infty}^{\infty} \psi^*(x) V(x) \psi(x) dx = E \int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx$$

$$\frac{1}{2m} \int_{-\infty}^{\infty} \psi^*(x) \left[-i\hbar \frac{d}{dx} \right] \left[i\hbar \frac{d}{dx} \right] \psi(x) dx + \int_{-\infty}^{\infty} \psi^*(x) V(x) \psi(x) dx = E$$

$$\text{pero } E = T + V = \frac{p^2}{2m} + V$$

Asociamos: $\int_{-\infty}^{\infty} \psi^* V(x) \psi dx = \langle V \rangle$ valor esperado de V
valor promedio

$$\frac{1}{2m} \int_{-\infty}^{\infty} \psi^* \left(-\hbar^2 \frac{d^2}{dx^2} \right) \psi dx = \langle T \rangle \quad \text{valor esperado de T}$$

→ asociar $-i\hbar \frac{d}{dx}$ = operador de momento $\vec{p}$

$$\Rightarrow \langle T \rangle = \int \psi^* \frac{\vec{p}^2}{2m} \psi dx = \left\langle \frac{\vec{p}^2}{2m} \right\rangle$$

$$\langle P_x \rangle = \int_{-\infty}^{\infty} \psi^*(x) (-i\hbar \frac{\partial}{\partial x}) \psi(x) dx$$

$$\text{Si } \psi(x) = e^{ik_0 x} \Rightarrow -i\hbar \frac{\partial \psi}{\partial x} = (-i\hbar) i k_0 \psi(x) = \hbar k_0 \psi$$

$$\dots -i\hbar \frac{\partial \psi}{\partial x} = \hbar k_0 \psi$$

$$\check{P}_x \psi = p_0 \psi$$

$$\text{En general, } \langle \check{\sigma} \rangle = \int_{-\infty}^{\infty} \psi^*(x) \sigma \psi(x) dx \quad (1)$$

$$\langle P_x^n \rangle = \int_{-\infty}^{\infty} \psi^*(x) (-i\hbar)^n \frac{\partial^n}{\partial x^n} \psi(x) dx \quad (2)$$

Values dispersion e interfeza

$$\Delta x = x - \langle x \rangle$$

$$\delta x = \sqrt{\langle (\Delta x)^2 \rangle} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \quad (3)$$

$$\text{Iguel'}. \quad \delta p = \sqrt{\langle P_x^2 \rangle - \langle P_x \rangle^2} \quad \nearrow \int_{-\infty}^{\infty} |\psi|^2 = 1 \quad (4)$$

$$\text{see } \psi(x) = \frac{1}{\sqrt{\sigma\sqrt{2\pi}}} e^{-\frac{x^2}{4\sigma^2}} \Rightarrow |\psi|^2 = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}}$$

$$\Rightarrow \langle x^2 \rangle - \langle x \rangle^2 = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{2\sigma^2}} dx - \left[\frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} x e^{-\frac{x^2}{2\sigma^2}} dx \right]^2 = \sigma^2$$

$$\Rightarrow \boxed{\delta x = \sqrt{\sigma^2 - 0} = \sigma} \quad (5)$$

$$\hat{p}\psi = -i\hbar \frac{\partial \psi}{\partial x} = (-i\hbar) \left(\frac{-2x}{4\sigma^2} \right) \psi = \frac{i\hbar x}{2\sigma^2} \psi$$

$$\begin{aligned} \hat{p}^2 \psi &= (-i\hbar)^2 \frac{\partial^2 \psi}{\partial x^2} = (-i\hbar) \left(\frac{i\hbar}{2\sigma^2} \right) \frac{\partial}{\partial x} (x\psi) \\ &= \frac{\hbar^2}{2\sigma^2} \left[\psi + x \frac{\partial \psi}{\partial x} \right] = \frac{\hbar^2}{2\sigma^2} \left(\psi + x \left(\frac{-x}{2\sigma^2} \right) \psi \right) \\ &= \frac{\hbar^2}{2\sigma^2} \left[1 - \frac{x^2}{2\sigma^2} \right] \psi \end{aligned}$$

$$\begin{aligned} \langle p^2 \rangle &= \frac{\hbar^2}{2\sigma^2} \underbrace{\int_{-\infty}^{\infty} |\psi|^2 dx}_1 - \frac{\hbar^2}{(2\sigma^2)} \underbrace{\int_{-\infty}^{\infty} x^2 |\psi|^2 dx}_{\sigma^2} \\ &= \frac{\hbar^2}{2\sigma^2} - \frac{\hbar^2}{4\sigma^2} = \frac{\hbar^2}{4\sigma^2} \end{aligned}$$

$$\Rightarrow \boxed{\delta p_x = \frac{\hbar}{2\sigma}} \quad (6)$$

$$\Rightarrow \delta x \delta p_x = \sigma \cdot \frac{\hbar}{2\sigma} = \frac{\hbar}{2} \quad (7)$$

$[\delta x \delta p_x > \hbar/2 \text{ per wave } \psi \text{ no gaussian}]$