

Another Argument

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

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

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

$$\text{toman } H\psi = \frac{\vec{p}^2}{2m} \psi + V(\vec{q}) \psi \quad (3)$$

Por otro lado, tenemos

$$\vec{p}\psi = \vec{p} e^{(i/\hbar)(\vec{p} \cdot \vec{q} - Ht)} = -i\hbar \nabla_{\vec{q}} \psi \quad (4)$$

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

reemplazando en (3), tenemos

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

válido para cualquier superposición de $\{\psi\} \Rightarrow$ válido para un pulso representando a una partícula.

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

Ec. de Schrödinger tiempo-independiente

Muchos veces, es posible $\psi(x,t) = \psi(x)\phi(t)$.

Sup. $V(x,t) = V(x)$.

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

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

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

$\Rightarrow \phi(t) \propto e^{+iCt/\hbar}$ $\rightarrow$ fn. compleja oscilatoria, con frecuencia ν , tq. $\nu = C/\hbar$

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

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

$\rightarrow$ "E.C. de S. t-indep"

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

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

$$\hat{L} \psi(x) = E \psi(x) \quad (19)$$

operador autofn. $\rightarrow$ autovalores

$$\rho(x,t) = \psi^* \psi$$

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \Rightarrow \frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} H\psi$$

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

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

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

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

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

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

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

$$\text{y } \boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J}} \text{ is to be conserved.}$$

(JUGANDO)

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

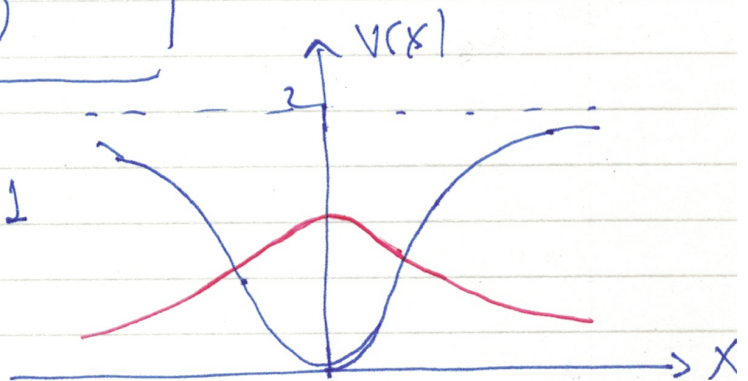
define $\bar{V}(x) \equiv \frac{2m}{\hbar^2} V(x)$; $\bar{E} \equiv \frac{2m}{\hbar^2} E$

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

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

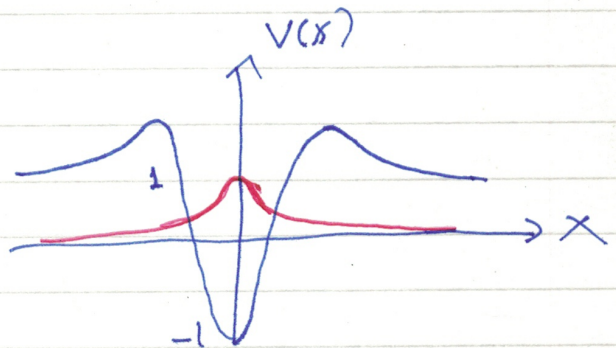
① $\psi(x) = \frac{1}{\sqrt{2}} \operatorname{sech}(x)$; $\bar{E} = 1$

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



② $\psi(x) = \frac{(1/\pi)}{(1+x^2)}$

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



Cuantización de la Energía

$$\text{sea } V(x, E) = V(x) \Rightarrow \Psi(x, E) = \psi(x) \phi(E)$$

$$\text{dado } -\frac{\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} + V(x) \Psi = E \Psi \quad (1)$$

Para que Ψ sea "aceptable", se requiere

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

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

tiempo lo cumplen

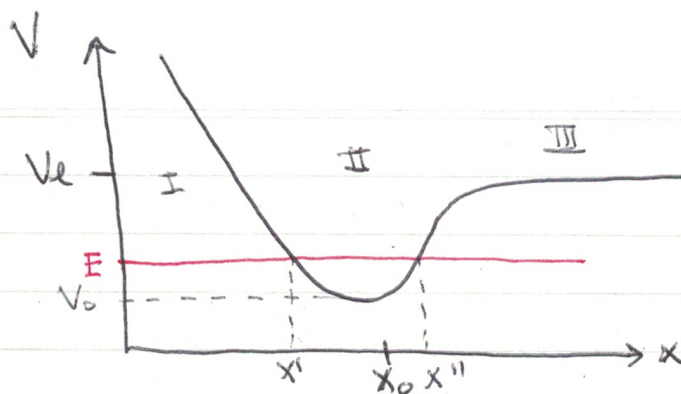
$$\Rightarrow P(x, E) = \Psi^*(x, E) \Psi(x, E)$$

$$\text{y } S(x, E) = -\frac{i\hbar}{2m} \left[\Psi^*(x, E) \frac{\partial \Psi(x, E)}{\partial x} - \text{c.c.} \right] \quad \text{No están bien definidos}$$

Por qué $(d\psi/dx)$ continua?

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

Cuantización de E : sólo $\exists$ soluciones "aceptables" para ciertos valores de la energía E



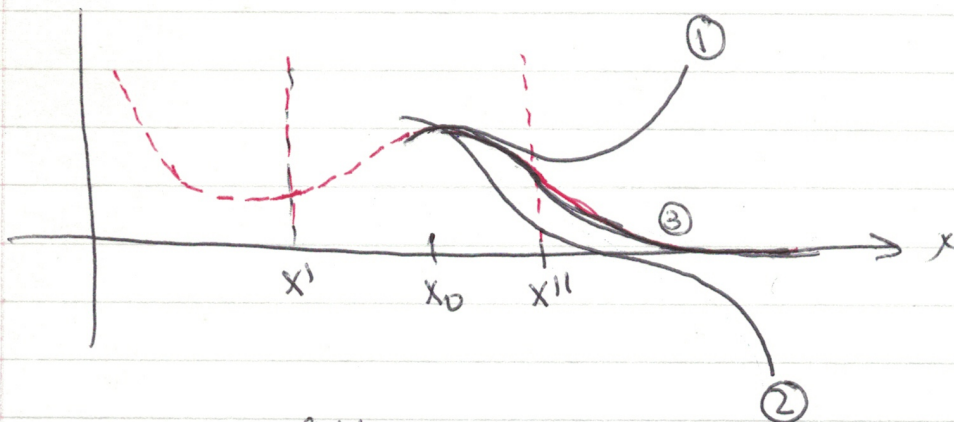
(i) Asumir value de E .

Si $V_0 < E < V_e \rightarrow 2$ "ptos. de retorno", x' , x''

$\rightarrow 3$ regiones:

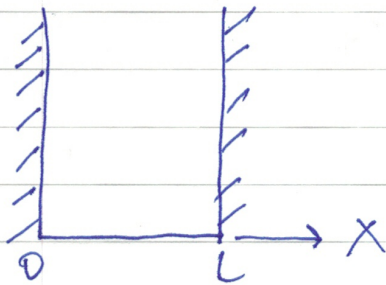
$0 < x < x'$	$V(x) - E > 0$	$\psi > 0 \rightarrow \psi'' > 0$	} oscilante
$x' < x < x''$	$V(x) - E < 0$	$\psi < 0 \rightarrow \psi'' < 0$	
		$\psi > 0 \Rightarrow \psi'' < 0$	
		$\psi < 0 \Rightarrow \psi'' > 0$	
$x'' < x$	$V(x) - E > 0$	$\psi > 0 \rightarrow \psi'' > 0$	
		$\psi < 0 \rightarrow \psi''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

Sup. que pertinamos la integración numérica en $x = x_0$
 sup. un valor $\psi(x_0)$ y un valor de $\left(\frac{d\psi}{dx}\right)_{x_0}$
 $\downarrow$
 no relevante



Escogiendo el $\left(\frac{d\psi}{dx}\right)_{x_0}$ 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 $\left(\frac{d\psi}{dx}\right)_{x_0}$, $\psi(x)$ divergirá (hacia $\pm\infty$) en general. Esto sig. que solo ciertos E son permitidos.

Problema: $V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & \text{cero continuos} \end{cases}$



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

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

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

$$\Rightarrow \psi(x) = A e^{ikx} + B e^{-ikx}$$

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

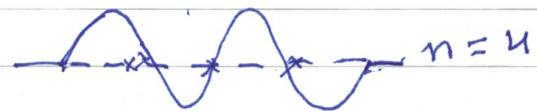
$$0 = \psi(L) \Rightarrow 0 = A e^{ikL} + B e^{-ikL} = A(e^{ikL} - e^{-ikL})$$

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

$$k_n = n\pi/L$$

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

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



ojo: $n(\text{mínimo}) = 1$ no ϕ .

cuantización surgió al imponer que la función de onda sea cero en los bordes