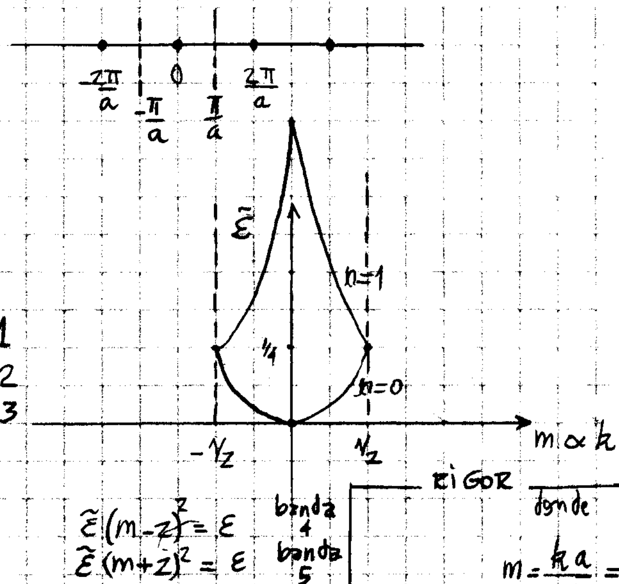
GUÍA 3 : Electrones en un Potencial Periódico

1. Átomos iguales a distancia a

i) $\longleftarrow a \longrightarrow$ $\quad \vec{a}_1 = a\hat{x} \qquad \vec{b}_1 = \frac{2\pi}{a}\hat{x}$



$$\frac{\hbar^2(k-K)^2}{2m} = \mathcal{E}$$

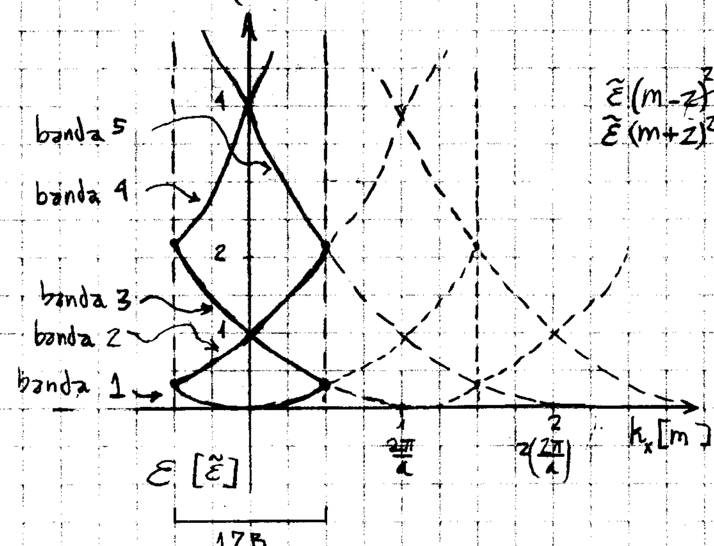
$$\underbrace{\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2}_{\tilde{\mathcal{E}}}(m-n)^2 = \mathcal{E}$$

$n=0 \qquad \tilde{\mathcal{E}}\, m^2 = \mathcal{E} \qquad$ banda 1

$n=1 \qquad \tilde{\mathcal{E}}.(m-1)^2 = \mathcal{E} \qquad$ banda 2

$n=-1 \qquad \tilde{\mathcal{E}}.(m+1)^2 = \mathcal{E} \qquad$ banda 3

$$\tilde{\mathcal{E}}(m-2)^2 = \mathcal{E}$$
$$\tilde{\mathcal{E}}(m+2)^2 = \mathcal{E}$$



RIGOR

donde m es

$$m = \frac{k\,a}{2\pi} = \frac{\cancel{2\pi}}{L}\tilde{m}\frac{a}{\cancel{2\pi}}$$

$$m = \frac{a}{L}\tilde{m}$$

$$k - K = \frac{2\pi}{L}\tilde{m} - \frac{2\pi}{a}n$$
$$= \frac{2\pi}{a}\left(\frac{a}{L}\tilde{m} - n\right)$$

$$k - K = \frac{2\pi}{a}(m - n)$$

$\# \in \mathbb{N}$ si $\tilde{m}$ es suficientemente grande

ii)

$$\mathcal{E}_n(k) = \frac{\hbar^2}{2m}(k-K_n)^2 \Rightarrow \left\{ K_n \rightarrow \text{banda} \right. \qquad K_1 = \frac{2\pi}{a} \qquad K_2 = -\frac{2\pi}{a}$$

$$\mathcal{E}_1(k) = \frac{\hbar^2}{2m}\left(k - \frac{2\pi}{a}\right)^2$$

$$\mathcal{E}_2(k) = \frac{\hbar^2}{2m}\left(k + \frac{2\pi}{a}\right)^2$$

$$\Delta k = \frac{2\pi}{L}$$

Por definición $\quad g_n(\varepsilon) = 2\int \frac{d\vec{k}}{(2\pi)^3}\,\delta(\varepsilon - \mathcal{E}_n(\vec{k}))$ (3D)

celda primitiva del espacio recíproco

$$d\mathcal{E} = \frac{\hbar^2}{2m}2(k-K_n)\,dk$$

$$\frac{1}{(k-K_n)}\frac{m}{\hbar^2}d\varepsilon = dk$$

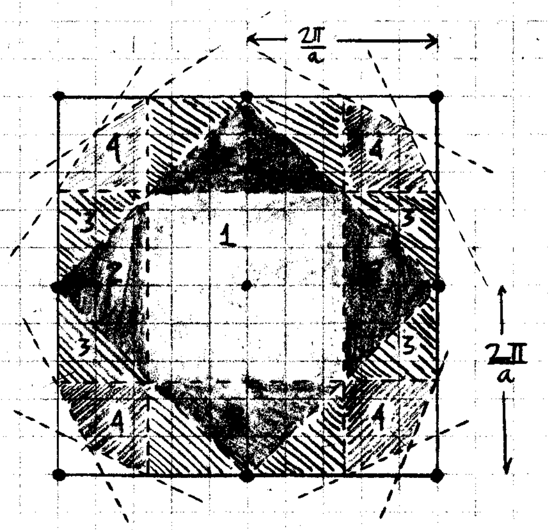
$$\frac{(k-K_n)}{2}d\varepsilon = \frac{\hbar^2}{2m}(\quad)^2 dk$$

* continúa 1 hoja luego

2.

$\vec{a}_1 = a\hat{x}$ $\qquad$ $\vec{b}_1 = 2\pi/a\ \hat{x}$

$\vec{a}_2 = a\hat{y}$ $\qquad$ $\vec{b}_2 = 2\pi/a\ \hat{y}$



i)

- A la 3^{ra} zona se llega atravesando $(3-1)=2$ planos
- A la 4^{ta} zona se llega atravesando $(4-1)=3$ planos
- etc

ii) En 2D

Usamos la discretización

$k_x = \left(\frac{2\pi}{L}\right) n_x$

$k_y = \left(\frac{2\pi}{L}\right) n_y$

donde L es macroscópico

electrones libres en una caja de lado L.

$\#$ puntos en el espacio discretizado $= \frac{\Omega L^2}{(2\pi)^2} = \frac{\pi k_F^2 L^2}{4\pi^2} = \frac{k_F^2 L^2}{4\pi}$

El # de electrones será dos veces el # de puntos

$\Rightarrow$ # electrones

Hay 2 electrones asociados a un $\vec{k}$

$N = 2 \cdot \frac{k_F^2 L^2}{4\pi} = \frac{k_F^2 L^2}{2\pi} \Rightarrow n = \frac{k_F^2}{2\pi}$

$k_F = \sqrt{2\pi n}$

densidad electrónica "Real" $\frac{\#\text{ electr.}}{\text{Área}}$

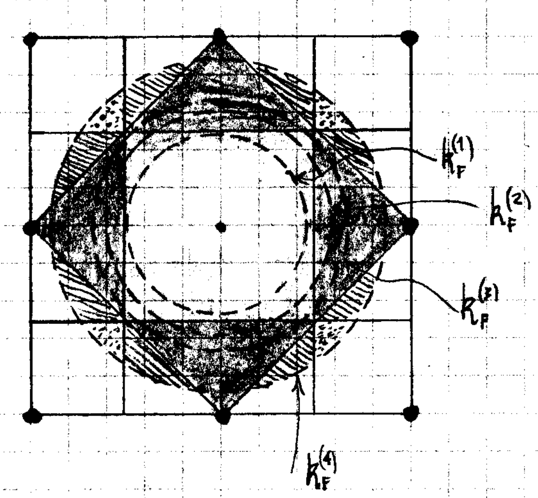
No se deben confundir las dos discretizaciones empleadas: $\left(\frac{2\pi}{L}\right) n_j = k_j$ divide al espacio en pequeñas celditas y $\frac{2\pi}{a} n_j = b_j$ son vectores de la red recíproca.

$\frac{N}{L^2} = n = \frac{N}{q \cdot a^2} = \frac{N}{q} \cdot \frac{1}{a^2} = \frac{N_q}{a^2}$ → # de electrones por celda; → Área de una celda

← Se mide k_F en términos del parámetro de la Red Recíproca

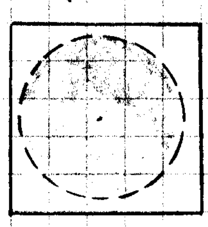
Esto lleva al siguiente set de valores de k_F $\qquad k_F = \frac{2\pi}{a}\sqrt{\frac{N_q}{2\pi}}$

$k_F^{(4)} \cong \left(\frac{2\pi}{a}\right) 0{,}79 \qquad k_F^{(1)} \cong \left(\frac{2\pi}{a}\right) 0{,}4 \;;\; k_F^{(2)} \cong \left(\frac{2\pi}{a}\right) 0{,}56 \;;\; k_F^{(3)} \cong \left(\frac{2\pi}{a}\right) 0{,}69$



iii) En un esquema de zona reducida tendremos:

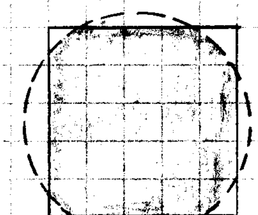
$N_q = 1$

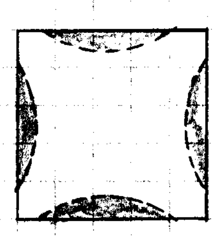


Todo queda en ZB1

$N_q = 2$

ZB1





ZB2

$N_q = 3$

Es idem que el anterior, pero con un factor de escala: todo queda en la 1^{er} y 2^{da} zona de Brillouin

$N_q = 4$

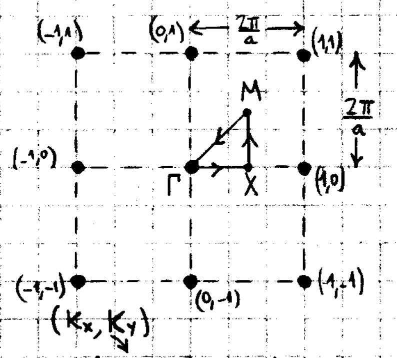
1er ZB | 2da ZB | 3er ZB | 4ta ZB

iv)

$$\left[\frac{\hbar^2}{2m}(\vec{k}-\vec{K})^2 - \varepsilon\right] C_{\vec{k}-\vec{K}} + \sum_{\vec{K}'} U_{\vec{K}'-\vec{K}}\, C_{\vec{k}-\vec{K}'} = 0$$

Como consideramos electrones libres, será $U_{\vec{K}'-\vec{K}} = 0$ con lo cual

$$\boxed{\frac{\hbar^2}{2m}(\vec{k}-\vec{K})^2 = \mathcal{E}}$$



Es conveniente trabajar en unidades de $2\pi/a$

$$\frac{\hbar^2}{2m}\left[(k_x - K_x)^2 + (k_y - K_y)^2\right]$$

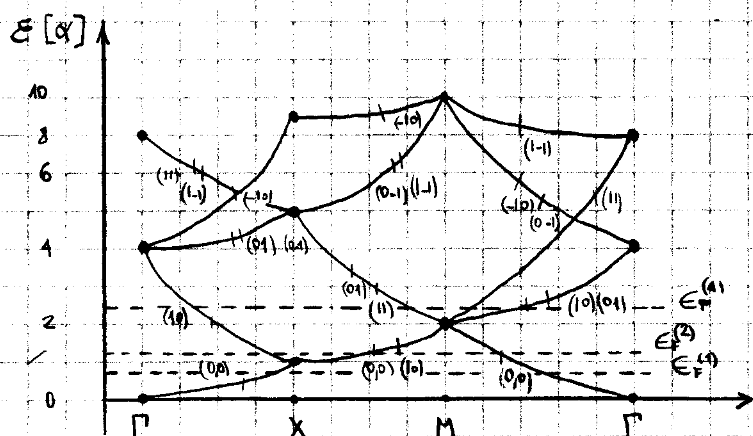
$$E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \left[(\tilde{k}_x - n_x)^2 + (\tilde{k}_y - n_y)^2\right]$$

$$E = 4\overbrace{\left(\frac{\pi^2\hbar^2}{a^2 2m}\right)}^{\alpha}\left[(\tilde{k}_x - n_x)^2 + (\tilde{k}_y - n_y)^2\right]$$

$\tilde{k} = \frac{a}{2\pi}k$

	$\mathcal{E}$	(0,0)	(1,0)	(0,1)	(-1,0)	(0,-1)	(1,1)	(1,-1)
$\vec{k}=(0,0)$	Γ	0	4	4	4	4	8	8
$\vec{k}=(1/2,0)$	X	1	1	5	9	5	5	5
$\vec{k}=(1/2,1/2)$	M	2	2	2	10	10	2	10

La energía se halla en unidades de α



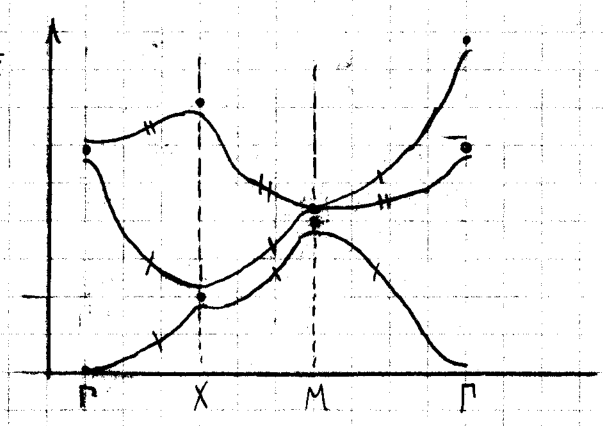
$$\epsilon_F^{(1)} = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 (0{,}4)^2$$

$$\epsilon_F^{(1)} = 4\underbrace{\left(\frac{\pi^2\hbar^2}{a^2 2m}\right)}_{\alpha} 0{,}16 \sim 0{,}64\,\alpha$$

$$\epsilon_F^{(2)} = 4\,.\,\alpha\,.\,0{,}3136 \sim 1{,}25\,\alpha$$

$$\epsilon_F^{(4)} = 4\,.\,\alpha\,.\,0{,}6241 \sim 2{,}5\,\alpha$$

I) La introducción de un potencial periódico débil provocará el desdoblamiento de algunas bandas con rompimiento de la degeneración.



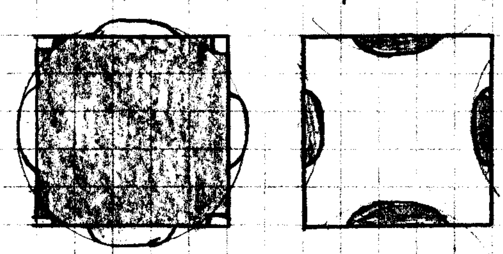
En particular la 1er banda (la más inferior) ve la deg. de orden 2 totalmente rota en X, pero no en M donde era de orden 4 y ha quedado degeneración remanente de orden 2.
Cualitativamente en los valores de energía ocurre un desdoblamiento como

$$\mathcal{E} = \mathcal{E}_0 \pm U_{\vec{k}}$$

, donde $U_{\vec{k}}$ es el coef. representativo del desarrollo de Fourier del potencial periódico.

Para $N_q = 1$ la superficie de Fermi no se modifica (no se atraviesan planos de Bragg).

Para $N_q = 2$ ya se empiezan a atravesar planos de Bragg y la superficie se ve modificada en torno a dichos planos de manera de ser $\perp$ al plano de Bragg.



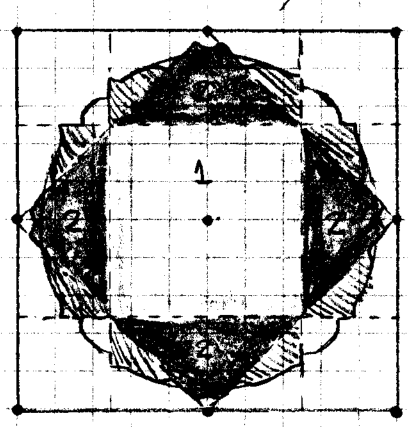
ZB1 ZB2

Se puede ver que esto hace que el nivel de fermi "llene" en mayor medida la primera zona

Para $N_q = 3$ es similar, con una variación de escala

Para $N_q = 4$ el dibujo ya es muy complicado se ven los bordes redondeados

ZB1 ZB2 ZB3 ZB4



La superficie de Fermi adquiere forma de "Bola con berrugas"

* CONTINUACIÓN EJERCICIO 1

$$g_n(\varepsilon) = \frac{dn}{d\varepsilon} = \frac{dn}{dk}\frac{dk}{d\varepsilon} = \frac{dn/dk}{d\varepsilon/dk} = \frac{2/\pi}{\frac{\hbar^2}{m}(k-K_n)} = \boxed{\frac{2m}{\pi\hbar^2(k-K_n)} = g_n(k)}$$

*** Análisis :**

de celdas prim. reales → $N = \#\ k$ permitidos → $\dfrac{\text{Volumen celda prim. red recíproca}}{\text{Volumen de un } k \text{ de Bloch permitido}} = \dfrac{\left(\frac{2\pi}{a}\right)^3}{\left(\frac{2\pi}{L}\right)^3} =$ # de k's permitidos en una celda red recíproca

$\dfrac{V}{v_{real}} = N$

$\#$ de k's por celda $= \left(\dfrac{L}{a}\right)^3 = \dfrac{V}{v} = \dfrac{N.a^3}{a^3}$

⇒ Hay N k's de Bloch por cada celda primitiva recíproca.

→ Hay 2N electrones

$$\frac{dn}{dk} \doteq \frac{\text{densidad de electrones}}{\text{densidad de vectores } k} = \frac{2\overbrace{\left(\frac{2N}{L}\right)}^{\text{por spin}}}{\frac{N}{L/2\pi}} = \cancel{2}\,\frac{2N}{\cancel{L}}\,\frac{\cancel{L}}{N\cancel{2}\pi} = \frac{2}{\pi}$$

Vol. espacio k ocupado por un k permitido $\Delta \vec{k} = \dfrac{\left(2\pi/a\right)^3}{N} = \left(\dfrac{2\pi}{L}\right)^3$

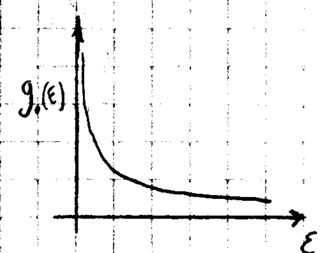
(Volumen de la celda; N: # de k's en una celda)

$n = \dfrac{2N}{L}$ (# de k' de Bloch) $\qquad \rho_k = \dfrac{N}{\left(\frac{2\pi}{a}\right)}$

$$g_0(k) = \frac{2m}{\pi\hbar^2 k} = \frac{2m}{\pi\hbar\sqrt{2m\varepsilon}} = \frac{\sqrt{2m}}{\pi\hbar\sqrt{\varepsilon}} = g_0(\varepsilon)\ ,$$

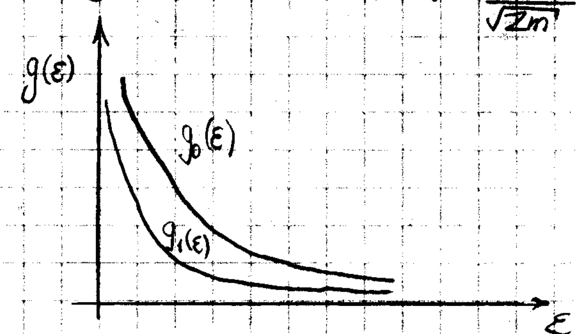
(Coincide con resultado electrón libre GUIA 2, Problema 5i))

banda n=0 es electrón libre →



$$g_1(\varepsilon) = \frac{2m}{\pi\hbar^2(k-K_1)} = \frac{2m}{\pi\hbar\sqrt{2m\varepsilon_1}} = \frac{\sqrt{2m}}{\pi\hbar\sqrt{\varepsilon_1}}$$

$$g_1(\varepsilon) = \frac{2m}{\pi\hbar^2 k - \pi\hbar^2 K_1} = \frac{2m}{\pi\hbar\sqrt{2m\varepsilon} - \pi\hbar^2 K_1} = \frac{\sqrt{2m}}{\pi\hbar\sqrt{\varepsilon_0} - \frac{\pi\hbar^2 K_1}{\sqrt{2m}}}$$

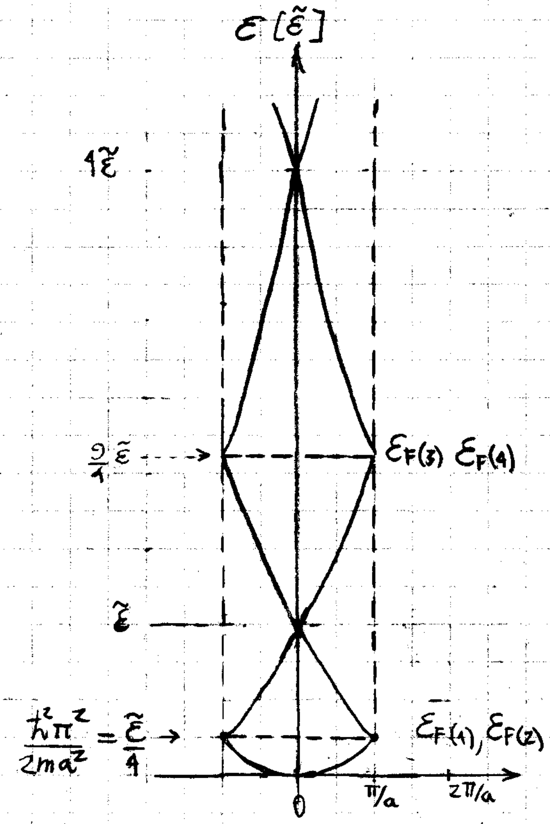


V) Para 1D es $n = \frac{k_F 2}{\pi}$ ← electrones libres

$$\frac{N}{L} = \frac{2k_F}{\pi} = \frac{N}{\underbrace{q}_{\#\text{celda}} \cdot a} = \frac{k_F 2}{\pi} \rightarrow \boxed{k_F = \frac{\pi}{2}\frac{N_q}{a}}$$; $N_q \equiv$ # de electrones por celda

Con $N_q = 2 \rightarrow k_F = \frac{\pi}{a} \rightarrow \mathcal{E}_{nF} = \frac{\hbar^2}{2m}(k - K_n)^2$

Comparando con el punto 1) vemos $\tilde{\mathcal{E}} = \frac{2\hbar^2\pi^2}{ma^2} \rightarrow \mathcal{E}_F = \tilde{\mathcal{E}} \Rightarrow$



$(k=0)$ banda 1 $\quad \mathcal{E}_{1F} = \frac{\hbar^2 k_F^2}{2m}$ ↗ $\frac{\hbar^2\pi^2}{2ma^2}$

$\left(k = \frac{2\pi}{a}\right)$ banda 2 $\quad \mathcal{E}_{2F} = \frac{\hbar^2}{2m}\left(k_F - \frac{2\pi}{a}\right)^2$

$\left(k = -\frac{2\pi}{a}\right)$ banda 3 $\quad \mathcal{E}_{3F} = \frac{\hbar^2}{2m}\left(k_F + \frac{2\pi}{a}\right)^2$

$\mathcal{E}_{1F} = \frac{\hbar^2\pi^2}{2ma^2} = \tilde{\mathcal{E}}/4 \qquad (0)$

$\mathcal{E}_{2F} = \frac{\hbar^2\pi^2}{2ma^2} = \tilde{\mathcal{E}}/4 \qquad \left(\frac{2\pi}{a}\right)$

$\mathcal{E}_{3F} = \frac{\hbar^2}{2m}\frac{9\pi^2}{a^2} = \frac{9}{4}\tilde{\mathcal{E}} \qquad \left(-\frac{2\pi}{a}\right)$

$\mathcal{E}_{4F} = \frac{9}{4}\tilde{\mathcal{E}} \qquad \left(\frac{4\pi}{a}\right)$

$\mathcal{E}_{5F} = \frac{\hbar^2}{2m}25\frac{\pi^2}{a^2} = \frac{25}{4}\tilde{\mathcal{E}} \qquad \left(-\frac{4\pi}{a}\right)$

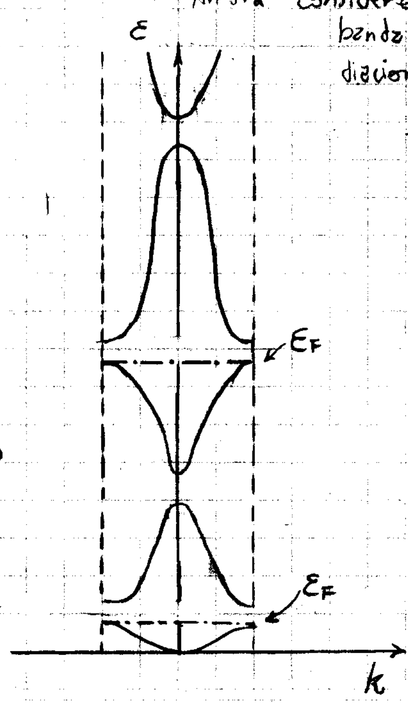
$\mathcal{E}_{6F} = \qquad \left(\frac{6\pi}{a}\right)$

$\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\pi^2}{2ma^2}$

$\frac{\hbar^2}{2m}\left(k - \frac{2\pi}{a}\right)^2 \rightarrow k=0 \quad \frac{\hbar^2}{2m}\frac{4\pi^2}{a^2}$

$\frac{\hbar^2}{2m}\left(k - \frac{4\pi}{a}\right)^2 \rightarrow k=0 \quad \frac{\hbar^2}{2m}\frac{16\pi^2}{a^2}$

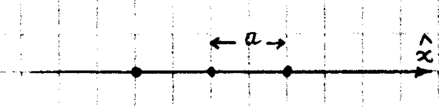
Ahora consideremos un potencial apreciable; las bandas de energía se deforman en las inmediaciones de los planos de Bragg

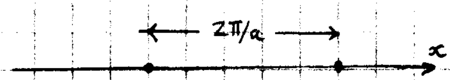


Tendremos sistema aislante si los electrones se hallan en la banda 1, puesto que la $\mathcal{E}_F$ queda por encima y no toca las siguientes bandas
Las $\mathcal{E}_F$ son ligeramente menores a las del caso electrón libre

El hecho de que se rompa la degeneración en los puntos donde ésta existe dependerá del potencial $U(\vec{r})$ que estemos considerando.

6.





$$\psi = \alpha e^{ikx} + \beta e^{i(k-\frac{2\pi}{a})x}$$

$$V = V_1 . \cos\left(\frac{2\pi x}{a}\right) \;\rightarrow\; V = \frac{V_1}{2} e^{\frac{i2\pi}{a}x} + \frac{V_1}{2} e^{-\frac{i2\pi}{a}x}$$

$$\frac{d\psi}{dx} = \alpha e^{ikx} ik + \beta e^{i(k-\frac{2\pi}{a})x} i\left(k-\frac{2\pi}{a}\right)$$

$$\frac{d^2\psi}{dx^2} = \alpha e^{ikx}(ik)^2 + \beta e^{i(k-\frac{2\pi}{a})x} i^2\left(k-\frac{2\pi}{a}\right)^2$$

$$= -\alpha k^2 e^{ikx} - \beta \cdot \left(k-\frac{2\pi}{a}\right)^2 e^{i(k-\frac{2\pi}{a})x}$$

$$+\frac{\hbar^2}{2m}\alpha k^2 e^{ikx} + \frac{\hbar^2}{2m}\beta\left(k-\frac{2\pi}{a}\right)^2 e^{i(k-\frac{2\pi}{a})x} + \frac{V_1}{2}\alpha e^{i(k+\frac{2\pi}{a})x} + \frac{V_1}{2}\alpha e^{i(k-\frac{2\pi}{a})x}$$
$$+\frac{V_1}{2}\beta e^{ikx} + \frac{V_1}{2}\beta e^{i(k-\frac{4\pi}{a})x} = \varepsilon\alpha e^{ikx} + \varepsilon\beta e^{i(k-\frac{2\pi}{a})x}$$

A) Multiplicando por e^{-ikx} se tiene:

$$\frac{V_1}{2}\beta + \frac{V_1}{2}\beta e^{\frac{i4\pi}{a}x}$$

$$\frac{\hbar^2}{2m}\alpha k^2 + \frac{\hbar^2}{2m}\beta\left[k-\frac{2\pi}{a}\right]^2 e^{-\frac{i2\pi x}{a}} + \frac{V_1}{2}\alpha e^{\frac{i2\pi x}{a}} + \frac{V_1}{2}\alpha e^{-\frac{i2\pi x}{a}} = \varepsilon\alpha + \varepsilon\beta e^{-\frac{i2\pi x}{a}}$$

B) Multiplicando por $e^{-i(k-\frac{2\pi}{a})x}$ se tiene:

$$\frac{\hbar^2}{2m}\alpha k^2 e^{\frac{i2\pi x}{a}} + \frac{\hbar^2}{2m}\beta\left[k-\frac{2\pi}{a}\right]^2 + \frac{V_1}{2}\alpha e^{\frac{i4\pi x}{a}} + \frac{V_1}{2}\alpha + \frac{V_1}{2}\beta e^{\frac{i2\pi x}{a}} + \frac{V_1}{2}\beta e^{-\frac{i2\pi x}{a}}$$
$$= \varepsilon\alpha e^{\frac{i2\pi x}{a}} + \varepsilon\beta$$

$$\int_{-L}^{L} e^{\frac{i2\pi x}{a}} dx = -\int_{-\frac{i2\pi L}{a}}^{\frac{i2\pi L}{a}} e^{u} \frac{a i}{\pi} du = \frac{ia}{\pi} 2 \,\text{sen}\left(\frac{2\pi L}{a}\right) = 0 \;\Rightarrow\; \text{usando esta integral:}$$

$2i\frac{\pi}{a}x = u$

$i\frac{\pi}{a}dx = du$

A) $$\frac{\hbar^2\alpha k^2}{2m}\cancel{2L} + \frac{V_1}{2}\beta\cancel{2L} = \varepsilon\alpha\cancel{2L}$$

$$\frac{\hbar^2 k^2\alpha}{2m} + \frac{V_1}{2}\beta = \varepsilon\alpha$$

B) $$\frac{\hbar^2\beta}{2m}\left[k-\frac{2\pi}{a}\right]^2\cancel{2L} + \frac{V_1}{2}\alpha\cancel{2L} = \varepsilon\beta\cancel{2L}$$

$$\frac{\hbar^2}{2m}\left[k-\frac{2\pi}{a}\right]^2\beta + \frac{V_1}{2}\alpha = \varepsilon\beta$$

Resolvemos el sistema de ecuaciones

$$\varepsilon^{\circ}\alpha + \frac{V_1}{2}\beta = \varepsilon\alpha \;\rightarrow\; (\varepsilon-\varepsilon^{\circ})\alpha = \frac{V_1}{2}\beta$$

$$\frac{V_1}{2}\alpha + \varepsilon'\beta = \varepsilon\beta \qquad (\varepsilon-\varepsilon')\beta = \frac{V_1}{2}\alpha$$

$$(\varepsilon-\varepsilon^{\circ})\frac{2}{V_1}(\varepsilon-\varepsilon') = \frac{V_1}{2}$$

$$(\mathcal{E}-\mathcal{E}^0)(\mathcal{E}-\mathcal{E}') = \frac{V_1^2}{4}$$

$$\mathcal{E}^2 - \mathcal{E}^0\mathcal{E} - \mathcal{E}\mathcal{E}' + \mathcal{E}^0\mathcal{E}' = \frac{V_1^2}{4}$$

$$\underset{a}{\mathcal{E}^2} - \underset{b}{(\mathcal{E}'+\mathcal{E}^0)}\mathcal{E} + \underset{c}{\left[\mathcal{E}^0\mathcal{E}' - \frac{V_1^2}{4}\right]} = 0$$

$$\mathcal{E}'^2 + \mathcal{E}^{0\,2} + 2\mathcal{E}'\mathcal{E}^0 - 4\mathcal{E}^0\mathcal{E}' + V_1^2$$
$$(\mathcal{E}'-\mathcal{E}^0)^2 + V_1^2$$

$$\mathcal{E} = \frac{\mathcal{E}^0+\mathcal{E}' \pm \sqrt{(\mathcal{E}'+\mathcal{E}^0)^2 - 4.(\mathcal{E}^0\mathcal{E}' - V_1^2/4)}}{2}$$

$$\mathcal{E} = \frac{1}{2}\left(\frac{\hbar^2k^2}{2m} + \frac{\hbar^2}{2m}\left(k-\frac{2\pi}{a}\right)^2 \pm \sqrt{\left(\frac{\hbar^2}{2m}\right)^2\left(k^2-\left(k-\frac{2\pi}{a}\right)^2\right)^2 + \left(\frac{\hbar^2}{2m}\right)^2\left(\frac{2m}{\hbar^2}\right)^2 V_1^2}\right.$$

$$\mathcal{E} = \frac{1}{2}\left(\frac{\hbar^2k^2}{2m} + \frac{\hbar^2k^2}{2m} + \frac{\hbar^2 k\pi 2}{ma} - \frac{\hbar^2 2\pi^2}{ma^2} \pm \left(\frac{\hbar^2}{2m}\right)^2 \cdot\right.$$
$$\cdot \sqrt{\left(k^2-\left[k-\frac{2\pi}{a}\right]^2\right)^2 + V_1^2\left(\frac{2m}{\hbar^2}\right)^2}$$

$$\mathcal{E} = \frac{1}{2}\left[\frac{\hbar^2k^2}{m} + \frac{\hbar^2\pi}{ma}2\left(k-\frac{\pi}{a}\right) \pm \left(\frac{\hbar^2}{2m}\right)\sqrt{\left(\frac{4\pi}{a}\right)^2\left(k-\frac{\pi}{a}\right)^2 + V_1^2\left(\frac{2m}{\hbar^2}\right)^2}\right.$$

* <u>Cálculo extra</u>

$$\left[k^2-\left(k-\frac{2\pi}{a}\right)^2\right]^2 = \left(\cancel{k^2} - \cancel{k^2} + 4\frac{k\pi}{a} - \frac{4\pi^2}{a^2}\right)^2 = \left(\frac{4\pi}{a}\right)^2\left(k-\frac{\pi}{a}\right)^2$$

$$\mathcal{E} = \frac{\hbar^2k^2}{2m} + \frac{\hbar^2\pi}{am}\left(k-\frac{\pi}{a}\right) \pm \frac{1}{\cancel{2}}\frac{\hbar^2}{\cancel{2}m}\left(\frac{4\pi}{a}\right)\sqrt{\left(k-\frac{\pi}{a}\right)^2 + V_1^2\left(\frac{\cancel{2}ma}{\cancel{4}_2\pi\hbar^2}\right)^2}$$

$$\mathcal{E} = \frac{\hbar^2k^2}{2m} + \frac{\hbar^2\pi}{am}\left[\left(k-\frac{\pi}{a}\right) \pm \left(\left(k-\frac{\pi}{a}\right)^2 + \left(\frac{V_1 am}{2\pi\hbar^2}\right)^2\right)^{1/2}\right]$$

En $k=\frac{\pi}{a}$ será: $\rightarrow$ $$\mathcal{E} = \frac{\hbar^2k^2}{2m} + \frac{\cancel{\hbar^2\pi}}{\cancel{am}}\cdot\left(\pm\frac{V_1\cancel{am}}{2\cancel{\pi\hbar^2}}\right) = \boxed{\frac{\hbar^2k^2}{2m} \pm \frac{V_1}{2} = \mathcal{E}}$$

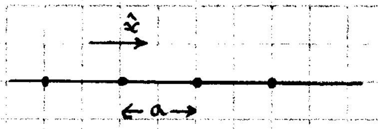
$$\mathcal{E} \cong \frac{\hbar^2k^2}{2m} + \frac{\hbar^2\pi}{am}\cdot\left(k-\frac{\pi}{a}\right)\left[1 \pm \sqrt{1 + \underbrace{\left(\frac{V_1am}{2\pi\hbar^2}\right)^2}_{\equiv v}\underbrace{\left(k-\frac{\pi}{a}\right)^{-2}}_{\equiv f}}\right]$$

$$+\frac{\hbar^2\pi}{am}\cdot f\left(1 \pm \left(1+\frac{v^2}{2f^2}\right)\right)$$

$$\frac{\hbar^2\pi}{am}\left(-\frac{v^2}{2f^1}\right) = \frac{\cancel{\hbar^2\pi}}{\cancel{am}}\left(-\frac{V_1}{4}\left(\frac{am}{\pi\hbar^2}\right)^2\frac{2a}{\pi}\right) = -\frac{V_1 a^2 m}{2\pi^2\hbar^2}$$

$$\frac{\hbar^2}{2m}\frac{9\pi^2}{4a^2} - \frac{V_1}{2}\frac{a^2m}{\pi^2\hbar^2}$$

7.



$\vec{a}_1 = a\hat{x}$

ii)

$$V(x) = -V_0\left(3 + 2\cos\left[\frac{2\pi}{a}x\right]\right)$$

$$V(x) = -V_0\left[3 + \frac{\cancel{2}}{\cancel{2}}\left(e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x}\right)\right]$$

$$V(x) = -3V_0 - V_0\, e^{i\frac{2\pi x}{a}} - V_0\, e^{-i\frac{2\pi x}{a}}$$

Descomposición Fourier del Potencial →

$$\boxed{V(x) = \underbrace{(-3V_0)}_{C_0} e^{i0x} + \underbrace{(-V_0)}_{C_{2\pi/a}} e^{i\frac{2\pi x}{a}} + \underbrace{(-V_0)}_{C_{-2\pi/a}} e^{-i\frac{2\pi x}{a}}}$$

$$\vec{K}_1 = 0,\quad \vec{K}_2 = \frac{2\pi}{a},\quad \vec{K}_2 = -\frac{2\pi}{a}$$

i) $\vec{b}_1 = \frac{2\pi}{a}\hat{x} \Rightarrow$

$\vec{K}_n = \frac{2\pi}{a} n\,\hat{x}$ → Vector de la red recíproca

iii) $\psi_k = e^{ikx}\sum_G C_G\, e^{-iGx}$

$G \in$ Red recíproca

$G = \pm\frac{2\pi}{a}, \pm\frac{4\pi}{a}, 0$

cinco G's de menor módulo

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_k + V(x)\psi_k - \varepsilon\psi_k = 0$$

$$\frac{\partial}{\partial x}\psi_k = e^{ikx}\, ik\sum_G C_G\, e^{-iGx} + e^{ikx}\sum_G C_G\, e^{-iGx}(-iG)$$

$$\frac{\partial^2}{\partial x^2}\psi_k = e^{ikx}(ik)^2\sum_G C_G\, e^{-iGx} + e^{ikx}\, ik\sum_G C_G\, e^{-iGx}(-iG)$$

$$+ e^{ikx}(ik)\sum_G C_G\, e^{-iGx}(-iG) + e^{ikx}\sum_G C_G\, e^{-iGx}(-iG)^2$$

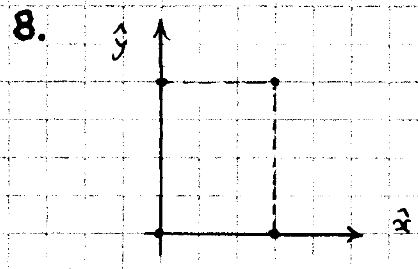
$$= -e^{ikx}k^2\sum_G C_G\, e^{-iGx} + e^{ikx}kG\sum_G C_G\, e^{-iGx}$$

$$+ e^{ikx}kG\sum_G C_G\, e^{-iGx} - e^{ikx}G^2\sum_G C_G\, e^{-iGx}$$

$$= \left(e^{ikx}\sum_G C_G\, e^{-iGx}\right)\left(-k^2 + kG + kG - G^2\right)$$

$$= -(\psi_k)(k+G)^2$$

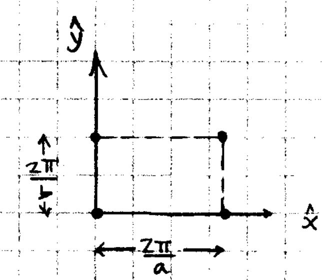
8.



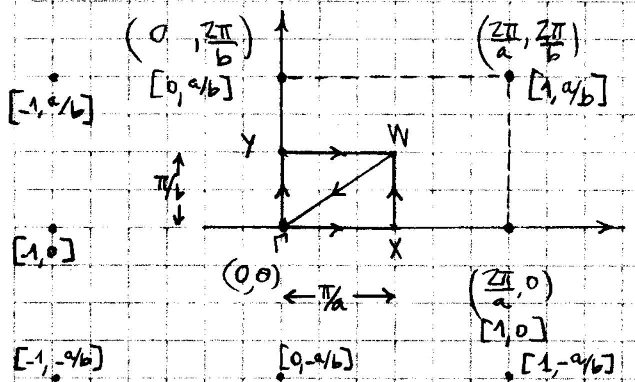
$\vec{a}_1 = a\,\hat{x}$ $\qquad$ $\vec{b}_1 = 2\pi/a\,\hat{x}$

$\vec{a}_2 = b\,\hat{y}$ $\qquad$ $\vec{b}_2 = \dfrac{2\pi}{b}\,\hat{y}$

$b > a$



1)



Trabajaremos en unidades de $\dfrac{2\pi}{a}$; entonces:

$$\mathcal{E} = \frac{\hbar^2}{2m}\left(\vec{k} - \vec{K}\right)^2$$

$$= \frac{\hbar^2}{2m}\left[(k_x - K_x)^2 + (k_y - K_y)^2\right]$$

$$\mathcal{E} = \frac{\hbar^2}{2m}\left[\left(\frac{2\pi}{a}\right)^2 (n_x - N_x)^2 + \left(\frac{2\pi}{b}\right)^2 (n_y - N_y)^2\right]$$

$$\mathcal{E} = \frac{\hbar^2 4\pi^2}{2m a^2}\left[(n_x - N_x)^2 + \left(\frac{a}{b}\right)^2 (n_y - N_y)^2\right]$$

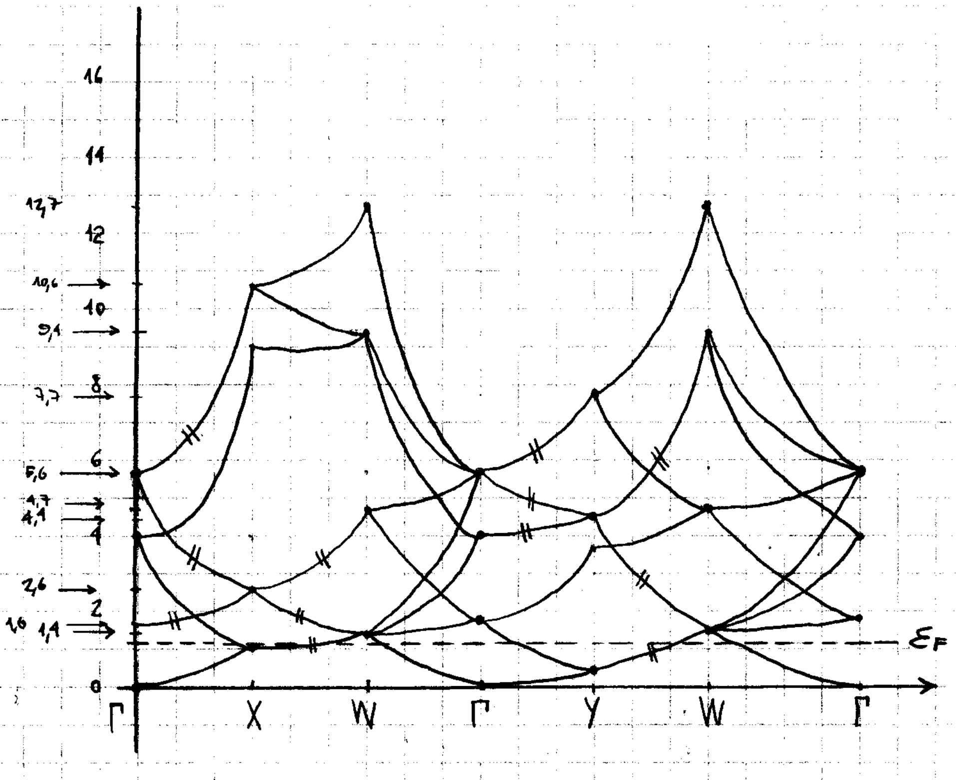
La energía depende del módulo $|\vec{k} - \vec{K}|$, con lo cual un punto como W tiene igual valor de energía en los cuatro vértices. Hasta qué $\vec{K}$ considerar se determinará por la limitación de que $\mathcal{E} < 16\alpha$ donde $\alpha \equiv \dfrac{\hbar^2 \pi^2}{2ma^2}$

	$\mathcal{E}\searrow$	$(0,0)$	$(1,0)$	$(1, a/b)$	$(0, a/b)$	$(-1, a/b)$	$(-1, 0)$
$(0,0)$	Γ	0	4	$4\left(1+\frac{a^4}{b^4}\right)$	$4a^4/b^4$	$4\left(1+a^4/b^4\right)$	4
$(1/2, 0)$	X	1	1	$4\left(1/4+[a/b]^4\right)$	$4\left(1/4+[a/b]^4\right)$	$4\left(\frac{9}{4}+\frac{a^4}{b^4}\right)$	$4\left(\frac{9}{4}\right)$
$(1/2, a/2b)$	W	$4\left(1/4+\frac{a^4}{4b^4}\right)$	$4\left(1/4+\frac{a^4}{4b^4}\right)$	$4\left(1/4+\frac{a^4}{4b^4}\right)$	$4\left(1/4+\frac{a^4}{4b^4}\right)$	$4\left(\frac{9}{4}+\frac{a^4}{4b^4}\right)$	$4\left(\frac{9}{4}+\frac{a^4}{4b^4}\right)$
$(0, a/2b)$	Y	$4\frac{a^4}{4b^4}$	$4\left(1+\frac{a^4}{4b^4}\right)$	$4\left(1+\frac{a^4}{4b^4}\right)$	$4\frac{a^4}{4b^4}$	$4\left(1+\frac{a^4}{4b^4}\right)$	$4\left(1+\frac{a^4}{4b^4}\right)$

	$\mathcal{E}\rightarrow$	$(-1, -a/b)$	$(0, -a/b)$	$(1, -a/b)$
$(0,0)$	Γ	$4\left(1+a^4/b^4\right)$	$4a^4/b^4$	$4\left(1+\frac{a^4}{b^4}\right)$
$(1/2, 0)$	X	$4\left(\frac{9}{4}+\frac{a^4}{b^4}\right)$	$4\left(\frac{1}{4}+\frac{a^4}{b^4}\right)$	$4\left(\frac{1}{4}+\frac{a^4}{b^4}\right)$
$(1/2, a/2b)$	W	$4\left(\frac{9}{4}+\frac{9a^4}{4b^4}\right)$	$4\left(\frac{1}{4}+\frac{9a^4}{4b^4}\right)$	$4\left(\frac{1}{4}+\frac{9a^4}{4b^4}\right)$
$(0, a/2b)$	Y	$4\left(1+\frac{9a^4}{4b^4}\right)$	$4\left(\frac{9a^4}{4b^4}\right)$	$4\left(1+\frac{9a^4}{4b^4}\right)$

supongo $a/b \sim 0.8$

	$(0,0)$	$(1,0)$	$(1, a/b)$	$(0, a/b)$	$(-1, a/b)$	$(-1, 0)$	$(-1, -a/b)$	$(0, -a/b)$	$(1, -a/b)$
Γ	0	4	5,6	1,6	5,6	4	5,6	1,6	5,6
X	1	1	2,6	2,6	10,6	9	10,6	2,6	2,6
W	1,4	1,4	1,4	1,4	9,4	9,4	12,7	4,7	4,7
Y	0,4	4,4	4,4	0,4	4,4	4,4	7,7	3,7	7,7

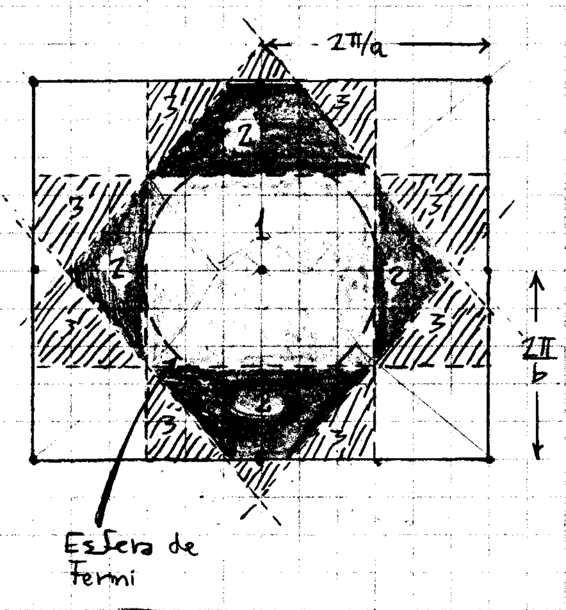


ii)

Dibujo
Escala

$$\frac{\cancel{2\pi}}{b}\frac{a}{\cancel{2\pi}}=\frac{5}{6}$$

$$\frac{a}{b}=\frac{5}{6}$$



← 1,2,3 eras Zonas de Brillouin

$$\frac{N}{L^2}=n=\frac{N}{\underbrace{q}_{\#\text{ de celdas}}\,a.b}=\frac{N_q}{a.b}$$

electrones por celda

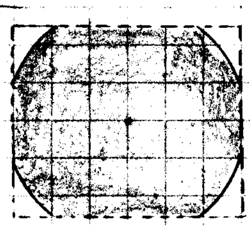
$$n=\frac{k_F^2}{2\pi}\;\rightarrow$$

$$k_F=\sqrt{\frac{2\pi N_q}{ab}}$$

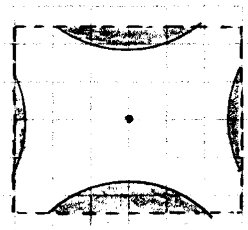
$$\boxed{k_F=\sqrt{\frac{4\pi}{ab}}}$$

$$k_F=\left(\frac{2\pi}{a}\right)\sqrt{\frac{a}{\pi b}}\cong\left(\frac{2\pi}{a}\right)0{,}51$$

1ºZB



2ºZB

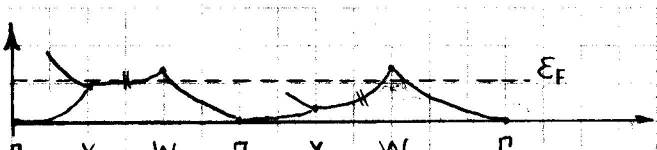


$$\varepsilon_F=\frac{\hbar^2k_F^2}{2m}=\frac{\hbar^2}{2m}\cdot\frac{4\pi}{ab}=\left(\frac{\hbar^2\pi^2}{2m\,a^2}\right)\frac{a\,4}{\pi b}$$

$$\varepsilon_F=\alpha\,\frac{a}{b}\frac{4}{\pi}$$

$$\boxed{\varepsilon_F\cong 1{,}01\,\alpha}$$ escala gráfico ε

$1{,}06\,\alpha$ ← escala dibujo ZB



Se puede ver que la banda 1 no se halla totalmente ocupada; lo cual se deduce de que la esfera de Fermi no llena íntegramente la 1ª ZB iii)

$$V(x,y) = -4V_0 \cos\left(\frac{2\pi}{a}x\right)\cos\left(\frac{2\pi}{b}y\right)$$

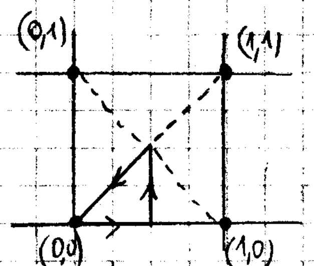
$$V(x,y) = -4V_0\left[\left(\frac{e^{i\frac{2\pi}{a}x}+e^{-i\frac{2\pi}{a}x}}{2}\right)\left(\frac{e^{i\frac{2\pi}{b}y}+e^{-i\frac{2\pi}{b}y}}{2}\right)\right]$$

$$V(x,y) = -V_0\left[e^{i\left(\frac{2\pi}{a}x+\frac{2\pi}{b}y\right)} + e^{i\left(-\frac{2\pi}{a}x+\frac{2\pi}{b}y\right)} + e^{i\left(\frac{2\pi}{a}x-\frac{2\pi}{b}y\right)} + e^{-\left(i\frac{2\pi}{a}x+i\frac{2\pi}{b}y\right)}\right]$$

Pero $U(\vec r)=\sum_k u_{\vec K}\, e^{i\vec K\cdot\vec r}$ $\rightarrow$ $\left(\frac{2\pi}{a}n_1, \frac{2\pi}{b}n_2\right)\cdot(x,y)$ $\rightarrow$

los $\vec K_i$ que aportan serán: $\vec K_1=(1,1)$, $\vec K_2=(-1,1)$, $\vec K_3=(1,-1)$, $\vec K_4=(-1,-1)$

(en unidades convenientes)



$\vec K'-\vec K=\vec K_i$ para que figure en la matriz

↳ visto los cuatro vértices que dan la degeneración entre sí

$*\;K'-K$

$(0,0)-\vec K$	$(1,0)-\vec K$	$(1,1)-\vec K$
$(-1,0)$ NO	$(0,-1)$ NO	$(1,0)$ NO
⇒ $(-1,-1)$ sí	⇒ $(1,-1)$ sí	
$(0,-1)$ NO		

$\rightarrow$ $K'-K=(-1,-1)$

$K'-K=(1,-1)$

10 - 01   00 - 11

K, K'

los coeficientes se labelearán $C_{\vec K-\vec K'}$ $\rightarrow$ $\begin{cases} C_{k-10}\neq 0 & \text{con el } 01 \\ C_{k-00}\neq 0 & \text{con el } 11\end{cases}$ $\Rightarrow$

Los K' labelearán los coeficientes $C_{\vec K-\vec K'}$

$$\begin{array}{c|cccc|}
 & C_{00} & C_{10} & C_{11} & C_{01} \\
C_{00} & \mathcal{E}^0_W-\mathcal{E} & 0 & -V_0 & 0 \\
C_{10} & 0 & \mathcal{E}^0_W-\mathcal{E} & 0 & -V_0 \\
C_{11} & -V_0 & 0 & \mathcal{E}^0_W-\mathcal{E} & 0 \\
C_{01} & 0 & -V_0 & 0 & \mathcal{E}^0_W-\mathcal{E}
\end{array}$$

Este determinante se puede escribir como:

$$= \begin{vmatrix} D & 0 & V & 0 \\ 0 & D & 0 & V \\ V & 0 & D & 0 \\ 0 & V & 0 & D \end{vmatrix} = \begin{vmatrix} D & V & 0 & 0 \\ 0 & 0 & D & V \\ V & D & 0 & 0 \\ 0 & 0 & V & D \end{vmatrix} = \begin{vmatrix} DV & 00 \\ VD & 00 \\ 00 & DV \\ 00 & VD \end{vmatrix}$$

C_{11} C_{10}

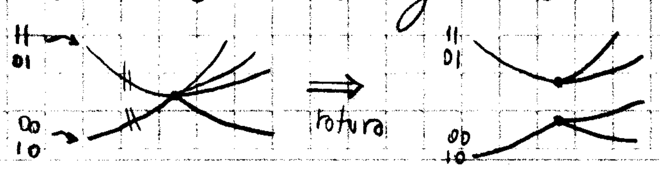
Un subespacio con $\{C_{00}, C_{10}$ $\{C_{11}\, C_{01}$

$$(\mathcal{E}^0_W-\mathcal{E})^2 - V_0^2 = 0$$

$$\mathcal{E} = \mathcal{E}^0_W \pm V_0$$

En el punto W el gap es, aprox., $\boxed{2V_0}$

Se tienden a separar las bandas; en W se rompe parcialmente la degeneración de orden 4 en dos ramas con degeneración de orden dos.



HOJA

FECHA

9. Red cuadrada de parámetro a $\rightarrow$ $\vec{K} = m\,\vec{b}_1 + n\,\vec{b}_2 = m\frac{2\pi}{a}\hat{x} + n\frac{2\pi}{a}\hat{y}$

$\vec{R} = p\,\vec{a}_1 + q\,\vec{a}_2$

$$V(x,y) = -V_0\left[\cos\left(\frac{2\pi}{a}x\right) + \cos\left(\frac{2\pi}{a}y\right)\right]$$

$$= -V_0\left(\frac{1}{2}\left[e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x}\right] + \frac{1}{2}\left[e^{i\frac{2\pi}{a}y} + e^{-i\frac{2\pi}{a}y}\right]\right)$$

$$V(x,y) = -\frac{V_0}{2}\left(e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x} + e^{i\frac{2\pi}{a}y} + e^{-i\frac{2\pi}{a}y}\right)$$

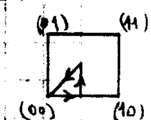
en unidades de $2\pi/a$

Como $U(\vec{r}) = \sum_{\vec{K}} U_{\vec{K}}\, e^{i\vec{K}\cdot\vec{r}} \Rightarrow \vec{K}_1 = (1,0)\ ;\ \vec{K}_2 = (-1,0)\ ;\ \vec{K}_3 = (0,1)\ ;\ \vec{K}_4 = (0,-1)$

la sumatoria se restringe a cuatro términos; los demás serán nulos

Los coeficientes de Fourier que aportarán

Considero la celda primitiva $\longrightarrow$



con $\vec{K} \neq \vec{K}'$

$$\left[\frac{\hbar^2}{2m}(\vec{k}-\vec{K})^2 - \mathcal{E}\right]C_{\vec{k}-\vec{K}} + \sum_{\vec{K}'} U_{\vec{K}'-\vec{K}}\cdot C_{\vec{k}-\vec{K}'} = 0$$

$\vec{K}' = (00)\,;(10)\,;(11)\,;(01)$

$\vec{K} = (00)\,;(10)\,;(11)\,;(01)$

$\vec{K}=(00)$ $\quad (\mathcal{E}^0_{k-00} - \mathcal{E})\,C_{k-00} + \qquad + U_{10-00}\cdot C_{k-10} + U_{11-00}\cdot C_{k-11} + U_{01-00}\cdot C_{k-01} = 0$

$\vec{K}=(10)$ $\quad (\mathcal{E}^0_{k-10} - \mathcal{E})\,C_{k-10} + U_{00-10}\,C_{k-00} + \qquad + U_{11-10}\cdot C_{k-11} + U_{01-10}\cdot C_{k-01} = 0$

$\vec{K}=(11)$ $\quad (\mathcal{E}^0_{k-11} - \mathcal{E})\,C_{k-11} + U_{00-11}\cdot C_{k-00} + U_{10-11}\cdot C_{k-10} + \qquad + U_{01-11}\cdot C_{k-01} = 0$

$\vec{K}=(01)$ $\quad \underbrace{(\mathcal{E}^0_{k-01} - \mathcal{E})}_{\equiv D}\,C_{k-01} + U_{00-01}\cdot C_{k-00} + U_{10-01}\cdot C_{k-10} + U_{11-01}\cdot C_{k-11} \qquad = 0$

$$D\cdot C_{00} + U_{10}\,C_{10} + U_{11}\cdot C_{11} + U_{10}\cdot C_{01} = 0$$

$$D\cdot C_{10} + U_{-10}\,C_{00} + U_{01}\cdot C_{11} + U_{-11}\cdot C_{01} = 0$$

$$D\cdot C_{11} + U_{11}\cdot C_{00} + U_{01}\cdot C_{10} + U_{-10}\cdot C_{01} = 0$$

$$D\cdot C_{01} + U_{0-1}\cdot C_{00} + U_{1-1}\cdot C_{10} + U_{10}\cdot C_{11} = 0$$

$$\begin{pmatrix} D & & & \\ & D & & \\ & & D & \\ & & & D \end{pmatrix}\begin{pmatrix} C_{00} \\ C_{10} \\ C_{11} \\ C_{01}\end{pmatrix} = 0$$

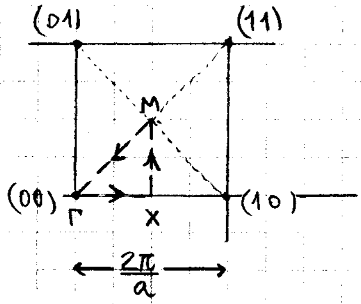
Pero como los coeficientes son $-\frac{V_0}{2} = U_{10} = U_{-10} = U_{01} = U_{0-1}$; se tendrá:

$$\begin{array}{c|cccc|} & C_{00} & C_{10} & C_{11} & C_{01} \\ C_{00} & D & -V_0/2 & 0 & -V_0/2 \\ C_{10} & -V_0/2 & D & -V_0/2 & 0 \\ C_{11} & 0 & -V_0/2 & D & -V_0/2 \\ C_{01} & -V_0/2 & 0 & -V_0/2 & D \end{array} = 0$$

Necesito determinante nulo

$D \equiv \mathcal{E}^0_{\vec{k}-\vec{K}} - \mathcal{E}(\vec{k})$

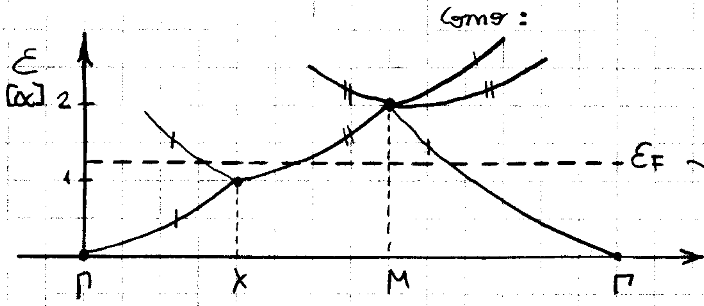
NOTA



Para $\vec{k} = \left(\frac{1}{2}, \frac{1}{2}\right)$ (en unidades de $\frac{2\pi}{a}$) se tiene que:

$$\left(\vec{k} - \vec{K}_i\right)^2 = \frac{1}{2} \quad \text{para} \quad i = 1,2,3,4 \Rightarrow$$

La energía, en unidades de $\alpha = \frac{\hbar^2 \pi^2}{2a^2 m}$, es 2. Entonces las bandas, para el electrón libre lucen como:



Calculamos el determinante de 4x4 anterior, obteniendo:

$$-\left(4 D^2 \left(-\frac{V_0}{2}\right)^2 - D^4\right) = 0$$

$$D^{\cancel{4}2} = \cancel{4} D^{\cancel{2}} \frac{V_0^2}{\cancel{4}}$$

$$D^2 = V_0^2 \longrightarrow D = \begin{cases} +V_0 \\ -V_0 \end{cases}$$

$$\left(\varepsilon^0_{\vec{k}-\vec{K}} - \varepsilon\right) = \pm V_0$$

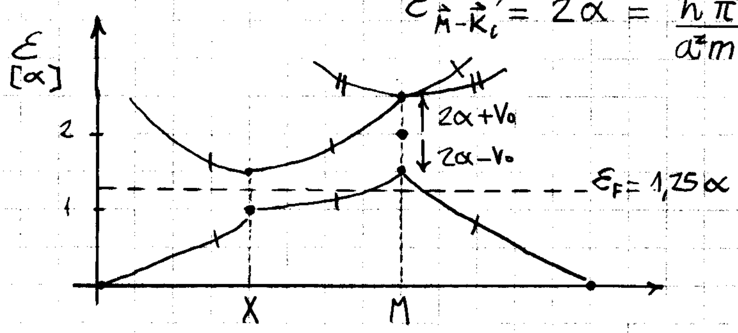
$$\boxed{\varepsilon_\pm = \varepsilon^0_{\vec{k}-\vec{K}} \pm V_0}$$

Para el punto $\vec{M} = \vec{k}$ era:

los vértices del cuadrado (00), (10), (11), (01)

$$\varepsilon^0_{\vec{M}-\vec{K}_i} = 2\alpha = \frac{\hbar^2 \pi^2}{a^2 m} \Rightarrow \boxed{\varepsilon_\pm = 2\alpha \pm V_0}$$

Se rompe la degeneración pero no en forma total

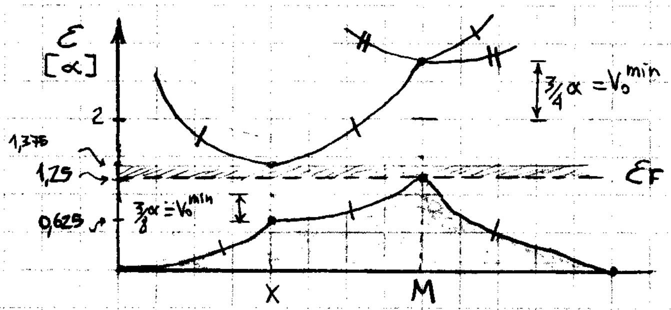


Para que el sistema sea aislante necesito que

$$0{,}75\,\alpha = V_0$$

$$\boxed{\frac{3}{4} \frac{\hbar^2 \pi^2}{2a^2 m} = V_0}$$

V_0 mínimo para sistema aislante



Para ver cuál es el ancho de banda en este caso necesito calcular cómo se desdobla la degeneración en el punto X

$$\vec{k} = (0,0)$$
$$\vec{k} = (1,0)$$

Planteando ecuación central llego a

$$\vec{k} = (00) \quad \left(\varepsilon^0_{k\cdot 00} - \varepsilon\right) C_{00} + U_{10-00} \cdot C_{10} = 0$$

$$\vec{k} = (10) \quad \left(\varepsilon^0_{k\cdot 10} - \varepsilon\right) C_{10} + U_{00-10} \cdot C_{00} = 0$$

$$\Rightarrow \begin{vmatrix} D & -V_0/2 \\ -V_0/2 & D \end{vmatrix} = 0$$

$$D^2 - \frac{V_0^2}{4} = 0 \rightarrow D = \pm \frac{V_0}{2}$$

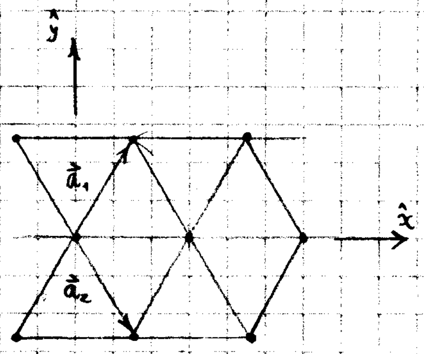
$$\varepsilon_\pm = \varepsilon^0_{\vec{X}-\vec{K}} \pm \frac{V_0}{2}$$

$$\varepsilon_\pm = 1\alpha \pm \frac{V_0}{2}$$

Con el V_0 min dado es $\varepsilon_\pm = 1\alpha \pm \frac{3}{8}\alpha \rightarrow$ Ancho de banda $= 1{,}375\alpha - 1{,}25\alpha = \boxed{0{,}125\,\alpha}$

10.

Red plana hexagonal con un átomo por sitio



$$\vec{a}_1 = a\left(\tfrac{1}{2}\hat{x} + \tfrac{\sqrt{3}}{2}\hat{y}\right) \quad ✓$$

$$\vec{a}_2 = a\left(\tfrac{1}{2}\hat{x} - \tfrac{\sqrt{3}}{2}\hat{y}\right) \quad ✓$$

$$\vec{b}_1 = \frac{2\pi\, a}{\frac{a^2\sqrt{3}}{2}}\left[-\tfrac{1}{2}\hat{y} - \tfrac{\sqrt{3}}{2}\hat{x}\right]$$

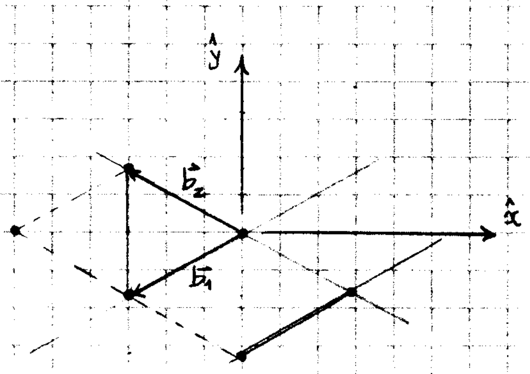
$$\vec{b}_2 = \frac{2\pi}{\frac{a^2\sqrt{3}}{2}}\, a\left[+\tfrac{1}{2}\hat{y} - \tfrac{\sqrt{3}}{2}\hat{x}\right]$$

$$V = \text{Área} = |\vec{a}_1 \times \vec{a}_2| = \left|a^2\left(-\frac{\sqrt{3}}{4}\hat{z} - \frac{\sqrt{3}}{4}\hat{z}\right)\right| =$$

$$\text{Área} = a^2 \cancel{2}^{1}\frac{\sqrt{3}}{\cancel{4}_2} = \frac{a^2\sqrt{3}}{2}$$

$$\vec{b}_1 = \frac{4\pi}{a\sqrt{3}}\left(-\frac{\hat{y}}{2} - \frac{\sqrt{3}}{2}\hat{x}\right) = \frac{2\pi}{a}\left(-\frac{1}{\sqrt{3}}\hat{y} - \hat{x}\right) ✓$$

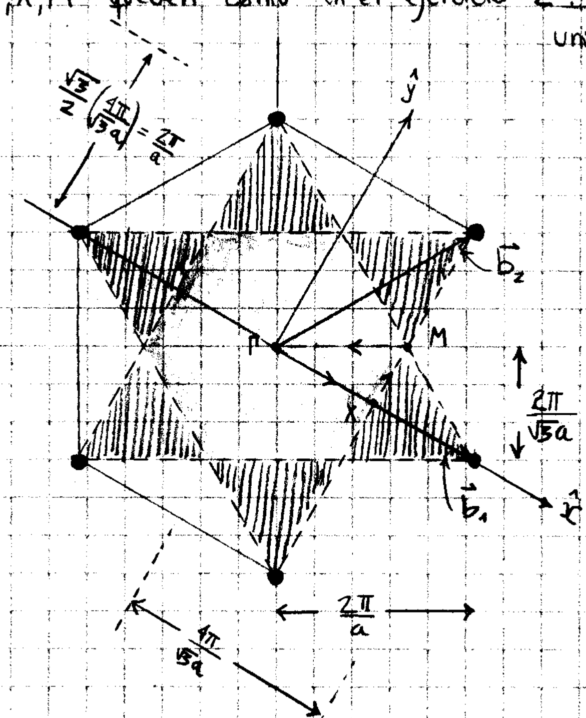
$$\vec{b}_2 = \frac{4\pi}{a\sqrt{3}}\left(\frac{\hat{y}}{2} - \frac{\sqrt{3}}{2}\hat{x}\right) = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{y} - \hat{x}\right) ✓$$

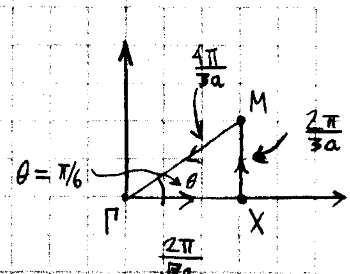


$$|\vec{b}_1| = \frac{2\pi}{a}\left(\frac{1}{3}+1\right) = \frac{2\pi}{a}\sqrt{\frac{4}{3}} = \frac{4\pi}{\sqrt{3}a}$$

i) y ii)

Hacemos una transformación de coordenadas para usar $\vec{b}_1 \parallel \hat{x}$ y que los puntos Γ, X, M queden como en el ejercicio 2. Conviene expresar todo en unidades de $2\pi/a$





Será $\Gamma = (0,0)$ $\quad X = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, 0\right)$ $\quad M = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, \frac{1}{3}\right)$

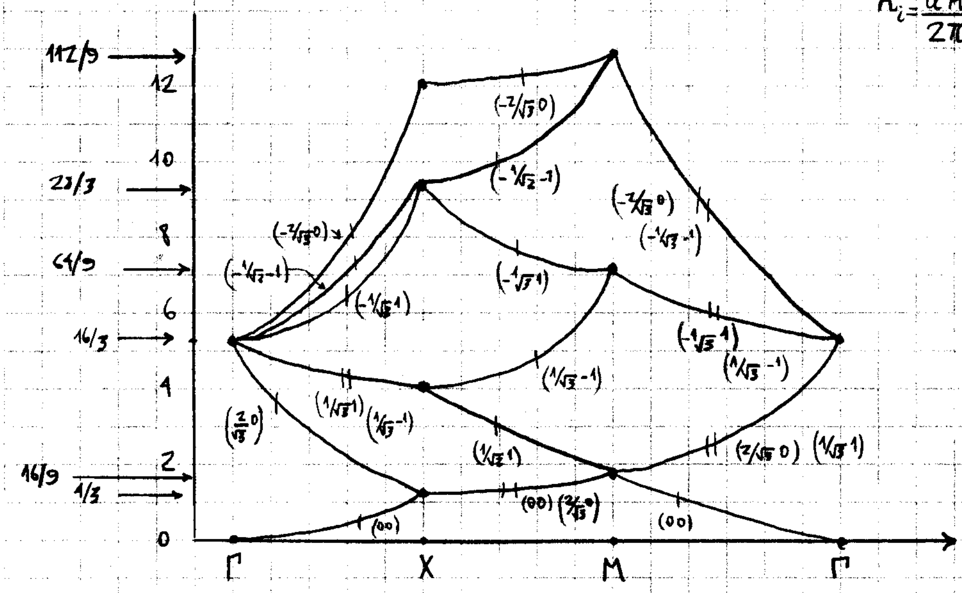
		(0,0)	$(2/\sqrt{3},0)$	$(1/\sqrt{3},1)$	$(-1/\sqrt{3},1)$	$(-2/\sqrt{3},0)$	$(-1/\sqrt{3},-1)$	$(1/\sqrt{3},-1)$
(0,0)	Γ	0	16/3	16/3	16/3	16/3	16/3	16/3
$(1/\sqrt{3},0)$	X	4/3	4/3	4	28/3	12	28/3	4
$(1/\sqrt{3},1/3)$	M	16/9	16/9	16/9	64/9	112/9	112/9	64/9

▲ Energía en unidades de α

$\frac{4}{3}$ $\frac{16}{9}$

$$E = 4\underbrace{\left(\frac{\pi^2\hbar^2}{a^2 2m}\right)}_{\alpha}\left[(\tilde{k}_x-n_x)^2+(\tilde{k}_y-n_y)^2\right]$$ donde (n_x,n_y) no son neces. $\in \mathbb{Z}$

$\tilde{k}_i = \frac{a k_i}{2\pi}$



iii)

$\#$ puntos en el $\vec{k}$-spa $= \frac{\Omega}{\frac{4\pi^2}{\sqrt{3}a^2}}$ NO! la discretización se hace en una caja de lado $L=L_x=L_y=L_z$ tenés que usar $V=\left(\frac{2\pi}{L}\right)^d$

si $\Omega = \pi k_F^2$

$= \frac{\pi k_F^2 \sqrt{3}a^2}{4\pi^2}$

El área de la celda primitiva será: (en la RR)

$$A = \left(\frac{1}{\cancel{2}}\left(\frac{2\pi}{a}\right)\frac{2\pi}{\sqrt{3}a}\right)\cancel{2} = \frac{4\pi^2}{\sqrt{3}a^2}$$

ojo! $n = \frac{N}{V}$ → no. total de celdas → volumen macroscópico

$N = \frac{\sqrt{3}k_F^2 a^2}{4\pi} \longrightarrow$ NO $n = \frac{\sqrt{3}}{4\pi}k_F^2 \longrightarrow k_F = \sqrt{\frac{4\pi n}{\sqrt{3}}}$ $\boxed{k_F^2 = 2\pi n}$ siempre! (2D)

$k_F^{(\#\text{electrones aportados})} \rightarrow$

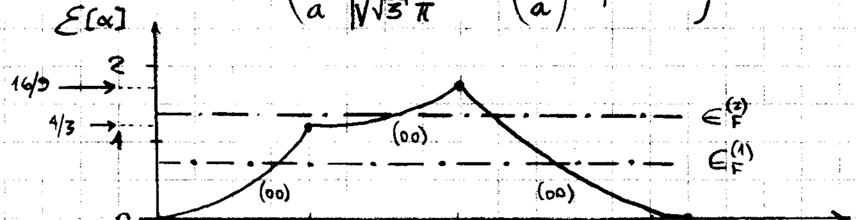
$$k_F^{(1)} = \left(\frac{2\pi}{a}\right)\sqrt{\frac{1}{\sqrt{3}\pi}} \approx \left(\frac{2\pi}{a}\right)\cdot 0{,}42$$

$$k_F^{(2)} = \left(\frac{2\pi}{a}\right)\sqrt{\frac{2}{\sqrt{3}\pi}} \approx \left(\frac{2\pi}{a}\right)\cdot 0{,}60$$

$\Rightarrow$

$$\epsilon_F^{(1)} = \frac{\hbar^2 k_F^{(1)2}}{2m} \cong \frac{\hbar^2}{2m}\frac{4\pi^2}{a^2}(0{,}42)^2 = 4\alpha(0{,}42)^2 \approx 0{,}70\,\alpha$$

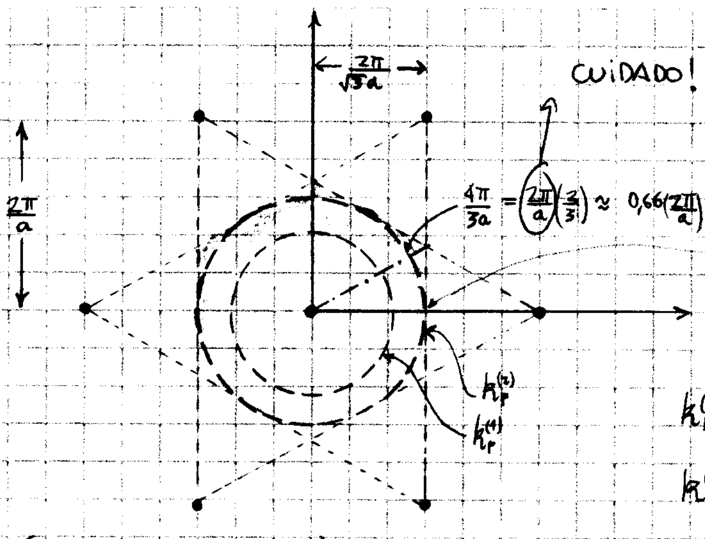
$$\epsilon_F^{(2)} = 4\alpha(0{,}60)^2 \approx 1{,}44\,\alpha$$



arrastrás el error

[Esto hecho al final nuevamente]

HOJA: LAVIA
FECHA: 684/01



CUIDADO! lo ideal es poner el k_F en unidades del límite de la 1ª ZB ie $\left(k_F = \left(\frac{2\pi}{a}\frac{2}{\sqrt{3}}\right)\alpha\right)$

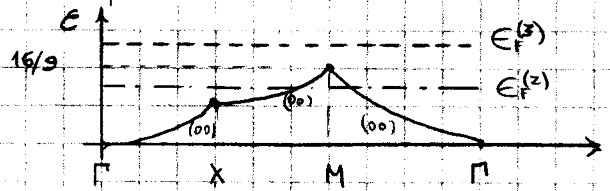
$k_F^{(1)}$ está totalmente dentro de la ZB1
$k_F^{(2)}$ tiene una ínfima parte en la ZB2

IV) (ANÁLISIS CUALITATIVO)

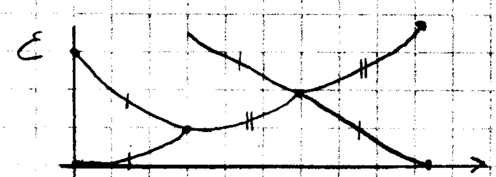
Cualitativamente podemos ver que

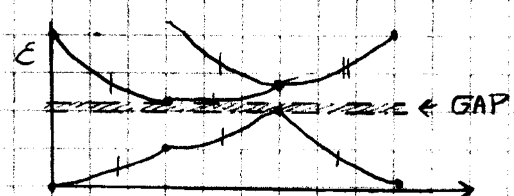
$$k_F^{(3)} = \left(\frac{2\pi}{a}\right)\sqrt{\frac{3}{\sqrt{3}\pi}} \approx \left(\frac{2\pi}{a}\right)0{,}74 \Rightarrow \varepsilon_F^{(3)} = 4\alpha(0{,}74)^2 \approx 2{,}20\,\alpha$$

La energía de fermi se ubica por encima de la primer banda si son 3 los electrones por sitio.



Para que el material resulte un aislante necesitamos un potencial débil que genere un GAP rompiendo la degeneración





Rotura de la degeneración

La idea era suponer $U_{(1,0)} = U_{(-1,0)} \neq 0$ y ver que se rompía la degeneración.

NOTA

Parte iii)

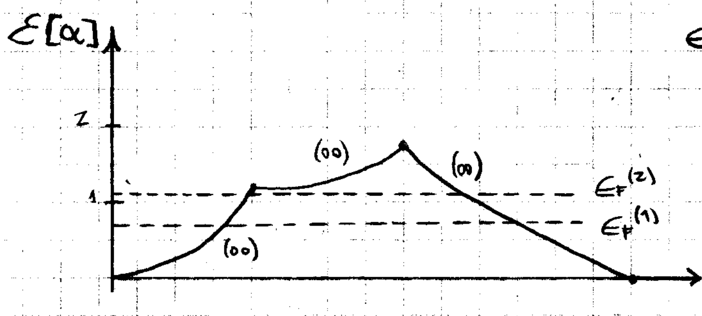
$$n = \frac{N}{A} = \frac{k_F^2}{2\pi} = \frac{N}{\underbrace{q}_{\#\text{de celdas}} \cdot \underbrace{\frac{a^2\sqrt{3}}{2}}_{\text{área de 1 celda}}} = \frac{N_q 2}{a^2\sqrt{3}} \rightarrow k_F = \left(\frac{4\pi N_q}{a^2\sqrt{3}}\right)^{1/2}$$

$$k_F^{(1)} = \frac{2\pi^{1/2}}{a} \cdot \frac{1}{3^{1/4}} \approx \frac{2\pi^{1/2}}{a} \cdot 0{,}76$$

$$k_F^{(2)} = \frac{2\pi^{1/2}}{a} \cdot \frac{2^{1/2}}{3^{1/4}} \approx \frac{2\pi^{1/2}}{a} \cdot 0{,}96$$

$$\epsilon_F^{(1)} = \frac{\hbar^2}{2m} k_F^{(1)2} \approx \frac{\hbar^2}{2m}\frac{4\pi^2}{a^2}\frac{(0{,}76)^2}{\pi} = \frac{4}{\pi}\alpha\,(0{,}76)^2$$

$$\epsilon_F^{(2)} = \frac{\hbar^2}{2m} k_F^{(2)2} \approx \frac{\hbar^2}{2m}\frac{4\pi^2}{a^2}\frac{(0{,}96)^2}{\pi} = \frac{4}{\pi}\alpha\,(0{,}96)^2$$



$$\boxed{\epsilon_F^{(1)} \approx 0{,}73\,\alpha}$$

$$\boxed{\epsilon_F^{(2)} \approx 1{,}17\,\alpha}$$

$$\frac{2\pi}{\sqrt{3}a} = \frac{\cancel{2\pi^{1/2}}}{\cancel{a}}\left(\frac{\pi^{1/2}}{\sqrt{3}}\right) > \frac{\cancel{2\pi^{1/2}}}{\cancel{a}} 0{,}76 = k_F^{(1)}$$

$$> \frac{2\pi^{1/2}}{a} 0{,}96 = k_F^{(2)}$$

$\Rightarrow$ Los k_F para $N_q = 1, 2$ caen ambos íntegramente en la 1ZB