Problema 5

a = paràmetre xarxa $= 4{,}05\,Å$.

$\varepsilon^0 = \dfrac{\hbar^2 k^2}{2m^*}$ $\quad m^* = 1{,}1716\, m_e$.

$U_1 = U_{\pm1,\pm1,\pm1} = 0{,}4\, eV$.

$U_2 = U_{\pm2,0,0} = U_{0,\pm2,0} = U_{0,0,\pm2} = 0{,}75\, eV$.

totes les altres components nul·les.

$$\Gamma K. \longrightarrow \left.\begin{array}{l} \Gamma = (0,0,0) \\ K = \frac{2\pi}{a}\left(\frac{3}{4}, 0, \frac{3}{4}\right). \end{array}\right\}$$

$$\vec{\Gamma K} = \vec{k}_k = \frac{2\pi}{a}\left(\frac{3}{4}, 0, \frac{3}{4}\right) = \left(\frac{2\pi}{a}\right)\xi\left(\hat{x} + \hat{z}\right)$$

$$0 \leq \xi \leq \frac{3}{4}$$

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

$$\vec{G} = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z})$$

$$\boxed{|\vec{k}_k - \vec{G}_i|^2 = \left(\frac{2\pi}{a}\right)^2\left[(\xi - h)^2 + k^2 + (\xi - l)^2\right] \qquad 0 \leq \xi \leq \frac{3}{4}.}$$

$$E_{hkl}(\xi) = \frac{\hbar^2}{2m^*}\underbrace{\left(\frac{2\pi}{a}\right)}_{K}^2\left[(\xi-h)^2 + k^2 + (\xi+l)^2\right]$$

a) - $E_{menor} = ?$

$\vec{G}_0 = \vec{0} \rightarrow \quad E_{000}(\xi=0) = 0.$

$$E_{000}(\xi = 3/4) = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 \cdot \frac{18}{16} =$$

$$= \boxed{\varepsilon_0 \cdot \frac{9}{8} = E_{000}\left(\xi = \frac{3}{4}\right)}$$

b) - $\underline{\text{model xarxa buida.}}$ ΓK {degeneració 2}.

excepte punts Γ ; K.

$$\left|\vec{K}_{\Gamma K} - \vec{G}\right| = \left(\frac{2\pi}{a}\right)\cdot\left((\xi-h), k, \xi-l\right) \quad 0<\xi<3/4$$

$\vec{G}_0 = (0,0,0) \rightarrow (hkl) = (000)$

$\vec{G}_1 \Rightarrow (111) = (hkl)$

$\vec{G}_2 \Rightarrow (\bar{1}\bar{1}\bar{1}) = (hkl)$

$\vec{G}_3 \Rightarrow (\bar{1}11) = (hkl)$

$\vec{G}_4 \Rightarrow (1\bar{1}1) = (hkl)$

$\vec{G}_5 \Rightarrow (11\bar{1}) = (hkl)$

$\vec{G}_6 \Rightarrow (\bar{1}\bar{1}1) = (hkl)$

$\vec{G}_7 \Rightarrow (\bar{1}1\bar{1}) = (hkl)$

$\vec{G}_8 \Rightarrow (1\bar{1}\bar{1}) = (hkl)$

PS,2

$$\left(\vec{K}_{\Gamma} - \vec{G}_{000}\right) = \frac{2\pi}{a}\left(0, 0, 0\right).$$

$$\left(\vec{K}(\xi = \tfrac{3}{4}) - \vec{G}_{000}\right) = \frac{2\pi}{a}\left(\frac{3}{4}, 0, \frac{3}{4}\right).$$

$\vec{K}(\xi=0)$

$$E_{000}^{(1,1)}(\xi = 0) = 0.$$

$$E_{000}^{(1,1)}\left(\xi = \tfrac{3}{4}\right) = \boxed{\varepsilon_0 \cdot \frac{9}{8}.}$$

$$E_{111}\left(\xi = \tfrac{3}{4}\right) = \varepsilon_0\left(\frac{1}{16} + 1 + \frac{1}{16}\right) = \frac{18}{16} = \boxed{\frac{9}{8}\varepsilon_0.}$$

$$E_{1\bar{1}\bar{1}}\left(\xi = \tfrac{3}{4}\right) = \varepsilon_0\left(\frac{49}{16} + 1 + \frac{49}{16}\right) = \frac{114}{16}\varepsilon_0 = \frac{57}{8}\varepsilon_0$$

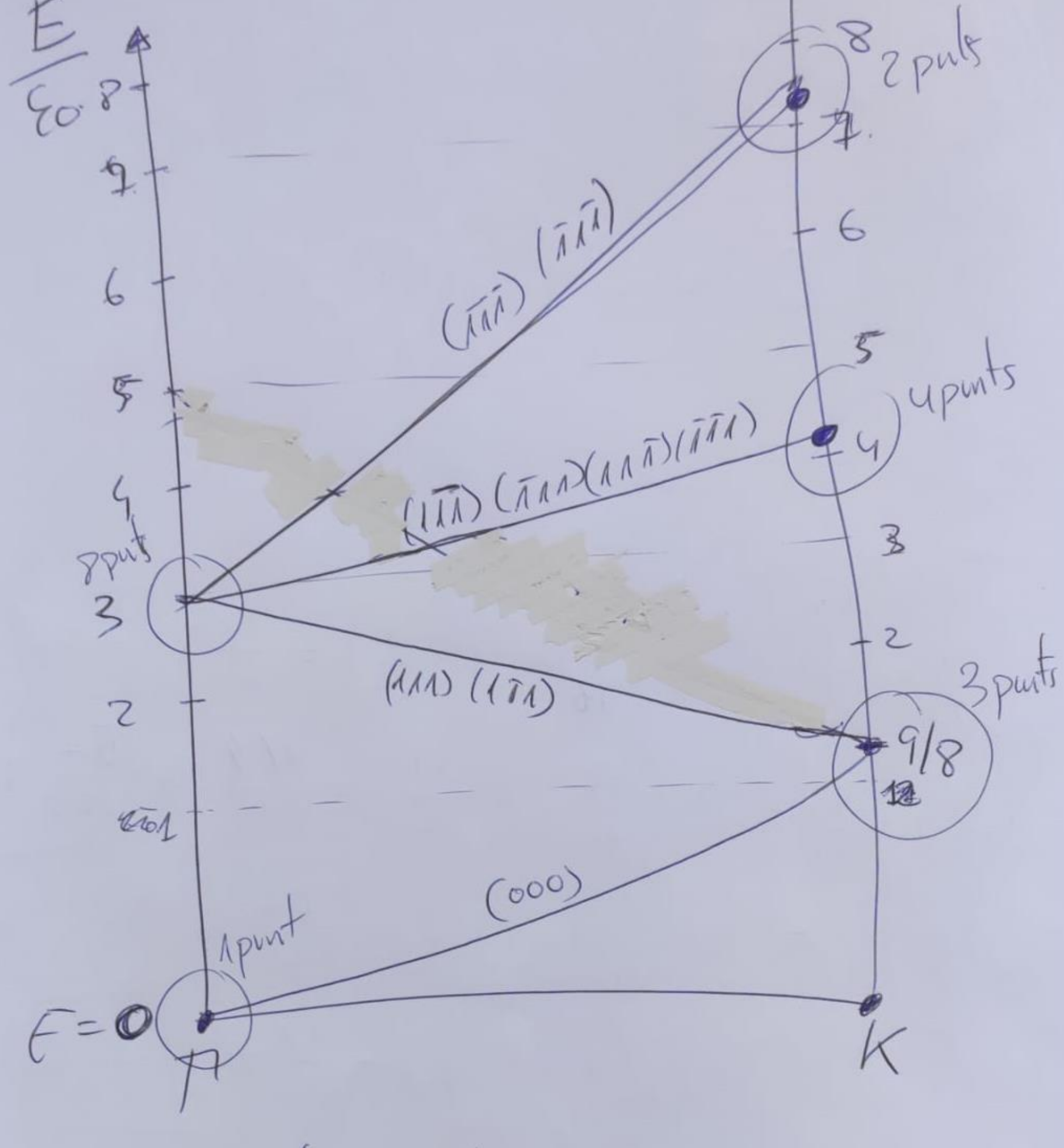
$$E_{\bar{1}11}\left(\xi = \tfrac{3}{4}\right) = \varepsilon_0\left(\frac{49}{16} + 1 + \frac{1}{16}\right) = \frac{66}{16}\varepsilon_0 = \boxed{\frac{33}{8}\varepsilon_0.}$$

$$E_{1\bar{1}1}\left(\xi = \tfrac{3}{4}\right) = \varepsilon_0\left(\frac{1}{16} + 1 + \frac{1}{16}\right) = \frac{18}{16}\varepsilon_0 = \boxed{\frac{9}{8}\varepsilon_0.}$$

$$E_{11\bar{1}}\left(\xi = \tfrac{3}{4}\right) = E_{\bar{1}11} = \boxed{\frac{33}{8}\varepsilon_0.}$$

$$E_{\bar{1}\bar{1}1}\left(\xi = \tfrac{3}{4}\right) = E_{11\bar{1}}\left(\xi = \tfrac{3}{4}\right) = \varepsilon_0\left(\frac{1}{16} + 1 + \frac{49}{16}\right) = \boxed{\frac{33}{8}\varepsilon_0.}$$

$$E_{\bar{1}1\bar{1}}\left(\xi = \tfrac{3}{4}\right) = \varepsilon_0\left(\frac{49}{16} + 1 + \frac{49}{16}\right) = \frac{114}{16}\varepsilon_0 = \frac{57}{8}\varepsilon_0.$$



$E_{111}(\xi=0) = \varepsilon_0(1+1+1) = 3\varepsilon_0.$

$E_{1\bar{1}1}(\xi=0) = 3\varepsilon_0.$

$\vdots \qquad = 3\varepsilon_0$

put k (000) (111) $(1\bar{1}1)$

PS/3

$\vec{G}_0' = \vec{0}$

$\vec{G}_1'(111) = \frac{2\pi}{a}(h, k, l) = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z})$ 1 1 1

$\vec{G}_2'(1\bar{1}1) = \frac{2\pi}{a}(h\hat{x} - k\hat{y} + l\hat{z})$. 1 1 1.

$$\underbrace{\left(\frac{\hbar^2}{2m}|k-G_1|^2 - E\right)}_{\Delta E} C_{k-G} + \sum_{G''} V_{G''-G_1} C_{k-G_1} = 0.$$

$$\begin{cases} \Delta E\, C_{k-G_0} + V_{G_0-G_0} C_{k-G_0} + V_{G_1-G_0} C_{k-G_1} + V_{G_2-G_0} C_{k-G_2} = 0 \\ \Delta E\, C_{k-G_1} + V_{G_0-G_1} C_{k-G_0} + V_{G_1-G_1} C_{k-G_1} + V_{G_2-G_1} V_{k-G_2} = 0 \\ \Delta E\, C_{k-G_2} + V_{G_0-G_2} C_{k-G_0} + V_{G_1-G_2} C_{k-G_1} + V_{G_2-G_2} V_{k-G_2} = 0. \end{cases}$$

$\vec{G}_0 - \vec{G}_0 = 0$

$\vec{G}_1 - \vec{G}_0 = \frac{2\pi}{a}(1\cdot\hat{x} + 1\cdot\hat{y} + 1\cdot\hat{z}) = \frac{2\pi}{a}(\hat{x} + \hat{y} + \hat{z})$. $= \frac{2\pi}{a}(1,1,1)$

$\vec{G}_2 - \vec{G}_0 = \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z}) = \frac{2\pi}{a}(1,-1,1)$

$\vec{G}_1 - \vec{G}_2 = \frac{2\pi}{a}(+2\hat{y}) = \frac{2\pi}{a}(0,2,0)$.

$$\begin{vmatrix} \Delta E & M_1 & M_1 \\ M_1 & \Delta E & M_2 \\ M_1 & M_2 & \Delta E \end{vmatrix} \begin{pmatrix} C_{K-G0} \\ C_{K-G1} \\ C_{K-G2} \end{pmatrix} = 0$$

$$\begin{vmatrix} \Delta E & M_1 & M_1 \\ M_1 & \Delta E & M_2 \\ M_1 & M_2 & \Delta E \end{vmatrix} \underset{F_2 - F_3}{=} \begin{vmatrix} \Delta E & 0 & M_1 \\ M_1 & \Delta E - M_2 & M_2 \\ M_1 & M_2 - \Delta E & \Delta E \end{vmatrix} \underset{Co2+Co3}{=}$$

$$= \begin{vmatrix} \Delta E & 0 & M_1 \\ 2M_1 & 0 & \Delta E + M_2 \\ M_1 & M_2 - \Delta E & \Delta E \end{vmatrix} =$$

$$= -(M_2 - \Delta E) \begin{vmatrix} \Delta E & M_1 \\ 2M_1 & \Delta E + M_2 \end{vmatrix} = \longrightarrow$$

P5/4

$$= (\Delta E - M_2)\left[\Delta E^2 + \Delta E M_2 - 2M_1^2\right)$$

$$\boxed{\Delta E_1 = M_2}$$

$$\boxed{\Delta E_{24}^{+} = \frac{-M_2 \pm \sqrt{M_2^2 + 8M_1^2}}{2}}$$

$$\boxed{\Delta E_3^{-} = \frac{-M_2 - \sqrt{M_2^2 + 8M_1^2}}{2}}$$

$$E_1 = \varepsilon^0 - M_2 \qquad = 8{,}055\,eV.$$

$$E_2 = \varepsilon^0 + \frac{M_2 - \sqrt{(\,)}}{2} = 8{,}5\,eV.$$

$$E_3 = \varepsilon^0 + \frac{M_2 + \sqrt{(\,)}}{2} = 9{,}86\,eV.$$

amb el potencial ja no tenim estats degenerats → ~~x~~ es generen unes bandes al punt K amb energies diferents.

Problema. 6.

a = paràmetre xarxa.

$\Gamma \longrightarrow F$

$\Gamma = (0,0,0)$

$F = \frac{2\pi}{a}\left(\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right) = \frac{2\pi\,\varepsilon}{a}(1,3,1) \quad \varepsilon = \frac{1}{4}.$

$\vec{\Gamma F} = \vec{K}_{\Gamma F} = \frac{2\pi\,\varepsilon}{a}(1,3,1). = \left(\frac{2\pi}{a}\right)\varepsilon\left(\hat{x} + 3\hat{y} + \hat{z}\right)$

$0 \leq \varepsilon \leq \frac{1}{4}$

a).- aproximació xarxa buida.

(a1) $\quad E(\vec{k}-\vec{G}) = \frac{\hbar^2}{2m}|\vec{k} - \vec{G}|^2$

$\vec{G} = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z}).$

$E_{hkl}(\varepsilon) = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\left((\varepsilon - h)^2 + (3\varepsilon - k)^2 + (\varepsilon - l)^2\right)$

$0 \leq \varepsilon \leq \frac{1}{4}.$

si fem $E_0 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2.$

$E_{hkl}(\varepsilon) = E_0\left[(\varepsilon-h)^2 + (3\varepsilon - k)^2 + (\varepsilon - l)^2\right] \quad 0 \leq \varepsilon \leq \frac{1}{4}.$

(a2)

$\rightarrow E_{hkl}\left(\xi = \frac{1}{4}\right) = ?$

$\rightarrow$ degeneració.

$\rightarrow$ funcions d'ona corresponents

punt F.

$$E_{hkl}\left(\frac{1}{4} = \xi\right) = E_0\left[\left(\frac{1}{4} - h\right)^2 + \left(\frac{3}{4} - k\right)^2 + \left(\frac{1}{4} - l\right)^2\right]$$

$$\vec{G}_0 = (0,0,0)\frac{2\pi}{a} \Rightarrow (hkl) = (000).$$

$$E_{000} = E_0\left[\left(\frac{1}{4}\right)^2 + \left(\frac{3}{4}\right)^2 + \left(\frac{1}{4}\right)^2\right] = \frac{11}{16}E_0.$$

$\vec{G}_1 = (1\,1\,0)$

$\vec{G}_2 = (0\,1\,1).$

(100) (010) (001)
(110) (101) (011)
(111) $\rightarrow$ negats.

Índex de Miller.

$$E_{110}\left(\xi = \frac{1}{4}\right) = E_0\left[\left(\frac{1}{4} - 1\right)^2 + \left(\frac{3}{4} - 1\right)^2 + \left(\frac{1}{4} + 0\right)^2\right] = \frac{11}{16}E_0.$$

Fets tots.

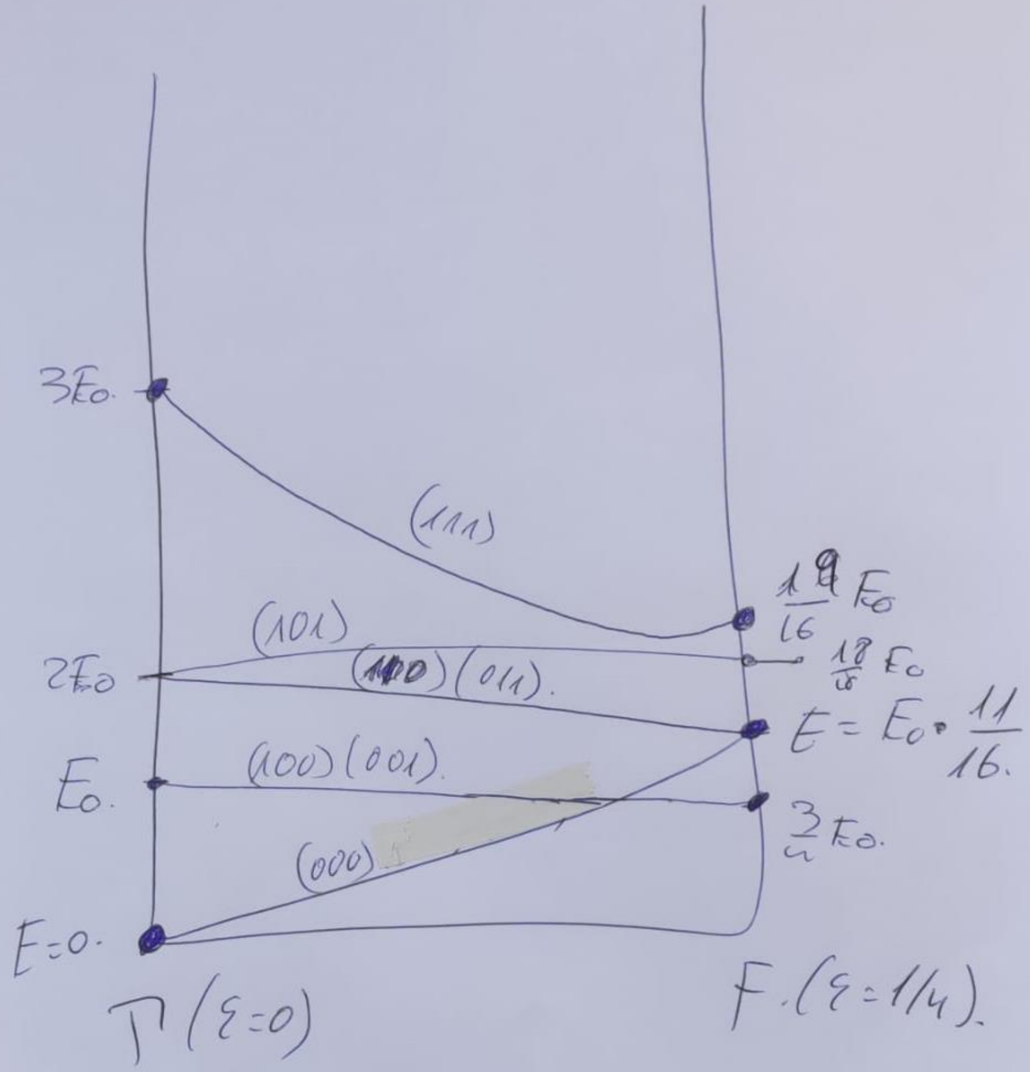
$$E_{011}\left(\xi = \frac{1}{4}\right) = \frac{11}{16}E_0.$$

$$\vec{G}_0 = \vec{0} \qquad \vec{G}_1 = \frac{2\pi}{a}(\hat{x} + \hat{y}) \qquad \vec{G}_2 = \frac{2\pi}{a}(\hat{y} + \hat{z}).$$

al punt F s'assoleix per tres valors iguals

$\Rightarrow$ degeneració $\underline{\underline{3}}$.

NOTA sig. a)2 Pb de 1a2



$E_{000}(0) = 0.$

$E_{100}(0) = E_{010}(0) = E_{001}(0) = \underline{E_0}$

$E_{110}(0) = \underline{2E_0} = E_{101}(0) = E_{011}(0).$

$E_{111}(0) = 3E_0$

CALCULAR.

$E_{hkl}(\varepsilon=0)$

$E_{hkl}(\varepsilon=\frac{1}{4}).$

Funcions d'ona:

$$\phi_{\vec{K}_F-\vec{G}_i}(\vec{r}) = C_{\vec{K}_F-\vec{G}_i}\, e^{i(\vec{K}_F-\vec{G}_i)\vec{r}}$$

$$\vec{K}_F = \left(\frac{2\pi}{a}\right) = \left(\frac{1}{4}\hat{x} + \frac{3}{4}\hat{y} + \frac{1}{4}\hat{z}\right)\left(\frac{2\pi}{a}\right).$$

$$i\ \vec{G} \Longrightarrow \vec{G}_0 = \vec{0}$$

$$\vec{G}_1 = \frac{2\pi}{a}(\hat{x}+\hat{y})$$

$$\vec{G}_2 = \frac{2\pi}{a}(\hat{y}+\hat{z}).$$

$$\vec{K}_F - \vec{G}_i \Rightarrow \begin{cases} \vec{K}_F - \vec{G}_0 = \frac{2\pi}{a}\left(\frac{1}{4}\hat{x} + \frac{3}{4}\hat{y} + \frac{1}{4}\hat{z}\right) \\ \vec{K}_F - \vec{G}_1 = \frac{2\pi}{a}\left(-\frac{3}{4}\hat{x} - \frac{1}{4}\hat{y} + \frac{1}{4}\hat{z}\right) \\ \vec{K}_F - \vec{G}_2 = \frac{2\pi}{a}\left(\frac{1}{4}\hat{x} - \frac{1}{4}\hat{y} - \frac{3}{4}\hat{z}\right) \end{cases}$$

b).- potencial associat $V_{h'k'l'} = \dfrac{6M}{h'^2+k'^2+l'^2}$

$$\vec{G}' = \frac{2\pi}{a}(h'\hat{x} + k'\hat{y} + l'\hat{z})$$

$$V_{200} = 0.$$

b) sistema homogeni.

equació central:

$$\underbrace{\left(\frac{\hbar^2}{2m}\left|\vec{k}_F-\vec{G}\right|^2 - E\right)}_{\Delta E} C_{k-G} + \sum_{\vec{G}''} V_{\vec{G}''-\vec{G}}\, C_{k-G''} = 0.$$

$\vec{G}_0\,,\ \vec{G}_1\,,\ \vec{G}_2$

$$\left.\begin{aligned}
&\Delta E\, C_{k_F-G_0} + V_{G_0-G_0} C_{k_F-G_0} + V_{G_1-G_0} C_{k-G_1} + V_{G_2-G_0} C_{k-G_2} = 0\\
&\Delta E\, C_{k_F-G_1} + V_{G_0-G_1} C_{k_F-G_0} + V_{G_1-G_1} C_{k-G_1} + V_{G_2-G_0} C_{k-G_2} = 0.\\
&\Delta E\, C_{k_F-G_2} + V_{G_0-G_2} C_{k_F-G_0} + V_{G_1-G_2} C_{k-G_1} + V_{G_2-G_2} C_{k_F-G_2} = 0.
\end{aligned}\right\}$$

$$\left.\begin{aligned}
\vec{G}_0-\vec{G}_0 &= 0.\\
\vec{G}_0-\vec{G}_1 &= -(\vec{G}_1-\vec{G}_0) = \frac{2\pi}{a}\left(-\hat{x}-\hat{y}\right)\\
\vec{G}_0-\vec{G}_2 &= -(\vec{G}_2-\vec{G}_0) = \frac{2\pi}{a}\left(-\hat{y}-\hat{z}\right).\\
\vec{G}_1-\vec{G}_2 &= -(\vec{G}_2-\vec{G}_1) = \frac{2\pi}{a}\left(\hat{x}-\hat{z}\right).
\end{aligned}\right\}\ (h'k'l').$$

$$V_{110} = V_{\bar{1}\bar{1}0} = 3M$$

$$V_{011} = V_{0\bar{1}\bar{1}} = 3M$$

$$V_{10\bar{1}} = V_{\bar{1}01} = 3M.$$

Pb. 3

$$\begin{pmatrix} \Delta E & 3M & 3M \\ 3M & \Delta E & 3M \\ 3M & 3M & \Delta E \end{pmatrix} \begin{pmatrix} C_{K_F - G_0} \\ C_{K_F - G_1} \\ C_{K_F - G_2} \end{pmatrix} = 0$$

b2 Resolem.

$$x = \frac{\Delta E}{3M} \Rightarrow \begin{vmatrix} x & 3 & 3 \\ 3 & x & 3 \\ 3 & 3 & x \end{vmatrix} = 0.$$

F2 - F3.

$$\underset{F2-F3}{=} \begin{vmatrix} x & 0 & 3 \\ 3 & x-3 & 3 \\ 3 & 3-x & x \end{vmatrix} \underset{C2+C3}{=} \begin{vmatrix} x & 0 & 3 \\ 6 & 0 & x+3 \\ 3 & 3-x & x \end{vmatrix} =$$

$$= -(3-x)\begin{vmatrix} x & 3 \\ 6 & x+3 \end{vmatrix} = -(3-x)(x^2+3x-18) =$$

$$= (+3-x)(x+6)(x-3) = (x+6)(x-3)^2 = 0.$$

$\Delta E = -6M.$

$\Delta E = 3M$ (degeneració 2).

$\Delta E = 3\mu.$

$\downarrow$

punt F $\rightarrow$ $\Delta E = \frac{11}{16} E_0 - E.$

$$\frac{11}{16} E_0 - E = 3\mu \Rightarrow \boxed{E_1 = \frac{11}{16} E_0 - 3\mu}$$

degeneració 2.

$\Delta E = -6\mu.$

$$\boxed{E_2 = \frac{11}{16} E_0 + 6\mu}$$

degeneració al punt F la trenquem parcialment. ja que apareix un valor E_1 (2 vectors iguals) i E_2 (1 vector igual).

Problema 7

$$\varepsilon(\vec{k}) = \varepsilon_0 + \frac{\hbar^2}{2m}(k_x^2 + k_y^2)$$

$\vec{k}(t=0) = k_0\,\hat{x}$

(a) per $\vec{E} = E_0\,\hat{x}$

$$\hbar\frac{d\vec{k}}{dt} = \vec{F} = -e\left(\vec{E} + \vec{v}\times\vec{B}\right) \Rightarrow \hbar\frac{d\vec{k}}{dt} = -e\vec{E}$$

$$\left.\begin{array}{l} \text{en } x \rightarrow \hbar\dfrac{dk_x}{dt} = -eE_0 \\ \text{en } y \rightarrow \hbar\dfrac{dk_y}{dt} = 0 \end{array}\right\} \begin{array}{l} k_x(t) = \dfrac{-eE_0}{\hbar}t + C_1 \\ k_y(t) = C_2. \end{array}$$

$$\text{per } t=0 \left\{\begin{array}{l} \rightarrow k_0 = C_1 \Rightarrow k_x(t) = k_0 - \dfrac{eE_0}{\hbar}t \\ \rightarrow 0 = C_2 \Rightarrow k_y(t) = 0. \end{array}\right.$$

$$\left.\begin{array}{l} k_x = k_0 - \dfrac{eE_0}{\hbar}t \\ k_y = 0 \end{array}\right\} \boxed{\vec{k}(t) = \left(k_0 - \frac{eE_0}{\hbar}t\right)\hat{x}.}$$

(b) $\vec{B} = B_0 \hat{z}$

$$\hbar \frac{d\vec{k}}{dt} = -e \vec{v} \times \vec{B}$$

$$v = \frac{1}{\hbar} \frac{dE}{d\vec{k}} = \frac{1}{\hbar} \frac{\hbar^2}{2m} \left(2k_x \hat{x} + 2k_y \hat{y} \right) =$$

$$= \frac{\hbar}{m} \left(k_x \hat{x} + k_y \hat{y} \right).$$

$$\hbar \frac{d\vec{k}}{dt} = -e \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ k_x & k_y & 0 \\ 0 & 0 & B_0 \end{vmatrix} \frac{\hbar}{m} = \frac{-e\hbar B_0}{m} \left(k_y \hat{x} - k_x \hat{y} \right)$$

$$\frac{d\vec{k}}{dt} = -\frac{eB_0}{m} \left(k_y \hat{x} - k_x \hat{y} \right)$$

$\frac{eB_0}{m}$ '' ω.

$$\begin{cases} \frac{dk_x}{dt} = -\omega k_y \rightarrow \dot{k}_x = -\omega k_y \rightarrow \ddot{k}_x = -\omega \dot{k}_y \\ \frac{dk_y}{dt} = +\omega k_x \rightarrow \dot{k}_y = \omega k_x \rightarrow \ddot{k}_y = \omega \dot{k}_x \end{cases} \Rightarrow$$

$$\Rightarrow \begin{matrix} \ddot{k}_x = -\omega \dot{k}_y = -\omega^2 k_x \\ \ddot{k}_y = \omega \dot{k}_x = -\omega^2 k_y \end{matrix} \quad \boxed{\begin{matrix} \ddot{k}_x = -\omega^2 k_x \\ \ddot{k}_y = -\omega^2 k_y. \end{matrix}}$$

solució $\Rightarrow$

7.3

per $\vec{k}(t=0) = k_0 \hat{x}$

$$\left.\begin{aligned} \ddot{k}_x &= -\omega^2 k_x \\ \ddot{k}_y &= -\omega^2 k_y \end{aligned}\right\} \begin{aligned} &\longrightarrow k_x(t) = k_0 \cos(\omega t) \\ &\longrightarrow k_y(t) = k_0 \sin(\omega t) \end{aligned}$$

per $\omega = \dfrac{eB_0}{m}$.