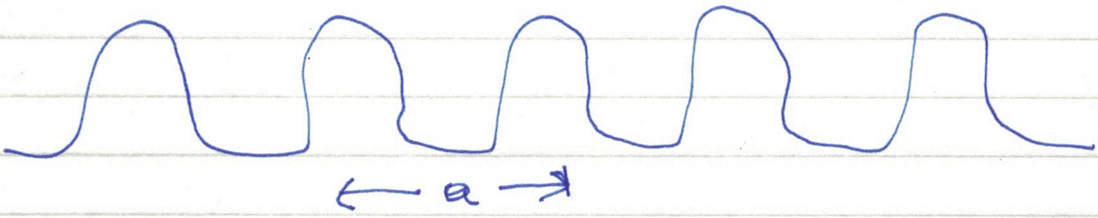
Potenciales Periódicos en 1D

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



<u>ej</u>: e^- en red cristalina 1D

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

$\Rightarrow \psi(x+a) = e^{i\theta}\psi(x)$, pongamos $\theta = ka$

$$\psi(x+a) = e^{ika}\psi(x) \qquad (1)$$

<u>Definimos</u> $u_k(x) \equiv e^{-ikx}\psi(x) \qquad (2)$

$u_k(x)$ es periódica con periodo a.

<u>Dem</u>: $u_k(x+a) = e^{-ik(x+a)}\psi(x+a) = e^{-ikx}\cancel{e^{-ika}}\,\cancel{e^{ika}}\psi(x)$

$$= e^{-ikx}\psi(x) = u_k(x)$$

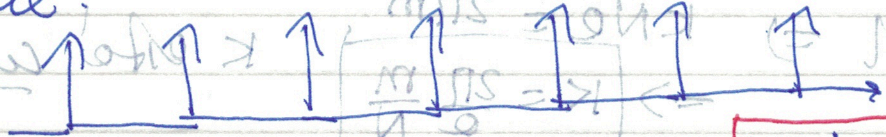
o sea, $u_k(x+a) = u_k(x)$ //

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

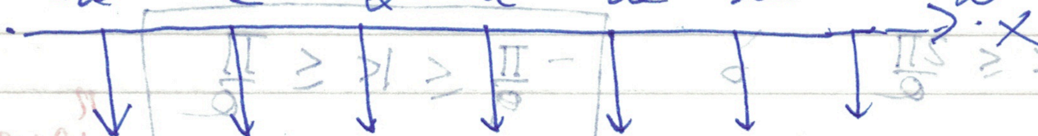
Nota: Podemos elegir $-\frac{\pi}{a} \le k \le \frac{\pi}{a}$

Modelo de Kronig-Penney

Más fácil:



$$\boxed{V(x) = \sum_{n=-\infty}^{\infty} w_0\, \delta(x-na)} \qquad (4)$$



Basta considerar $0<x<a$

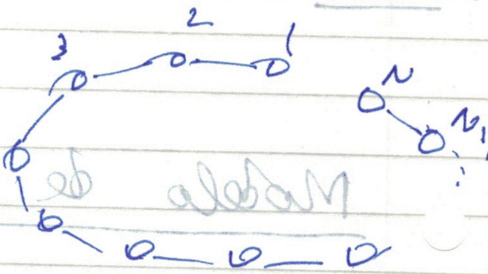
$0<x<a$, $V=0$ $\Rightarrow$ $\psi(x) = A e^{iqx} + B e^{-iqx}$ (5)

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

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

condición de borde periódico

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



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

usando Teo. de Bloch

$$e^{ikNa}\,\psi(x) = \psi(x)$$

$$\Rightarrow e^{ikNa} = 1 \Rightarrow kNa = 2\pi m$$

$$\Rightarrow \boxed{k = \frac{2\pi}{a}\frac{m}{N}}$$ k está cuantizado → cuasi-continuo

$0 \leq k \leq \frac{2\pi}{a}$ ó $\boxed{-\frac{\pi}{a} < k \leq \frac{\pi}{a}}$ "1era zona de Brillouin"

Para evaluar A, B, usamos las condiciones de borde

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

$\Rightarrow u_k(x)$ también debe ser continua:

$$u_k(\varepsilon) - u_k(-\varepsilon) \xrightarrow[\varepsilon \to 0]{} 0$$

Como conocemos sólo $u_k(x)$ para $0 < x < a$, no conocemos $u_k(-\varepsilon)$, pero usamos la periodicidad de u_k:

$$u_k(-\varepsilon) = u_k(-\varepsilon + a)$$

$$\Rightarrow u_k(\varepsilon) - u_k(a-\varepsilon) \xrightarrow[\varepsilon \to 0]{} 0 \qquad (7)$$

Insertando (7) en (6):

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

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

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

$$\left(\frac{d\psi}{dx}\right)_{\varepsilon} = iqAe^{iq\varepsilon} - iqBe^{-iq\varepsilon} \longrightarrow iq(A-B) \qquad (10)$$

$$y \ \left(\frac{d\psi}{dx}\right)_{x=-\varepsilon} = \frac{d}{dx}\left[u_k(x)e^{ikx}\right]_{x=-\varepsilon} = \frac{d}{d(x-a)}\left[u_k(x-a)e^{ik(x-a)}\right]_{x=-\varepsilon+a}$$

$$= \frac{d}{dx}\left[u_k(x)e^{ikx}e^{-ika}\right]_{x=a-\varepsilon} = e^{-ika}\left(\frac{d\psi}{dx}\right)_{x=a-\varepsilon}$$

$$= e^{-ika}\, iq\left(Ae^{iqa} - Be^{-iqa}\right) \qquad (11)$$

Por último $\psi(0) = A + B$

$$\Rightarrow iq\left[A - B - Ae^{+i(q-k)a} + Be^{-i(q+k)a}\right] = \frac{2m w_0}{\hbar^2}(A+B) \qquad (12)$$

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

Insertando (13) en (12)

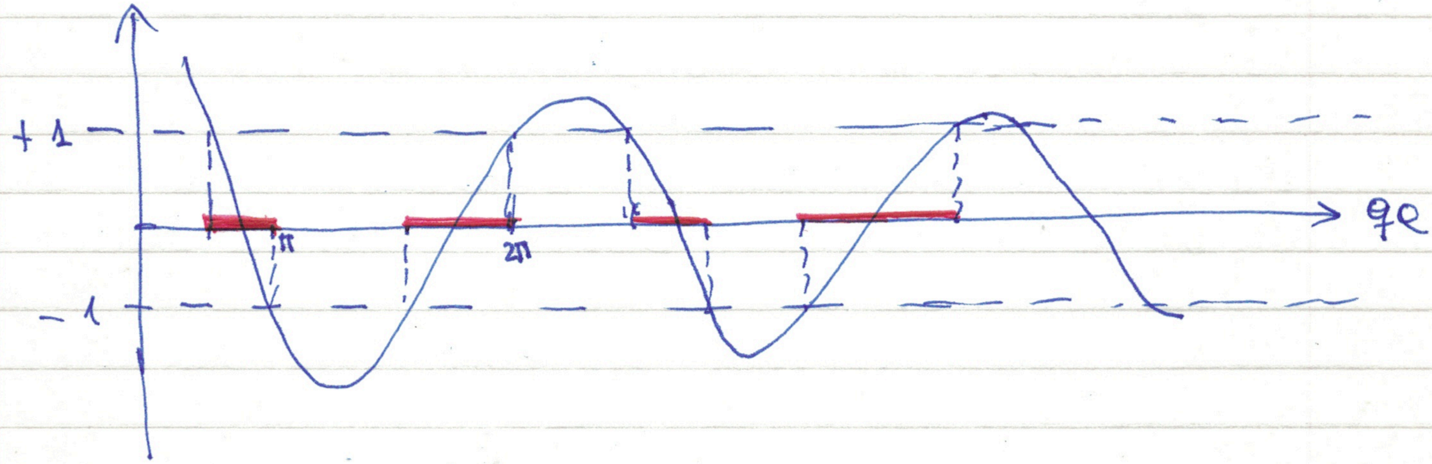
$$A\left(e^{ika} - e^{-iqa} - e^{iqa} + e^{-ika}\right) = A\,\frac{m w_0}{\hbar^2 iq}\left(e^{iqa} - e^{-iqa}\right)$$

$$\Rightarrow \left(\cos(ka) - \cos(qa) - \frac{m w_0}{q\hbar^2}\sin(qa)\right)A = 0 \qquad (14)$$

solución no-trivial $\Rightarrow$

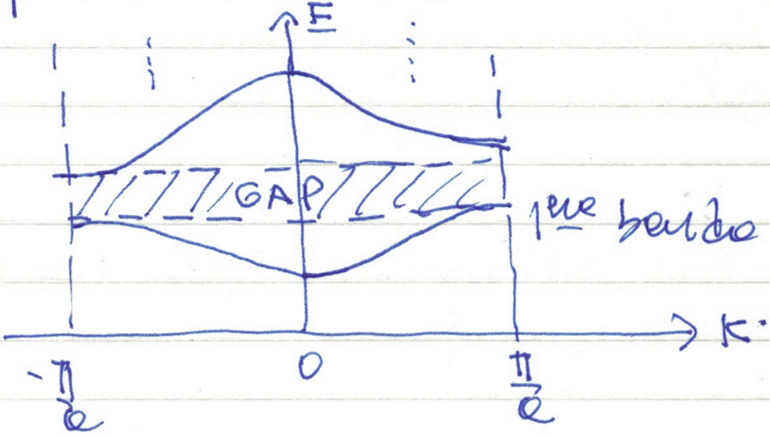
$$\boxed{\cos(ka) = \cos(qa) + \frac{mW_0 a}{\hbar^2}\,\frac{\sin(qa)}{qa}}$$

Solución gráfica..



los valores permitidos de qa caen dentro de las "zonas permitidas" (BANDAS), las cuales están separadas unas de otras por "zonas prohibidas" (GAPS).

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



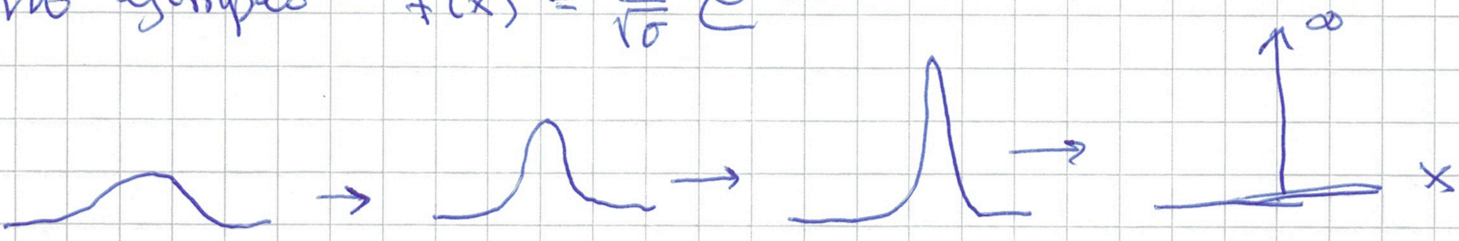
La función $\delta(x)$

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

toman límite $a \to 0$

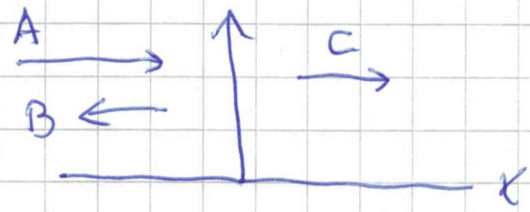
$$\lim_{a \to 0} f(x) = \delta(x) \quad , \text{ donde } \int_{-\infty}^{\infty} \delta(x)\,dx = 1$$

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



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

Scattering a través de una función $\delta(x)$



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

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

$k^2 = \frac{2mE}{\hbar^2}$

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

$x<0$: $-\psi'' = k^2\psi \Rightarrow \psi = \{e^{\pm ik}\}$

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

$x>0$: $\psi(x) = Ce^{ikx}$

cont. de ψ en $x=0$: $A + B = C$ (2)

discontinuidad de ψ en $x=0$

(1) $\rightarrow$ $-\psi'' + \gamma\,\delta(x)\psi = k^2\psi \quad \Big/ \int_{-\epsilon}^{\epsilon}$

$$-\psi'(x)\Big|_{-\epsilon}^{\epsilon} + \gamma\int_{-\epsilon}^{\epsilon}\delta(x)\psi = k^2\int_{-\epsilon}^{\epsilon}\psi\,dx$$

$$-\psi'(+\epsilon) + \psi'(\bar{\epsilon}) + \gamma\psi(0) = 0$$

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

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

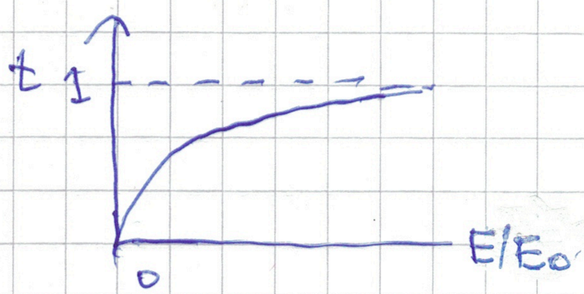
$$A - B = \frac{(ik-\gamma)}{ik}\,C \qquad (3)$$

$$A + B = C$$

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

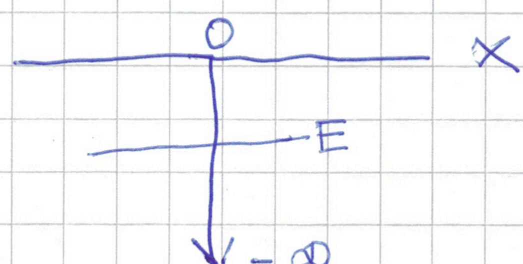
$$\Rightarrow \frac{C}{A} = \frac{2ik}{2ik-\gamma} \Rightarrow t = \left|\frac{C}{A}\right|^2 = \frac{1}{1+(\gamma/2k)^2}$$

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



<u>Nota</u>: t es el <u>mismo</u> si $\Omega \to -\Omega$

<u>Estado ligado de $V(x) = -\Omega\,\delta(x)$</u>



$$V(x) = -\Omega\,\delta(x)$$

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

$$-\psi'' - \gamma\,\delta(x)\psi = -k^2\psi$$

donde $\gamma = \frac{2m\Omega}{\hbar^2}$ y $k^2 = -\frac{2mE}{\hbar^2}$ $\qquad (E<0)$

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

Si $x \neq 0$, $\psi'' = K^2\psi \Rightarrow \psi = \{e^{\pm Kx}\}$

$\psi(x) = A\, e^{-K|x|}$ cont. de ψ en $x=0$ ✓

iscont. de ψ' en $x=0$:

$+ \quad \psi'(\epsilon) - \psi'(-\epsilon) + \gamma\psi(0) = 0$

$-AK - AK + \gamma A \Rightarrow +2\cancel{A}K = \gamma\cancel{A} \Rightarrow \gamma = 2K$ (5)

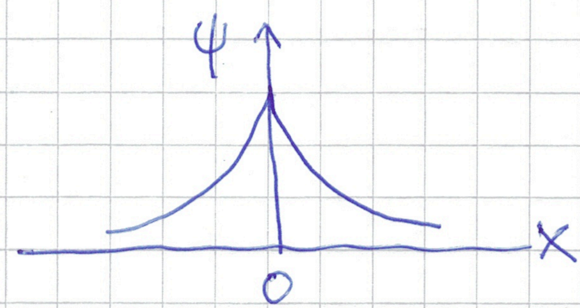
$\gamma^2 = 4K^2 = 4\left(\frac{-2mE}{\hbar^2}\right)$

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

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

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

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



Ec. Schrödinger en 2D: caso fácil

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

Sea $H(x,y) = H_x(x) + H_y(y)$

entonces $\Psi(x,y) = X(x)\,Y(y)$ (separación variable)

con $H_x(x)X(x) = E_x X$

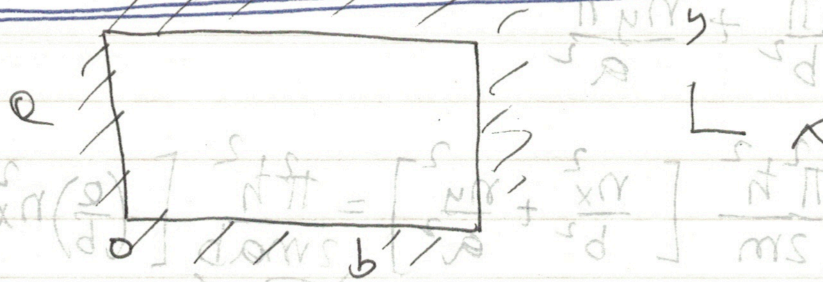
$H_y(y)Y(y) = E_y Y$

$$\Rightarrow (H_x + H_y)XY = (H_x X)Y + X(H_y Y) = E_x XY + E_y XY$$

$$= (E_x + E_y)XY$$

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

Schrödinger Eq. in 2-D



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

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

$\psi(x,y) = X(x)\,Y(y)$ >> Generalized <<

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

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

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

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

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

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

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

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

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

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

$$\Rightarrow E_{n_x,n_y} = \frac{\pi^2\hbar^2}{2m}\left[\frac{n_x^2}{b^2} + \frac{n_y^2}{a^2}\right] = \underbrace{\frac{\pi^2\hbar^2}{2mab}}_{E_0}\left[\left(\frac{a}{b}\right)n_x^2 + \left(\frac{b}{a}\right)n_y^2\right]$$

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	$\longrightarrow E_1$
1	2	17/4	$\longrightarrow E_3$
2	1	2	$\longrightarrow E_2$
2	2	5	$\longrightarrow E_4$

si $\boxed{b = 10a}$

n_x	n_y	E/E_0
1	1	10.1
2	1	10.4
3	1	10.9
4	1	11.6
⋮	⋮	
17	1	38.9
1	2	40.1
(18)	(1)	(42.4)

} dimension Y "congelada"