

Regla de cuantización de Bohr-Sommerfeld



$$\oint \frac{dq}{\lambda(q)} = n, \quad n \in \mathbb{N} \quad (1)$$

Condición para q' de
onda interferencia
constructivamente
consigo mismo

Se puede re-expressar como:

$$\oint p(q) dq = nh \quad (2)$$

$$dq = v dt$$

$$p = mv$$

$$\oint p dq = \oint mv^2 dt = 2 \oint T dt = 2\tau \langle T \rangle = nh$$

Si el potencial es del tipo $V(q) = Aq^s$

← energía total

$$\Rightarrow \langle T \rangle = \frac{s}{s+2} E$$

→ Demostración como
ejercicio ←

$$\Rightarrow 2\tau \frac{s}{s+2} E = nh \Rightarrow E_n = h\nu \left(\frac{s+2}{2s} \right) n \quad (3)$$

$$(\nu \equiv 1/\tau)$$

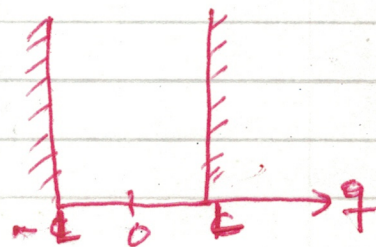
→ puede ser función de E_n .

(i) Oscilador armónico: $V(q) = \frac{1}{2} m\omega^2 q^2 \Rightarrow s=2$

$$\Rightarrow E_n = n h \nu \quad (\text{igual que Planck})$$

(ii) Partícula en pozo-infinito:

$$V(q) = \begin{cases} 0 & |q| < c \\ \infty & |q| > c \end{cases} = \lim_{m \rightarrow \infty} \left(\frac{q}{c} \right)^m$$



En este caso, $S = m$ con $m \rightarrow \infty$

$$\lambda = \frac{1}{\nu_E} = \frac{4L}{\nu} = 4L \sqrt{\frac{m}{2E}} \quad \left(\begin{array}{l} \text{este es un ejemplo de} \\ \nu = \nu(E) \end{array} \right)$$

$$\Rightarrow E_n = h\nu_E \left(\frac{m+2}{m} \right) n \xrightarrow{m \rightarrow \infty} \frac{h\nu_E n}{2} = \frac{h n}{8L} \sqrt{\frac{2E_n}{m}}$$

$$\Rightarrow \boxed{E_n = \frac{\pi^2 \hbar^2}{2mL^2} \cdot n^2}$$

Teo. del Virial : $E = T + V \Rightarrow E = \langle T \rangle + \langle V \rangle$

$$\text{si } V = Aq^S \Rightarrow q \frac{\partial V}{\partial q} = S V \Rightarrow \boxed{\left\langle q \frac{\partial V}{\partial q} \right\rangle = S \langle V(q) \rangle}$$

$$\text{ luego, } \left\langle q \frac{\partial V}{\partial q} \right\rangle = \frac{1}{2} \oint q \frac{\partial V}{\partial q} dt \stackrel{\text{Newton}}{=} -\frac{m}{2} \oint q \frac{dv}{dt} \cdot dt =$$

$$= -\frac{1}{2} \oint q dp \stackrel{pp}{=} \frac{1}{2} \oint p dq = \frac{1}{2} \oint mv^2 dt = 2 \langle T \rangle$$

$$\Rightarrow S \langle V \rangle = 2 \langle T \rangle \Rightarrow \langle V \rangle = (2/S) \langle T \rangle$$

$$E = \langle T \rangle + \frac{2}{S} \langle T \rangle = \left(\frac{S+2}{S} \right) \langle T \rangle$$

$$\boxed{\langle T \rangle = \left(\frac{S}{S+2} \right) E}$$

A. Sommerfeld: considers orbits elliptical.



$$V(r) = -\frac{e^2 Z^2}{r} \quad (0 \text{ see, } s = -1)$$

$$s = -1 \Rightarrow \langle T \rangle = -E \quad (1)$$

$$T = \frac{1}{2} m \dot{r}^2 + \frac{1}{2} m r^2 \dot{\theta}^2 = T_r + T_\theta$$

$$\langle T_\theta \rangle = \left\langle \frac{1}{2} m r^2 \dot{\theta}^2 \right\rangle = \left\langle m r^2 \dot{\theta} \cdot \frac{1}{2} \dot{\theta} \right\rangle = \frac{L}{2} \langle \dot{\theta} \rangle = \frac{\hbar l}{2} \langle \dot{\theta} \rangle$$

$$\text{pero } \langle \dot{\theta} \rangle = 2\pi \nu_E \Rightarrow \langle T_\theta \rangle = \frac{\hbar l}{2} \cdot 2\pi \nu_E = \boxed{\frac{\hbar l \nu_E}{2}}$$

$$\text{end } \langle T_r \rangle = \frac{\hbar h}{2l} = \boxed{\frac{\hbar h \nu_E}{2}}$$

$$\Rightarrow E = -\langle T \rangle = -\frac{\hbar \nu_E}{2} (n+l) = -\frac{\hbar \nu_E}{2} N$$

$$\text{Kepler: } r^2 = \frac{m \pi^2}{2 Z e^2} R^3, \text{ end } E = -\frac{Z e^2}{R}$$

$$\Rightarrow E^2 = \frac{\hbar^2 N^2}{4 r^2} = \frac{\hbar^2 N^2}{4} \cdot \frac{2 Z e^2}{m \pi^2 R^3} = \frac{\hbar^2 N^2 Z e^2}{2 \pi^2 m} \cdot \frac{E^3}{Z^3 e^6}$$

$$\Rightarrow 1 = \frac{N^2 \hbar^2 E}{(ze^2)^2 2\pi^2 m}$$

$$\Rightarrow \boxed{E_{n\ell} = -\frac{m z^2 e^4}{2\hbar^2} \cdot \frac{1}{(n+\ell)^2}}$$

N	n	ℓ	Ω ← degeneración
1	1	0	1
2	1	1	3
	2	0	1
3	3	0	5
	2	1	3
	1	2	1

Una partícula no-relativista de masa m es mantenida en órbita circular alrededor del origen por una fuerza $f(r) = -kr$, donde k es una constante positiva.

(a) Demuestre que la energía potencial se puede escribir como

$$U(r) = kr^2/2$$

Asumiendo $U(r) = 0$ cuando $r = 0$.

(b) Asumiendo la cuantización de Bohr del momento angular de la partícula, muestre que el radio de la órbita de la partícula y su velocidad v pueden ser escritos como

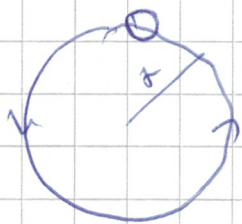
$$v^2 = \left(\frac{n\hbar}{m}\right) \left(\frac{k}{m}\right)^{1/2} \qquad r^2 = \left(\frac{n\hbar}{k}\right) \left(\frac{k}{m}\right)^{1/2}$$

donde n es un entero.

(c) Por lo tanto, demuestre que la energía total de la partícula es

$$E_n = n\hbar \left(\frac{k}{m}\right)^{1/2}$$

(d) Si $m = 3 \times 10^{-26}$ kg y $k = 1180 \text{ Nm}^{-1}$, determine numericamente la longitud de onda del fotón en nm que causará una transición entre niveles sucesivos de energía.



$$f = -kr$$

$$(a) \quad U = - \int f \cdot dr = + \int kr dr = \frac{k}{2} r^2 \quad U(0) \text{ si } r=0$$

$$(b) \quad 2\pi r = n\lambda = \frac{nh}{p} = \frac{nh}{mvr}$$

$$\Rightarrow \boxed{r = \frac{nh}{mvr}} \quad \text{but} \quad \frac{mv^2}{r} = kr \Rightarrow \boxed{v^2 = \frac{kr^2}{m}}$$

$$\Rightarrow r^2 = \frac{n^2 h^2}{m^2 v^2} = \left(\frac{nh}{m} \right)^2 \cdot \frac{m}{kr^2} \Rightarrow r^4 = \left(\frac{m}{k} \right) \left(\frac{nh}{m} \right)^2$$

$$\Rightarrow r^2 = \left(\frac{nh}{m} \right) \sqrt{\frac{m}{k}} = \frac{nh}{\sqrt{mk}} = \frac{nh}{\sqrt{mk}} \sqrt{\frac{k}{k}} = \boxed{\left(\frac{nh}{k} \right) \sqrt{\frac{k}{m}}}$$

$$c = \lambda v$$

$$\text{Wegol, } v^2 = \frac{k}{m} \cdot \left(\frac{nh}{k} \right) \sqrt{\frac{k}{m}} = \boxed{\left(\frac{nh}{m} \right) \sqrt{\frac{k}{m}}}$$

$$E = \hbar \omega$$

$$E = K + U = \frac{1}{2} m \cdot \left(\frac{nh}{m} \right) \left(\frac{k}{m} \right)^{1/2} + \frac{1}{2} k \cdot \left(\frac{nh}{k} \right) \left(\frac{k}{m} \right)^{1/2} = \boxed{nh \left(\frac{k}{m} \right)^{1/2}}$$

$$(c) \quad m = 3 \times 10^{-26} \text{ kg}, \quad k = 1180 \text{ N m}^{-1} \Rightarrow \omega = \sqrt{\frac{k}{m}} = \boxed{1.983 \times 10^{14} \text{ Hz}}$$

$$\left. \begin{array}{l} E_n = (n + \frac{1}{2}) \hbar \omega \\ E_{n+1} = (n + \frac{3}{2}) \hbar \omega \end{array} \right\} \Delta E = \hbar \omega = 6.626 \times 10^{-34} \frac{\text{m}^2 \text{kg}}{\text{s}} \times 1.983 \times 10^{14} =$$

$$= \frac{h c}{\lambda} \Rightarrow \lambda = \frac{h c}{\Delta E} = \boxed{240 \text{ nm}} \quad \boxed{9511 \text{ nm}}$$

Construyendo la ec. de Schrödinger

$\lambda = \frac{h}{p} \rightarrow$ ¿cuál es la "ec. de onda" para una partícula?

onda infinita: $\psi = A \cos(kx - \omega t)$ (0)

Pulso finito = superposición de ondas planas,
aunque q' el pulso finito también satisficiera
la misma ec. q' la onda plana $\Rightarrow$ Ec. debe ser LINEAL

E. total partícula = $\hbar\omega$ $\leftarrow$ frec. onda.

$$\begin{aligned} E &= \hbar\omega \\ &= \frac{p^2}{2m} + V = \frac{\hbar^2 k^2}{2m} + V \end{aligned} \quad (1)$$

$$(0) \rightarrow \frac{\partial \psi}{\partial x} = -Ak \sin(kx - \omega t)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -Ak^2 \cos(kx - \omega t) = -k^2 \psi$$

$$\text{pero } k^2 = \frac{2m(E-V)}{\hbar^2}$$

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

$k = 2\pi/\lambda$, sea $V = c\epsilon \Rightarrow$ (2) solo reformulada de Broglie.

Idea de Schrödinger: E.c. (2) es válida también cuando $V = V(x)$.

Introduciendo el tiempo:

$$\psi = A \cos(kx - \omega t)$$

$$\frac{\partial \psi}{\partial t} = \omega A \sin(kx - \omega t)$$

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 A \cos(kx - \omega t) = -\omega^2 \psi \quad (3)$$

de $E\psi = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V\psi$ y usando $\omega = E/\hbar$

$$\Rightarrow \hbar \omega \psi = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V\psi \quad (3')$$

si' interponemos entre (3) en (3'):

$$\hbar^2 \omega^2 \psi^2 = \left[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V\psi \right]^2$$

$$-\hbar^2 \psi \frac{d^2 \psi}{dt^2} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \right]^2 \quad \text{NO LINEAL}$$

→ ←

Idea: usar $\psi = A e^{i(kx - \omega t)}$ (como en óptica)

$$\Rightarrow \frac{\partial \psi}{\partial t} = -i\omega A e^{i(kx - \omega t)} = -i\omega \psi$$

$$\Rightarrow \frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar} \psi \quad (4)$$

$$\Rightarrow \boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi} \quad (5)$$

Ec. de S. t-dependiente en 1D.

$\psi(x) \rightarrow$ no observable

$$\text{Intensidad} \equiv |\psi|^2 = \psi\psi^* = A^*A = |A|^2 \in \mathbb{R}$$

Justificación : acuerdo con incontable experimentos

$|\psi(x,t)|^2 :=$ densidad de probabilidad de hallar la partícula en posición x , ~~mas~~ en el instante t $= |\psi(x,t)|^2 dx dt$

CONSTRUYENDO LA EC. DE SCHRÖDINGER

Schrodinger 1^{er} intento

$$E^2 = p^2 c^2 + m^2 c^4 \quad (\text{partícula libre})$$

$$\Psi = A e^{i(kx - \omega t)} \quad E = \hbar \omega, \quad \vec{P} = -i\hbar \vec{\nabla}$$

$$\frac{\partial \Psi}{\partial t} = -i\omega \Psi \Rightarrow \frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 \Psi = -\frac{E^2}{\hbar^2} \Rightarrow \boxed{E^2 = -\hbar^2 \frac{\partial^2 \Psi}{\partial t^2}}$$

$$\Rightarrow \boxed{-\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \Psi + m^2 c^4 \Psi} \quad \text{Ec. de Klein-Gordon}$$

No resulta para los e^- !

$\Rightarrow$ tomar límite no-relativista

$$E = (p^2 c^2 + m^2 c^4)^{1/2} \simeq mc^2 + \frac{p^2}{2m} + \dots$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[mc^2 + \frac{p^2}{2m} + \dots \right] \Psi$$

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + mc^2 \Psi}$$

$\swarrow$ puede eliminarse

$$\Psi \rightarrow e^{-\frac{imc^2}{\hbar} t} \Psi$$

desaparece el término cte.
No afecta $|\Psi|^2$.

Ec. de Schrödinger tiempo-independiente

mucho más, $\Rightarrow$ 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. $\nu = c/h$

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

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

" E de S. t-indep"

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

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

$$L\psi(x) = E\psi(x)$$

(19)

operador $\downarrow$ autofn. $\rightarrow$ autovalores

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

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

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

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

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

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

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

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

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

$$\text{y } \boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J}} \quad \text{is continuous.}$$

(JUGANDO)

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

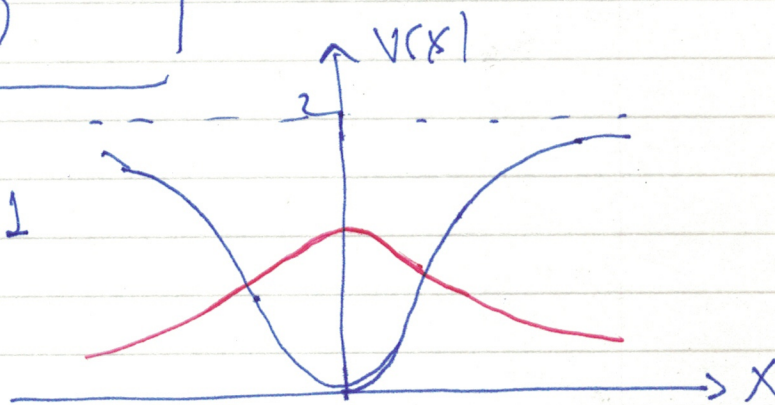
define $\bar{V}(x) \equiv \frac{2m}{\hbar^2} V(x)$; $\bar{E} \equiv \frac{2m}{\hbar^2} E$

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

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

