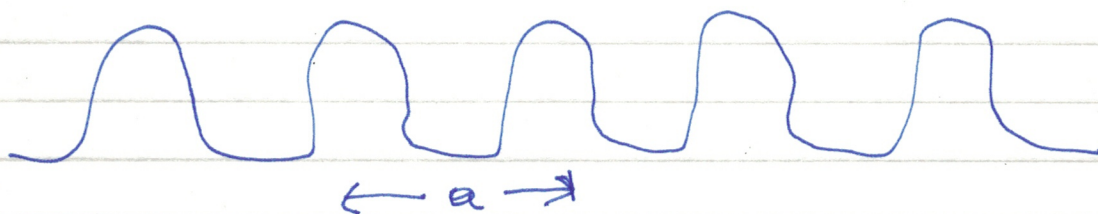


Potenciales Periódicos en 1D

$$V(x) = V(x-a) \quad \forall x$$



ej.: e^- en red cristalina 1D

Debido a la periodicidad, $|\psi(x)|^2 = |\psi(x-a)|^2$

$$\Rightarrow \psi(x+a) = e^{i\theta} \psi(x) \quad \text{porque } \theta = k a$$

$$\psi(x+a) = e^{i k a} \psi(x) \quad (1)$$

$$\text{Definimos } u_k(x) \equiv e^{-i k x} \psi(x) \quad (2)$$

$u_k(x)$ es periódica con período a .

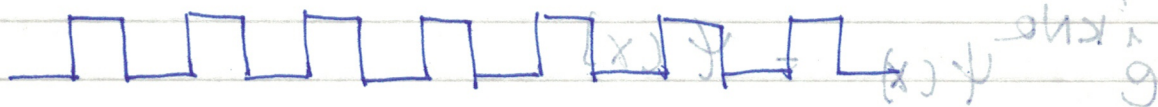
$$\begin{aligned} \text{Dem: } u_k(x+a) &= e^{-i k (x+a)} \psi(x+a) = e^{-i k x - i k a} e^{i k a} \psi(x) \\ &= e^{-i k x} \psi(x) = u_k(x) \end{aligned}$$

$$\circ \text{ see, } u_k(x+a) = u_k(x) //$$

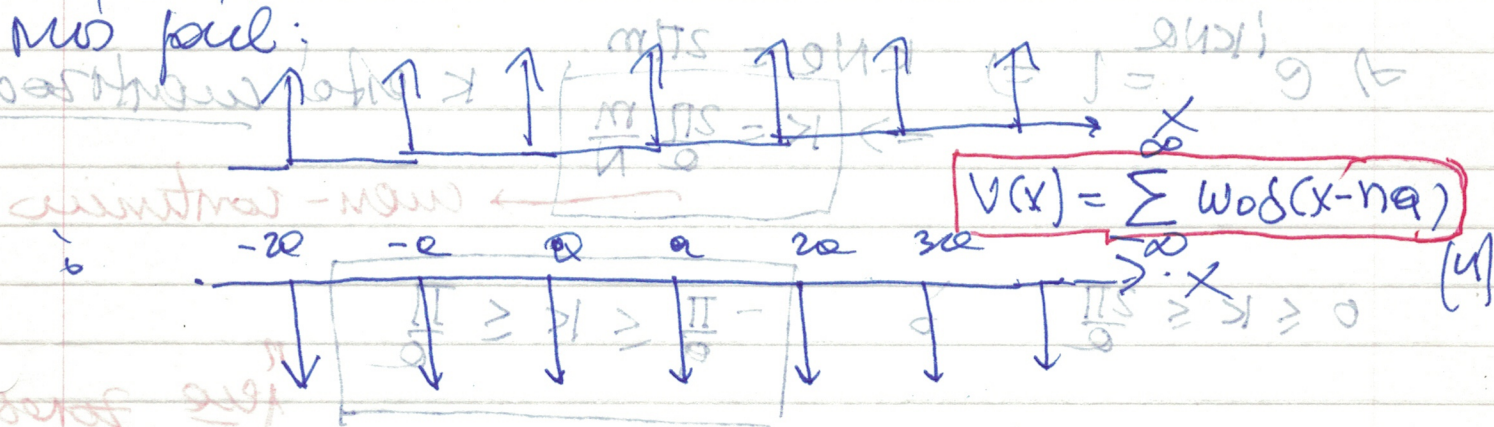
Se concluye que $\psi(x) = u_k(x) e^{ikx}$ (3)
 es la forma gen. de las autofunciones de H
 cuando $V(x)$ es periódico.

Note: Podemos elegir $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$ $\rightarrow$

Modelo de Kronig-Penney



mo pul:



Para considerar $0 < x < a$

$$0 < x < a, V=0 \Rightarrow \psi(x) = A e^{iqx} + B e^{-iqx} \quad (5)$$

donde $q = \sqrt{2mE/\hbar^2}$

$$\Rightarrow u_k(x) = A e^{i(q-k)x} + B e^{-i(q+k)x} \quad (6)$$

Condición de borde periódica

Para q' el sistema sea periódico no puede tener bordes, pero no necesita ser infinito

$$\psi(x + Na) = \psi(x)$$

usando Teo. de Bloch

$$e^{iKNa} \psi(x) = \psi(x)$$

$$\Rightarrow e^{iKNa} = 1 \Rightarrow KNa = 2\pi m$$

$$\Rightarrow K = \frac{2\pi}{a} \frac{m}{N}$$

K este cuantizado

$$(p(x-x)) \delta(x) = (x) \delta(x)$$

cuen-continuo

$$0 \leq K \leq \frac{2\pi}{a}$$

$$-\frac{\pi}{a} \leq K \leq \frac{\pi}{a}$$

esta zona de Brillouin

(2)

$$\psi(x) = \psi(x) \Rightarrow \psi(x) = \psi(x)$$

(1)

$$\psi(x) = \psi(x) \Rightarrow \psi(x) = \psi(x)$$

Pero evaluamos $A+B$, usando las condiciones de borde

(1) Continuidad de ψ : en $x = na$, $n \in \mathbb{Z}$

$\Rightarrow U_k(x)$ también debe ser continuo:

$$U_k(\epsilon) - U_k(-\epsilon) \xrightarrow{\epsilon \rightarrow 0} 0$$

Como conocemos solo $U_k(x)$ para $0 < x < a$, lo conocemos $U_k(-\epsilon)$, pero usando la periodicidad de U_k :

$$U_k(-\epsilon) = U_k(-\epsilon + a)$$

$$\Rightarrow U_k(\epsilon) - U_k(a - \epsilon) \xrightarrow{\epsilon \rightarrow 0} 0 \quad (7)$$

Usando (7) en (6):

$$A+B = A e^{i(q-k)a} + B e^{-i(q+k)a} \quad (8)$$

(2) Debido a la presencia de los potenciales $\delta(x-na)$ la derivada de $\psi(x)$ experimenta un salto en $x=0$.

$$\left(\frac{d\psi}{dx} \right)_{x=\epsilon} - \left(\frac{d\psi}{dx} \right)_{x=-\epsilon} = \frac{2mW_0}{\hbar^2} \psi(0) \quad (9)$$

$$\left(\frac{d\psi}{dx} \right)_\epsilon = iq A e^{iq\epsilon} - iq B e^{-iq\epsilon} \rightarrow iq(A-B) \quad (10)$$

$$\begin{aligned}
 \psi \left(\frac{d\psi}{dx} \right)_{x=-\epsilon} &= \frac{d}{dx} \left[u_k(x) e^{ikx} \right]_{x=-\epsilon} = \frac{d}{d(x-\epsilon)} \left[u_k(x-\epsilon) e^{ik(x-\epsilon)} \right]_{x=-\epsilon+\epsilon} \\
 &= \frac{d}{dx} \left[u_k(x) e^{ikx} e^{-ik\epsilon} \right]_{x=a-\epsilon} = e^{-ik\epsilon} \left(\frac{d\psi}{dx} \right)_{x=a-\epsilon} \\
 &= e^{-ik\epsilon} i q (A e^{iq\epsilon} - B e^{-iq\epsilon}) \quad (11)
 \end{aligned}$$

Por último $\psi(0) = A + B$

$$\Rightarrow i q \left[A - B - A e^{+i(q-k)\epsilon} + B e^{-i(q+k)\epsilon} \right] = \frac{2mW_0}{\hbar^2} (A+B) \quad (12)$$

$$(8) \Rightarrow B = \left[\frac{1 - e^{i(q-k)\epsilon}}{e^{-i(q+k)\epsilon} - 1} \right] A \quad (13)$$

Insertando (13) en (12)

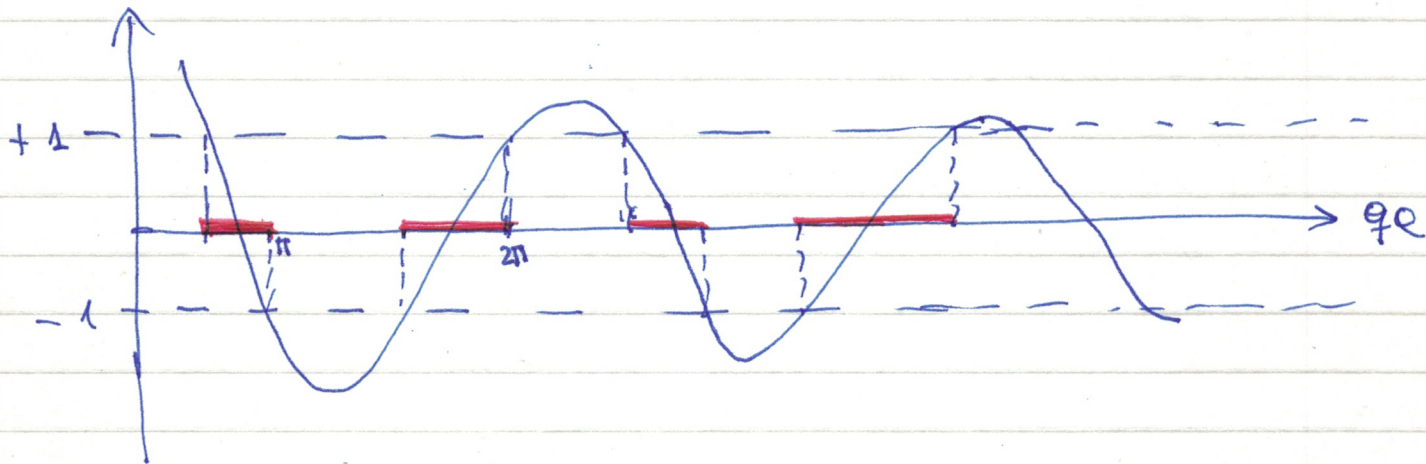
$$A \left(e^{ik\epsilon} - e^{-iq\epsilon} - e^{iq\epsilon} + e^{-ik\epsilon} \right) = A \frac{mW_0}{\hbar^2 i q} (e^{iq\epsilon} - e^{-iq\epsilon})$$

$$\Rightarrow \left(\cos(k\epsilon) - \cos(q\epsilon) - \frac{mW_0}{q\hbar^2} \sin(q\epsilon) \right) A = 0 \quad (14)$$

Solución no-trivial $\Rightarrow$

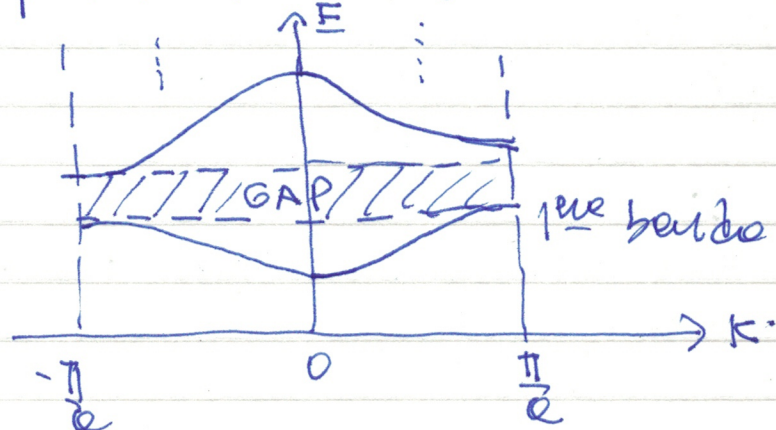
$$\cos(ka) = \cos(qa) + \frac{mW_0a}{\hbar^2} \frac{\sin(qa)}{qR}$$

Solución gráfica..



Los valores permitidos de qa caen dentro de los "zonas permitidas" (BANDAS), los cuales están separados unos de otros por "zonas prohibidas" (GAPS).

$$E = \frac{\hbar^2 q^2}{2m}$$



La función $\delta(x)$

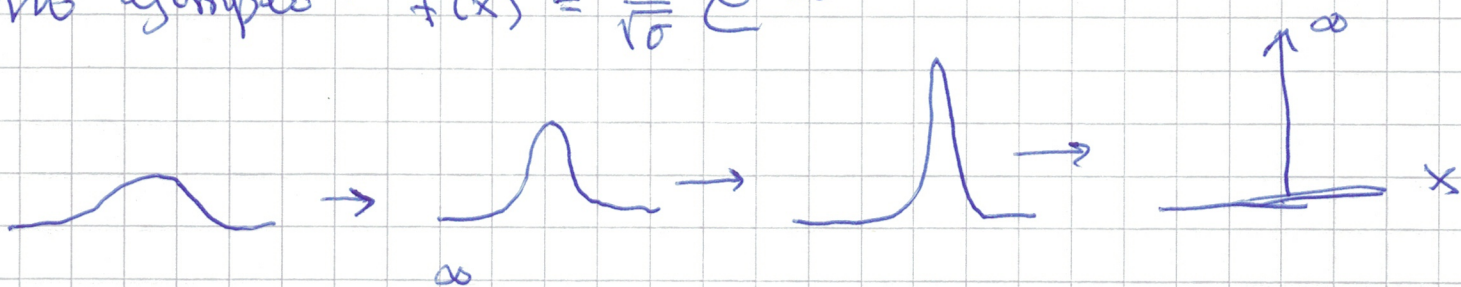
considere $f(x) = \begin{cases} 1/a & 0 < x < a \\ 0 & \text{caso contrario} \end{cases}$

toman límite $a \rightarrow 0$



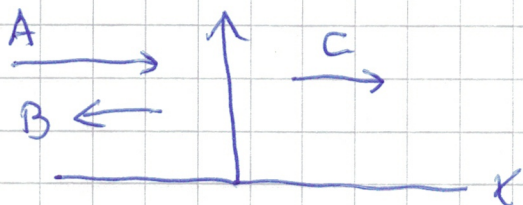
$$\lim_{a \rightarrow 0} f(x) = \delta(x), \text{ donde } \int_{-\infty}^{\infty} \delta(x) dx = 1$$

otro ejemplo: $f(x) = \frac{1}{\sqrt{a}} e^{-\frac{x^2}{2a^2}}$



se cumple: $\int_{-\infty}^{\infty} f(x) \delta(x-b) dx = f(b)$

Scattering a través de una función $S(x)$



$$-\frac{\hbar^2}{2m} \psi'' + \Omega S(x) \psi(x) = E \psi$$

$$(1) \quad -\psi'' + \left(\frac{2m\Omega}{\hbar^2}\right) S(x) \psi = \frac{2mE}{\hbar^2} \psi$$

def: $\gamma = \frac{2m\Omega}{\hbar^2}$
 $K^2 = \frac{2mE}{\hbar^2}$

$$x < 0: \quad -\psi'' = K^2 \psi \Rightarrow \psi = \{ e^{\pm iKx} \}$$

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

$$x > 0: \quad \psi(x) = C e^{iKx}$$

cont. de ψ en $x=0$: $A + B = C$ (2)

discontinuidad de ψ en $x=0$

$$(1) \rightarrow -\psi'' + \gamma S(x) \psi = K^2 \psi \quad \Bigg| \int_{-e}^e$$

$$-\psi'(x) \Bigg|_{-e}^e + \gamma \int_{-e}^e S(x) \psi = K^2 \int_{-e}^e \psi dx$$

$$-\psi'(+e) + \psi'(-e) + \gamma \psi(0) = 0$$

$$-iK C + iK(A - B) + \gamma C = 0$$

$$ik(A-B) = (ik-\gamma)C$$

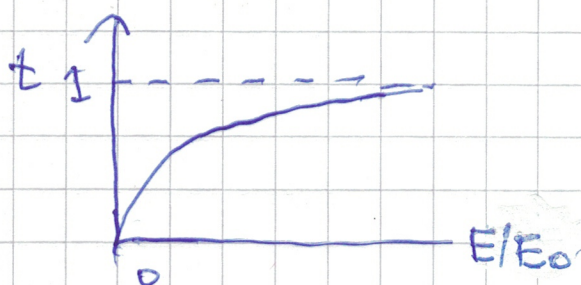
$$A-B = \frac{(ik-\gamma)}{ik} C \quad (3)$$

$$A+B = C$$

$$\frac{A+B = C}{A-B = \frac{(ik-\gamma)}{ik} C} \Rightarrow 2A = C \left\{ 1 + \frac{(ik-\gamma)}{ik} \right\} = \left(\frac{2ik-\gamma}{ik} \right) C$$

$$\Rightarrow \frac{C}{A} = \frac{2ik}{2ik-\gamma} \Rightarrow t = \left| \frac{C}{A} \right|^2 = \frac{1}{1 + (\gamma/2k)^2}$$

$$\therefore t = \frac{1}{1 + (E_0/E)} \quad , \quad \text{donde } E_0 = \frac{m\Omega^2}{2\hbar^2}$$



Nota: t es el mismo si $\Omega \rightarrow -\Omega$

Estado ligado de $V(x) = -\Omega S(x)$

$$V(x) = -\Omega S(x)$$

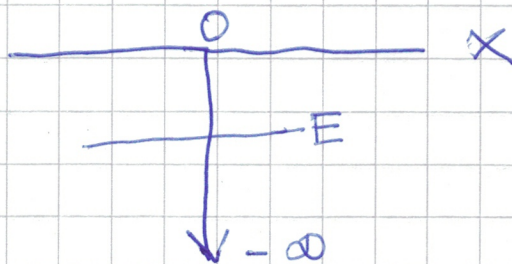
$$-\frac{\hbar^2}{2m} \psi'' - \Omega S(x) \psi = E \psi$$

$$-\psi'' - \gamma S(x) \psi = -K^2 \psi$$

$$\text{donde } \gamma = \frac{2m\Omega}{\hbar^2}$$

$$\text{y } K^2 = -\frac{2mE}{\hbar^2}$$

$$(E < 0)$$



entonces, $\psi'' + \gamma \delta(x) \psi = k^2 \psi$ (4)

Si $x \neq 0$, $\psi'' = k^2 \psi \Rightarrow \psi = \begin{cases} e^{\pm kx} \end{cases}$

$\psi(x) = A e^{-k|x|}$

cont. de ψ en $x=0$ ✓

discont. de ψ' en $x=0$:

$\psi'(0^+) - \psi'(0^-) + \gamma \psi(0) = 0$

$-Ak - Ak + \gamma A \Rightarrow +2Ak = \gamma A \Rightarrow \gamma = 2K$ (5)

$\gamma^2 = 4K^2 = 4\left(-\frac{2mE}{\hbar^2}\right)$

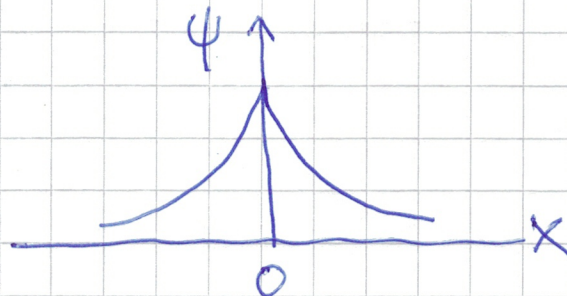
$\left(\frac{2m\Omega}{\hbar^2}\right)^2 = \frac{8m|E|}{\hbar^2} \Rightarrow |E| = \frac{m\Omega^2}{2\hbar^2}$ (6)

Normalización

$1 = \int_{-\infty}^{\infty} |\psi|^2 dx = \int_{-\infty}^{\infty} A^2 e^{-2k|x|} dx$

$\Rightarrow A = \sqrt{\frac{m\Omega}{2\hbar^2}}$

$\psi(x) = \sqrt{\frac{m\Omega}{2\hbar^2}} e^{-\left(\frac{m\Omega}{\hbar^2}\right)|x|}$



Ec. Schrödinger en 2D: caso fácil

$$H(x,y) \Psi(x,y) = E \Psi(x,y)$$

$$\text{Sea } H(x,y) = H_x(x) + H_y(y)$$

$$\text{entonces } \Psi(x,y) = X(x) Y(y) \quad (\text{separación variable})$$

$$\text{con } H_x(x) X(x) = E_x X$$

$$H_y(y) Y(y) = E_y Y$$

$$\begin{aligned} \Rightarrow (H_x + H_y) X Y &= (H_x X) Y + X (H_y Y) = E_x X Y + E_y X Y \\ &= (E_x + E_y) X Y \end{aligned}$$

$$\therefore \boxed{\begin{aligned} E &= E_x + E_y \\ \Psi(x,y) &= X(x) Y(y) \end{aligned}}$$

Schrödinger Eq. in 2-D



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

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi(x,y) = -k^2 \psi(x,y)$$

$$\psi(x,y) = X(x)Y(y)$$

$$\Rightarrow -X''Y + XY'' = -k^2 XY$$

$$\Rightarrow \underbrace{-\frac{X''}{X}}_{k_x^2} + \underbrace{\frac{Y''}{Y}}_{k_y^2} = -k^2$$

$$\Rightarrow X'' = -k_x^2 X \Rightarrow X(x) = A \cos(k_x x) + B \sin(k_x x)$$

$$Y'' = -k_y^2 Y \Rightarrow Y(y) = C \cos(k_y y) + D \sin(k_y y)$$

$$X(0) = X(a) = 0 \Rightarrow X(x) = B \sin\left(\frac{n_x \pi}{a} x\right)$$

$$Y(0) = Y(b) = 0 \Rightarrow Y(y) = D \sin\left(\frac{n_y \pi}{b} y\right)$$

$$\Rightarrow \psi(x,y) = \tilde{A} \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{b} y\right)$$

$$\boxed{\psi(x,y) = \frac{2}{\sqrt{ab}} \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{b} y\right)}$$

$$n_x, n_y = 1, 2, \dots$$

$$\frac{2mE}{\hbar^2} = \frac{n_x^2 \pi^2}{b^2} + \frac{n_y^2 \pi^2}{a^2}$$

$$\Rightarrow E_{n_x, n_y} = \frac{\pi^2 \hbar^2}{2m} \left[\frac{n_x^2}{b^2} + \frac{n_y^2}{a^2} \right] = \frac{\pi^2 \hbar^2}{2mab} \left[\left(\frac{a}{b}\right) n_x^2 + \left(\frac{b}{a}\right) n_y^2 \right]$$

si' $b = 2a$

$$E_{n_x, n_y} = \frac{\pi^2 \hbar^2}{2ma^2} \left[\frac{n_x^2}{4} + n_y^2 \right] = E_0 \left[\left(\frac{n_x}{2}\right)^2 + n_y^2 \right]$$

n_x	n_y	E/E_0	
1	1	5/4	$\rightarrow E_1$
1	2	17/4	$\rightarrow E_3$
2	1	2	$\rightarrow E_2$
2	2	5	$\rightarrow E_4$

si' $b = 10a$

n_x	n_y	E/E_0	
1	1	10.1	dimension 1 congelade
2	1	10.4	
3	1	10.9	
4	1	11.6	
...	...	...	
17	1	38.9	
1	2	40.1	