Another Argument

Sea H el Hamiltoniano de una partícula con posición $\vec{q}$ y momento $\vec{p}$, en un potencial $V(\vec{q})$

$$H = \frac{\vec{p}^{\,2}}{2m} + V(\vec{q}) \qquad (1)$$

$$\text{Sea } \Psi = e^{(i/\hbar)(\vec{p}\cdot\vec{q} - Ht)} \qquad (2)$$

$$\text{tomar } H\Psi = \frac{\vec{p}^{\,2}}{2m}\Psi + V(\vec{q})\Psi \qquad (3)$$

$\frac{-i}{\hbar}H$

Por otro lado, tenemos

$$\vec{p}\Psi = \vec{p}\, e^{(i/\hbar)(\vec{p}\cdot\vec{q} - Ht)} = -i\hbar\nabla_q \Psi \qquad (4)$$

$$H\Psi = H e^{(i/\hbar)(p\cdot q - Ht)} = i\hbar\frac{\partial\Psi}{\partial t} \qquad (5)$$

reemplazando en (3), tenemos

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(\vec{q})\Psi \qquad (6)$$

valido para cualquier superposición de $\{\Psi\}$ ⇒ valido para un pulso representando a una partícula.

⇒ Ec (6) se presume válida en todos los casos, no solamente ondas planas.

Ec. de Schrödinger tiempo-independiente

Muchas veces, es posible $\Psi(x,t) = \psi(x)\phi(t)$.
Sup. $V(x,t) = V(x)$.

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\psi''(x)\phi(t) + V(x)\psi(x)\phi(t) = i\hbar\left(\frac{\partial\phi}{\partial t}\right)\psi \qquad / \frac{1}{\psi(x)\phi(t)}$$

$$\Rightarrow \quad \underbrace{\frac{1}{\psi(x)}\left\{-\frac{\hbar^2}{2m}\psi'' + V(x)\psi(x)\right\}}_{\text{solo fn. de } x} = \underbrace{i\hbar\frac{1}{\phi(t)}\frac{d\phi}{dt}}_{\text{solo fn. de } t} \qquad (17)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\psi'' + V\psi = c\psi \quad y \quad i\hbar\frac{d\phi}{dt} = c\phi$$

$\Rightarrow \phi(t) \propto e^{+ict/\hbar}$ → fn. complejo oscilatorio, con frecuencia ν, tq. $\nu = c/h$

Pero, se debe tener $\nu = E/h$ $\Rightarrow$ $\boxed{C = E}$

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi} \qquad (18)$$

"Ec. de S. t-indep"

$\psi(x)$ es también una "autofunción" del operador

$$\check{L} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$$\check{L}\,\psi(x) = E\,\psi(x) \qquad (19)$$

operador autofn. autovalor

Corriente de probabilidad

$$\rho(x,t) = \psi^* \psi \qquad i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \Rightarrow \frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} H\Psi$$

$$y \quad \frac{\partial \Psi^*}{\partial t} = \frac{i}{\hbar}(H\Psi)^*$$

$$\frac{\partial \rho}{\partial t} = \frac{\partial \Psi^*}{\partial t}\cdot\psi + \psi^* \frac{\partial \psi}{\partial t} = \frac{i}{\hbar}(H\psi^*)\psi - \frac{i}{\hbar}\psi^* H\Psi$$

$$= -\frac{i}{\hbar}\left[\psi^* H\psi - (H\psi^*)\psi\right]$$

$$= -\frac{i}{\hbar}\left[\Psi^*\left(-\frac{\hbar^2}{2m}\nabla^2\Psi\right) + \underbrace{\psi^* V\Psi}_{} + \left(\frac{\hbar^2}{2m}\nabla^2\Psi^*\right)\psi - \underbrace{\psi V\psi^*}_{}\right]$$

$$\frac{i\hbar}{2m}\left[\psi^*\nabla^2\Psi - \psi\nabla^2\psi^*\right] =$$

$$\frac{i\hbar}{2m}\vec{\nabla}\cdot\left[\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right] = \vec{\nabla}\cdot\vec{J}$$

$$\vec{J} = -\frac{i\hbar}{2m}(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*)$$

$$y \quad \boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0} \text{ Ec. de continuidad}$$

(JUGANDO)

Playing: $-\psi'' + \bar{V}(x)\psi = \bar{E}\psi$

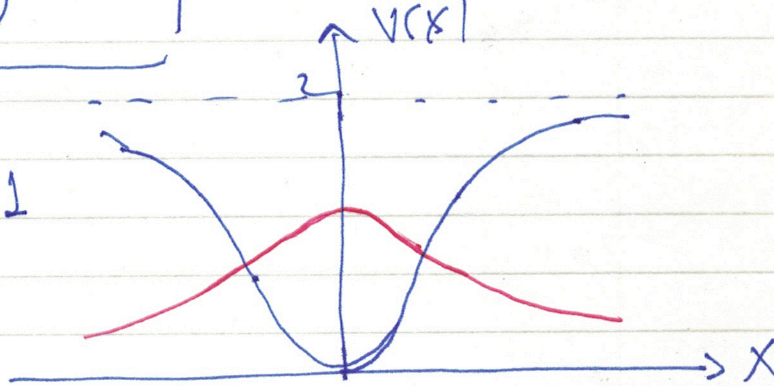
donde $\bar{V}(x) \equiv \frac{2m}{\hbar^2} V(x)$; $\bar{E} \equiv \frac{2m}{\hbar^2} E$

Given $\psi(x) \neq 0$, $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$, and given $\bar{E}$,

$$\Rightarrow \boxed{\bar{V}(x) = \frac{\psi''(x) + \bar{E}\psi(x)}{\psi(x)}}$$

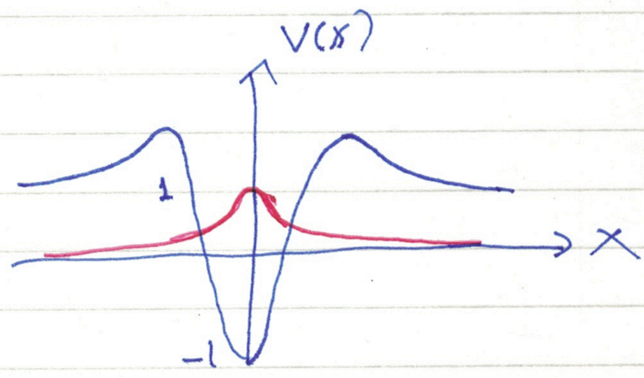
(1) $\psi(x) = \frac{1}{\sqrt{2}} \operatorname{sech}(x)$; $\bar{E} = 1$

$\Rightarrow \bar{V}(x) = 2\tanh^2(x)$



(2) $\psi(x) = \frac{(1/\pi)}{1+x^2}$, E=1

$\Rightarrow \bar{V}(x) = \frac{x^4 + 8x^2 - 1}{(x^2+1)^2}$



Cuantización de la Energía

sea $V(x,t) = V(x) \Rightarrow \Psi(x,t) = \psi(x)\phi(t)$

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

Para que ψ sea "aceptable", se requiere

(1) $\psi(x)$ debe ser finita
(2) $\psi(x)$ debe ser continua
(3) $d\psi/dx$ continua
(4) $d\psi/dx$ finita

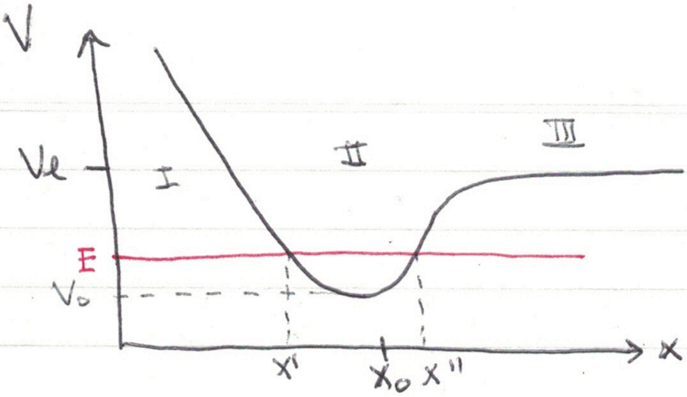
Si no se cumple (1) y/ó (4) $\Rightarrow \Psi(x,t) = e^{-iEt/\hbar}\psi(x)$
y $\frac{\partial\Psi(x,t)}{\partial x} = e^{-iEt/\hbar}\frac{d\psi}{dx}$

tampoco lo cumplen
$\Rightarrow P(x,t) = \Psi^*(x,t)\Psi(x,t)$
y $S(x,t) = -\frac{i\hbar}{2m}\left[\Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial x} - c.c.\right]$ No estarían bien definidos

Por qué $(d\psi/dx)$ continua?

$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}[V(x)-E]\psi(x) \Rightarrow$ para $V(x)$, E y $\psi(x)$ FINITO
$\Rightarrow \frac{d^2\psi}{dx^2}$ finita $\Rightarrow$ (3)

Cuantización de E: $\boxed{\text{sólo } \exists \text{ soluciones "aceptables" para \underline{ciertos} valores de la energía } E}$



(i) Asumir valor de E.

Si $V_0 < E < V_e$ → 2 "ptos. de retorno": x', x''

→ 3 regiones:

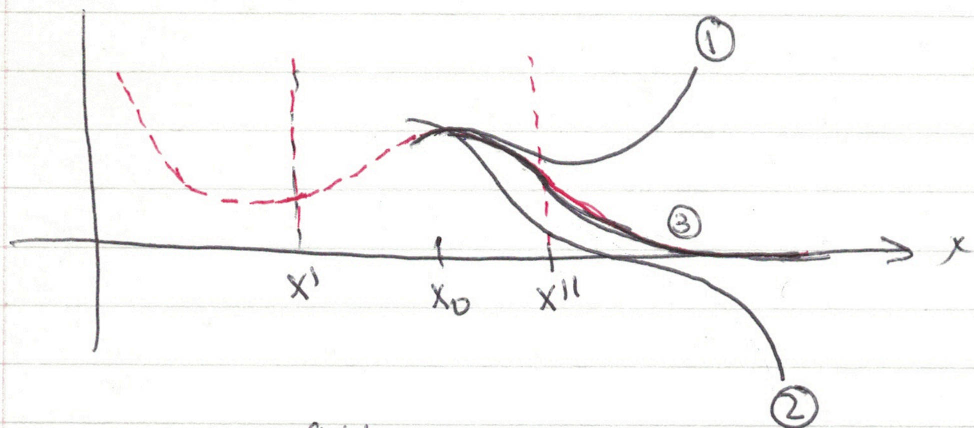
$0 < x < x'$:	$V(x) - E > 0$	$\psi > 0 \rightarrow \psi'' > 0$; $\psi < 0 \rightarrow \psi'' < 0$
$x' < x < x''$:	$V(x) - E < 0$	$\psi > 0 \Rightarrow \psi'' < 0$; $\psi < 0 \rightarrow \psi'' > 0$ } oscilante
$x'' < x$:	$V(x) - E > 0$	$\psi > 0 \rightarrow \psi'' > 0$; $\psi < 0 \rightarrow \psi'' < 0$

Sup. que partimos la integración numérica en $x = x_0$

sup. un valor $\psi(x_0)$ y un valor de $\left(\frac{d\psi}{dx}\right)_{x_0}$

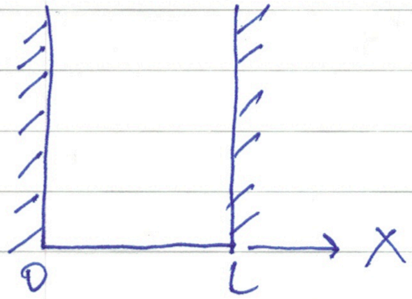
↓

no relevante



Escogiendo el $(d\psi/dx)_{x_0}$ adecuado, se puede hallar un $\psi(x)$ aceptable para $x \geq x_0$. Pero queda hallar $\psi(x)$ para $-\infty < x < x_0$. Como ya no podemos ajustar $(d\psi/dx)_{x_0}$, $\psi(x)$ divergerá (hacia $\pm\infty$) en gral. Esto sug. que sólo ciertos E son permitidos.

POZO ∞: $V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & \text{caso contrario} \end{cases}$



$\psi(x) = 0 \quad x < 0\ ;\ x > L$

$0 < x < L$: $\quad -\frac{\hbar^2}{2m}\psi''(x) = E\psi$

$\Rightarrow \psi''(x) + k^2\psi(x) = 0$, con $k^2 \equiv 2mE/\hbar^2$

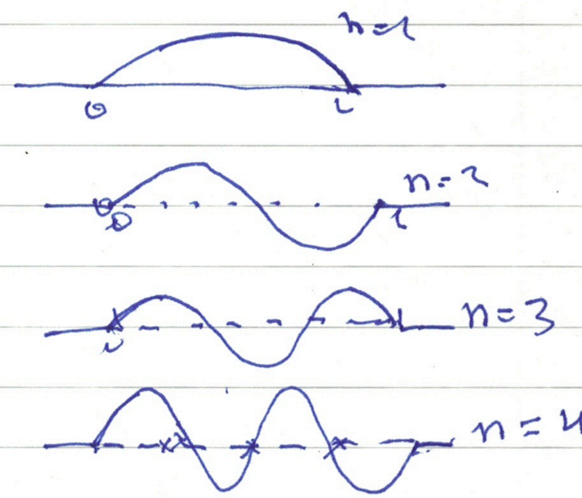
$\Rightarrow \psi(x) = Ae^{ikx} + Be^{-ikx}$

$0 = \psi(0) \Rightarrow A + B = 0 \Rightarrow B = -A$

$0 = \psi(L) \Rightarrow 0 = Ae^{ikL} + Be^{-ikL} = A(e^{ikL} - e^{-ikL})$

$0 = +2iA\sin(kL) \Rightarrow kL = n\pi$

$$\boxed{k_n = n\pi/L}$$



$$\Rightarrow \boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\pi^2\hbar^2}{2mL^2}\,n^2.}$$

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{n\pi}{L}x\right)}$$

OJO: n(mínimo) = 1 no ϕ.

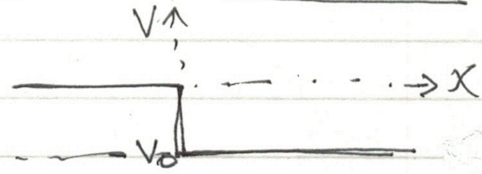
cuantizacion surgio al imponer que la funcion de onda sea cero en los bordes

condiciones de borde..

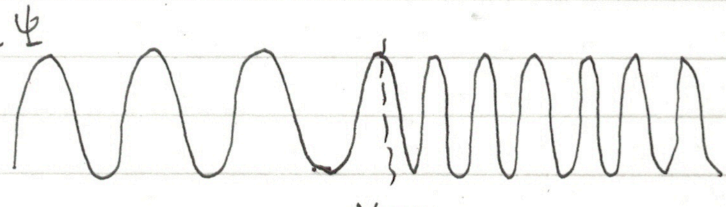
pedimos que ψ sea finita. Luego si E y V son finitos, ψ'' existe $\Rightarrow$ $\frac{\partial \psi}{\partial x}$ y ψ son continuas. (aun si V es discontinuo)

Ejemplo..

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



$$\lambda = \frac{h}{\sqrt{2m(E-V)}} \qquad (6)$$



$$\psi(x,t) = e^{-\frac{iEt}{\hbar}}\,\psi(x) \qquad (7)$$

$$\Rightarrow \quad E\psi(x) = -\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) \qquad (8)$$

$x<0$: $\quad E\psi = -\frac{\hbar^2}{2m}\psi'' \Rightarrow \psi'' + \frac{2mE}{\hbar^2}\psi = 0$

o sea $\quad \psi'' + k_1^2\psi = 0 \Rightarrow \psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad (9)$

$x>0$: $\quad E\psi = -\frac{\hbar^2}{2m}\psi'' - V_0\psi \Rightarrow \psi'' + \frac{2m}{\hbar^2}(E+V_0)\psi = 0$

o sea, $\quad \psi'' + k_2^2\psi = 0 \Rightarrow \psi(x) = Ce^{ik_2x} \qquad (10)$

cont. de ψ, $\quad A + B = C$

cont. de ψ', $\quad ik_1A - ik_1B = ik_2C$

$$\left.\begin{aligned} A+B&=C \\ ik_1A - ik_1B &= ik_2C \end{aligned}\right\} \quad (11)$$

$$\Rightarrow \quad \frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \quad ; \quad \frac{C}{A} = \frac{2k_1}{k_1 + k_2}$$

Coefics. de transmisión y reflexión:

Intensidad incidente $\longrightarrow$

intensidad transmitida $\longrightarrow$

$\longleftarrow$ intensidad reflejada

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

$p = mv$ $\therefore mv = \hbar k$

$$\boxed{v = \hbar k/m}$$

densidad de numero

velocidad

$$\text{Intensidad} = \rho v = |\psi|^2 \frac{\hbar k}{m}$$

Reflexión:
$$R = \frac{|B|^2 (\hbar/m) k_1}{|A|^2 (\hbar/m) k_1} = \frac{|B|^2}{|A|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad (12)$$

Transmisión:
$$T = \frac{|C|^2 (\hbar/m) k_2}{|A|^2 (\hbar/m) k_1} = \frac{|C|^2 k_2}{|A|^2 k_1} = \frac{4 k_1 k_2}{(k_1 + k_2)^2} \qquad (13)$$

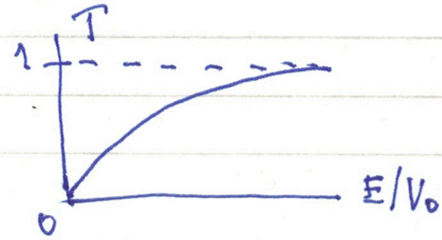
y se cumple, $\boxed{R + T = 1}$ (14)

cuando $k_1 = \sqrt{2mE/\hbar^2}$ y $k_2 = \sqrt{(2m/\hbar^2)(E+V_0)}$

$$\Rightarrow \quad R = \left(\frac{\sqrt{E} - \sqrt{E+V_0}}{\sqrt{E} + \sqrt{E+V_0}}\right)^2$$

No ∃ cuantización de E.

$$T = \frac{4\sqrt{E}\sqrt{E+V_0}}{(\sqrt{E} + \sqrt{E+V_0})^2}$$



Paridad de las soluciones

cuando $V(x)$ es par, i.e., $V(-x) = V(x)$, las autofn. poseen paridad definida, o sea son pares ó impares.

Dem: $$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \qquad (1)$$

$x \Rightarrow -x$:
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + V(-x)\psi(-x) = E\psi(-x) \qquad (2)$$
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + V(x)\psi(-x) = E\psi(-x) \qquad (3)$$

o sea, $\psi(x)$ y $\psi(-x)$ satisfacen la misma ecuación y dado que sólo $\exists$ una autofunción para un E dado

$$\Rightarrow \quad \psi(-x) = c\,\psi(x) \qquad (4)$$

en particular, para $-x$, (4) queda

$$\psi(x) = c\,\psi(-x) = c^2\psi(x) \Rightarrow c^2 = 1 \Rightarrow c = \pm 1$$

$$\Rightarrow \boxed{\psi(-x) = \pm\psi(x)}$$

Si $\psi(-x) = \psi(x) \rightarrow \psi(x)$ es PAR

Si $\psi(-x) = -\psi(x) \rightarrow \psi(x)$ es IMPAR