Numerical Integration of the S. eqn

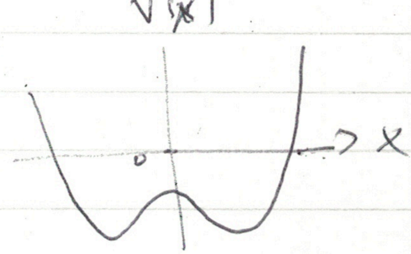
Caso simple: $V(-x) = V(x)$ (1)

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

Método primitivo:

$$\psi(x+\Delta x) \simeq \psi(x) + \Delta x\,\psi'(x) + O(\Delta x)^2 \qquad (3)$$

$$\Rightarrow \psi'(x+\Delta x) \simeq \psi'(x) + \Delta x\,\psi''(x) + O(\Delta x)^2 \qquad (4)$$



$x_1 = x_0 + \Delta x$; $x_2 = x_1 + \Delta x = x_0 + 2\Delta x$.

$$\psi(x_1) \simeq \psi(x_0) + \Delta x\,\psi'(x_0)$$

$$\psi'(x_1) \simeq \psi'(x_0) + \Delta x\,\psi''(x_0)$$

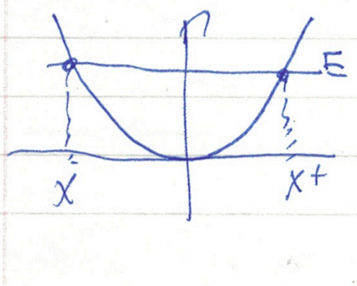
$$\overset{(2)}{=} \psi'(x_0) + \frac{2m}{\hbar^2}\Delta x\,(V(x_0)-E)\,\psi(x_0) \qquad (5)$$

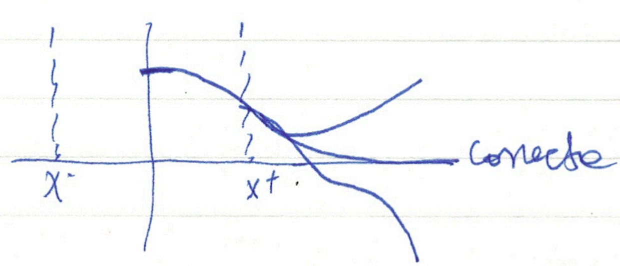
$x_0 = 0$, y $\psi(0)$, $\psi'(0)$ dados, integro desde $x_0 = 0$ hasta x_f.

Por E dado

También usar Taylor de orden superior.

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x)$$





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 × función = número × función

$$\boxed{\underset{\text{operador}}{\check{H}}\ \underset{\text{autofunción}}{\psi} = \underset{\text{autovalor}}{E}\ \psi}$$

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

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

o sea el autovalor de $\check{p}_x$ es $\hbar k$.

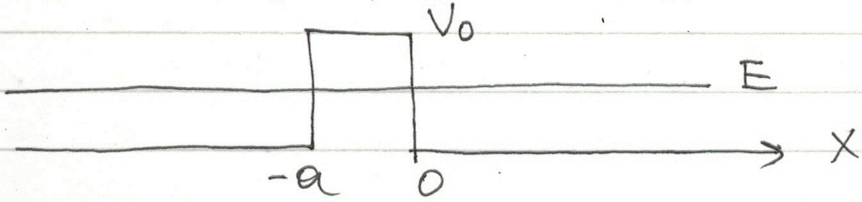
Consideremos $\check{L}_z = x p_y - y p_x = x(-i\hbar)\frac{\partial}{\partial y} - y(-i\hbar)\frac{\partial}{\partial x}$

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

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

Postulado 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

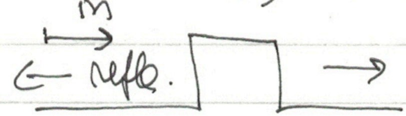


clásico: la partícula NO puede pasar si $E < V_0$:

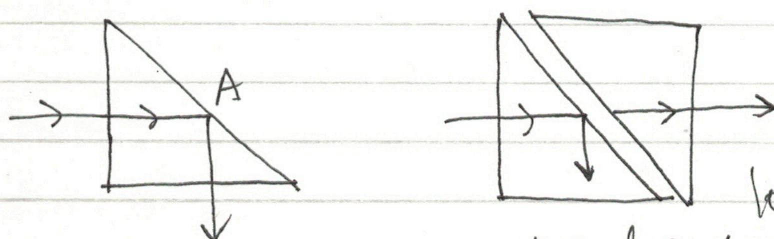
$E = \frac{p^2}{2m} + V \Rightarrow \frac{p^2}{2m} = E - V < 0$ dentro de la barrera

$\Rightarrow$ momento imaginario! →

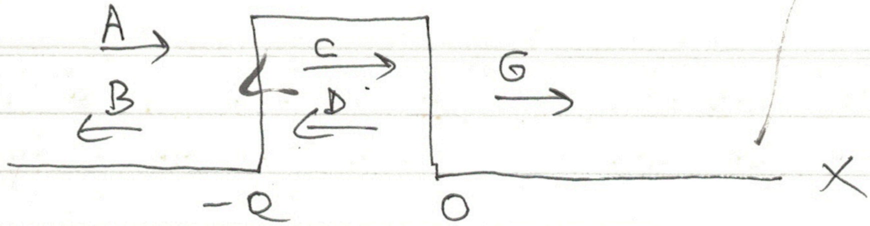
cuánticamente:



óptica: reflexión total interna:



los prismas se acoplan por los campos <u>evanescentes</u>



$$u = Ae^{ikx} + Be^{-ikx} \qquad x < -a$$
$$u = Ce^{\alpha x} + De^{-\alpha x} \qquad -a < x < 0$$
$$u = Ge^{ikx} \qquad x > 0$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Cont. en $x=0$;

u: $C + D = G$

u': $\alpha(C - D) = ikG$

cont. en $x = -a$

$$Ae^{-ika} + Be^{ika} = Ce^{-\alpha a} + De^{\alpha a}$$
$$ik(Ae^{-ika} - Be^{ika}) = \alpha(Ce^{-\alpha a} - De^{\alpha a})$$

$$\alpha C + \alpha D = \alpha G$$
$$\alpha C - \alpha D = ikG$$

$$2\alpha D = (\alpha - ik)G$$

$$\Rightarrow 2\alpha C = (\alpha + ik)G$$
$$C = \frac{(\alpha + ik)}{2\alpha}G \qquad D = \frac{(\alpha - ik)G}{2\alpha}$$

$$\Rightarrow Ce^{-\alpha a} + De^{\alpha a} = \left[\left(\frac{\alpha + ik}{2\alpha}\right)e^{-\alpha a} + \left(\frac{\alpha - ik}{2\alpha}\right)e^{\alpha a}\right]G = \left[\cosh(\alpha a) - \frac{ik}{\alpha}\sinh(\alpha a)\right]G$$

$$\text{y} \quad Ce^{-\alpha a} - De^{\alpha a} = \left[\left(\frac{\alpha + ik}{2\alpha}\right)e^{-\alpha a} - \left(\frac{\alpha - ik}{2\alpha}\right)e^{\alpha a}\right]G = \left[\frac{ik}{\alpha}\cosh(\alpha a) - \sinh(\alpha a)\right]G$$

$$Ae^{-ika} + Be^{ika} = G\left[\cosh(\alpha a) - \frac{ik}{\alpha}\sinh(\alpha a)\right]$$
$$Ae^{-ika} - Be^{ika} = G\frac{\alpha}{ik}\left[\frac{ik}{\alpha}\cosh(\alpha a) - \sinh(\alpha a)\right]$$
$$= G\left[\cosh(\alpha a) - \frac{\alpha}{ik}\sinh(\alpha a)\right]$$

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

$$\frac{Ae^{-ika}+Be^{ika}}{Ae^{-ika}-Be^{ika}} = \frac{\cosh(\alpha a)-\frac{ik}{\alpha}\sinh(\alpha a)}{\cosh(\alpha a)-\frac{\alpha}{ik}\sinh(\alpha a)}$$

$$\frac{\left(1+(B/A)e^{2ika}\right)\left(ch(\alpha a)-\frac{\alpha}{ik}sh(\alpha a)\right)}{\left(1-(B/A)e^{2ika}\right)\left(ch(\alpha a)-\frac{ik}{\alpha}sh(\alpha a)\right)} = 1$$

$$ch(\alpha)-\frac{\alpha}{ik}sh(\alpha a)+\left(\frac{B}{A}\right)e^{2ika}\left(ch(\alpha a)-\frac{\alpha}{ik}sh(\alpha a)\right) =$$

$$\left(ch(\alpha)-\frac{ik}{\alpha}sh(\alpha a)\right)-(B/A)e^{2ika}\left(ch(\alpha a)-\frac{ik}{\alpha}sh(\alpha a)\right)$$

$$\left(\frac{B}{A}\right)e^{2ika}\left[ch(\alpha a)-\frac{\alpha}{ik}sh(\alpha a)+ch(\alpha a)-\frac{ik}{\alpha}sh(\alpha a)\right] =$$

$$\cancel{ch(\alpha)}-\frac{ik}{\alpha}sh(\alpha a)-\cancel{ch(\alpha a)}+\frac{\alpha}{ik}sh(\alpha a)$$

$$e^{2ika}(B/A)\left[2ch(\alpha a)-\left(\frac{\alpha}{ik}+\frac{ik}{\alpha}\right)sh(\alpha a)\right] = \left(\frac{\alpha}{ik}-\frac{ik}{\alpha}\right)sh(\alpha a)$$

$$\frac{B}{A} = e^{-2ika}\frac{\left(\frac{\alpha}{ik}-\frac{ik}{\alpha}\right)sh(\alpha a)}{\left[2ch(\alpha a)-\left(\frac{\alpha}{ik}+\frac{ik}{\alpha}\right)sh(\alpha a)\right]} \qquad \begin{matrix} ik\alpha \\ ik\alpha \end{matrix}$$

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

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

pero $k^2 = 2mE/\hbar^2$, $\alpha^2 = 2m(V_0-E)/\hbar^3$

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

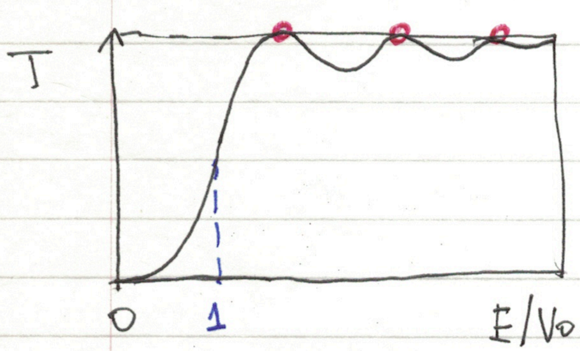
$$R = \left[1 + \frac{4(E/V_0)(1-(E/V_0))}{\sinh^2\left[\sqrt{\frac{2mV_0 a^2}{\hbar^2}\left(1-\frac{E}{V_0}\right)}\right]}\right]^{-1}$$

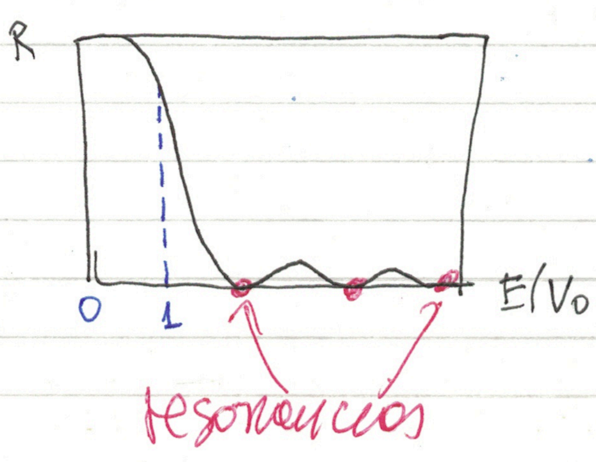
Graficar al para $V_0 = 8\hbar^2/ma^2 \Rightarrow R = \left[1 + \frac{4(E/V_0)(1-\frac{E}{V_0})}{\sinh^2\left[4\sqrt{1-\frac{E}{V_0}}\right]}\right]^{-1}$

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 $E > V_0$: $(\sinh(\alpha i) = i\sin(\alpha) \Rightarrow \sinh^2(i\alpha) = -\sin^2(\alpha))$





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

$E > V_0$:
$$T = \left[1 + \frac{\sin^2\left(\sqrt{\frac{2ma^2V_0}{\hbar^2}\left(\frac{E}{V_0}-1\right)}\right)}{4(E/V_0)\left(\frac{E}{V_0}-1\right)} \right]^{-1}$$

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

$$\Rightarrow \boxed{E_n = V_0 + \frac{\pi^2\hbar^2}{2ma^2}\, n^2} \qquad n = 0, 1, 2, \ldots$$

OJO: No es cuantización de energías; son energías resonantes.

Valores esperados

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

$$\int_{-\infty}^{\infty} \psi^*(x) \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}\,dx + \int_{-\infty}^{\infty} \psi^*(x) V(x)\psi(x)\,dx = E \underbrace{\int_{-\infty}^{\infty} \psi^*(x)\psi(x)\,dx}_{1}$$

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

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

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

$\rightarrow$ asocio $-i\hbar\frac{d}{dx}$ = operador de momento $\check{p}$

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

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

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

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

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

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

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

Valores esperados e incerteza

$\Delta x \equiv x - \langle x\rangle$

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

Igual'/. $\delta p \equiv \sqrt{\langle p_x^2\rangle - \langle p_x\rangle^2}$ $\quad\int_{-\infty}^{\infty}|\psi|^2 = 1$ (4)

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

$$\Rightarrow \langle x^2\rangle - \langle x\rangle^2 = \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty}x^2 e^{-\frac{x^2}{2\sigma^2}}dx - \left[\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty}\underbrace{x e^{-\frac{x^2}{2\sigma^2}}dx}_{0}\right]^2 = \sigma^2$$

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

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

$$\check{p}^2\psi = (-i\hbar)^2\frac{\partial^2\psi}{\partial x^2} = (-i\hbar)\frac{(i\hbar)}{2\sigma^2}\frac{\partial}{\partial x}(x\psi)$$

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

$$= \frac{\hbar^2}{2\sigma^2}\left[1 - \frac{x^2}{2\sigma^2}\right]\psi$$

$$\langle p_x^2\rangle = \frac{\hbar^2}{2\sigma^2}\underbrace{\int_{-\infty}^{\infty}|\psi|^2 dx}_{1} - \frac{\hbar^2}{(2\sigma^2)^2}\underbrace{\int_{-\infty}^{\infty}x^2|\psi|^2 dx}_{\sigma^2}$$

$$= \frac{\hbar^2}{2\sigma^2} - \frac{\hbar^2}{4\sigma^2} = \frac{\hbar^2}{4\sigma^2}$$

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

$$\Rightarrow \delta x\,\delta p_x = \sigma\cdot\frac{\hbar}{2\sigma} = \frac{\hbar}{2} \;/\!/ \qquad (7)$$

[$\delta x\,\delta p_x > \hbar/2$ pero wolq. ψ no gaussiana]