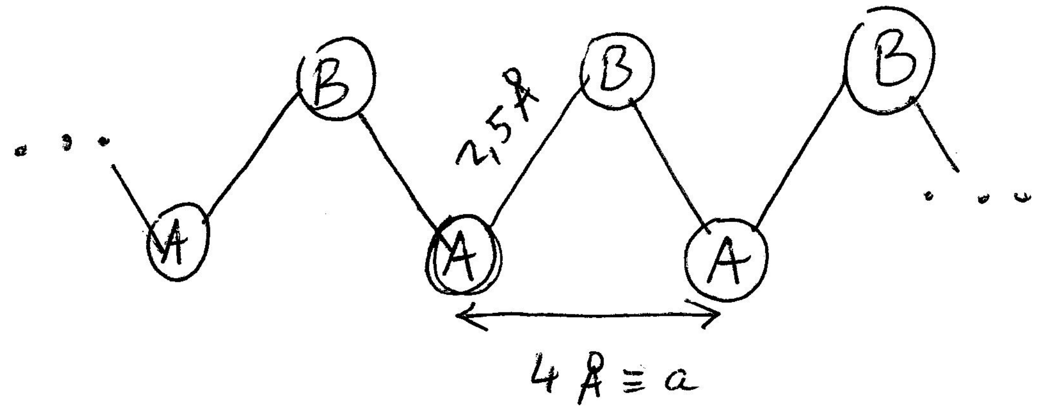
(1)



$E(k)$

$$e_A = \langle \phi_A(\vec{r}-\vec{R}_1) | \hat{H} | \phi_A(\vec{r}-\vec{R}_1) \rangle = 0$$

$$e_B = \langle \phi_B(\vec{r}-\vec{R}_2) | \hat{H} | \phi_B(\vec{r}-\vec{R}_2) \rangle = -3\,eV$$

$$V_{ss} = \langle \phi_A(\vec{r}-\vec{R}_1) | \hat{H} | \phi_B(\vec{r}-\vec{R}_2) \rangle \quad [n.n.] \quad = -1\,eV$$

$$H_{11} = e_A \qquad H_{12} = V_{ss}\left(1 + e^{-ika}\right)$$

$$H_{22} = e_B \qquad H_{21} = V_{ss}\left(1 + e^{ika}\right)$$

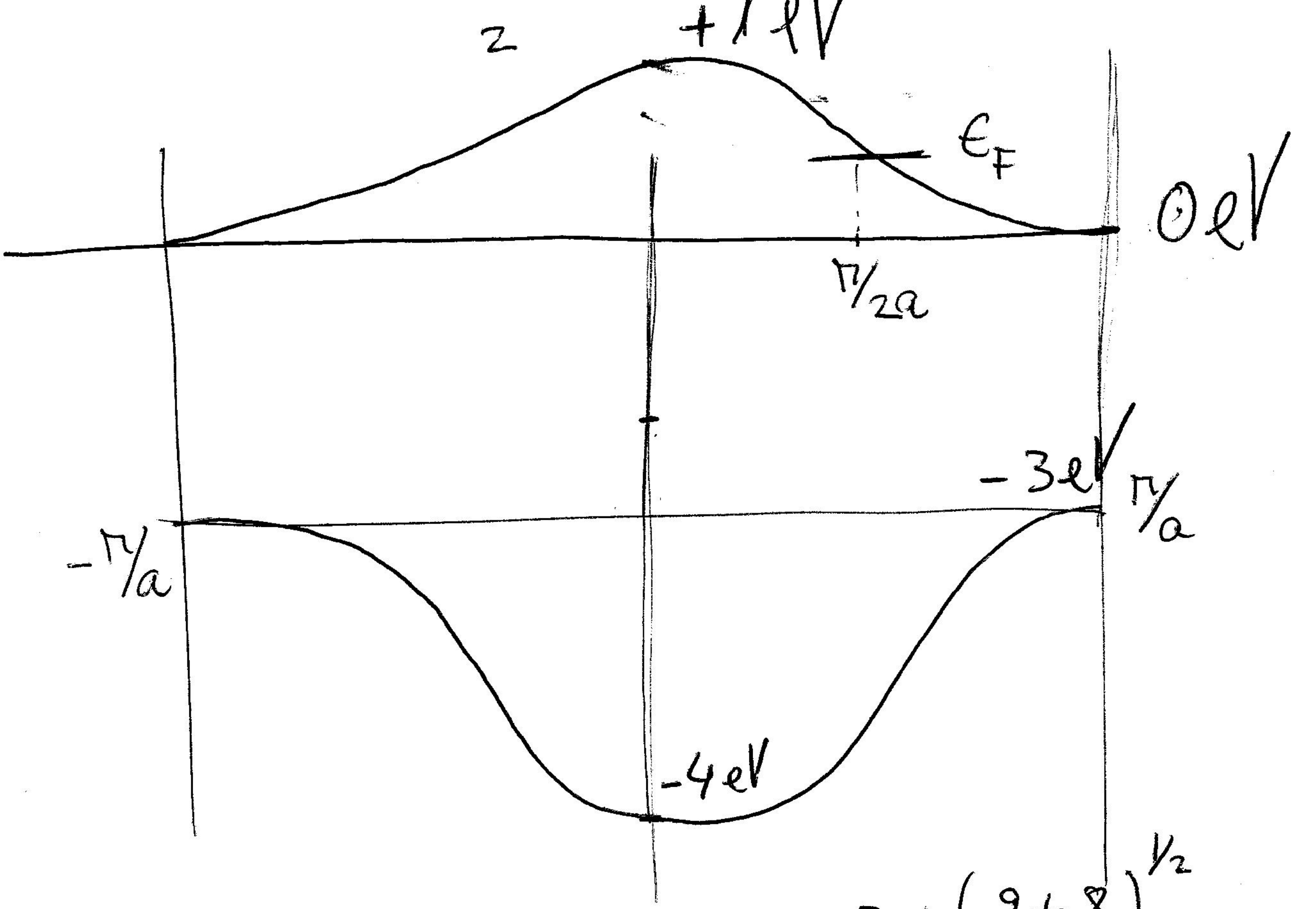
$$(e_A - \lambda)(e_B - \lambda) - V_{ss}^2\left(2 + 2\cos ka\right) = 0$$

$$(e_A = 0) \rightarrow \quad \lambda^2 - e_B\lambda - V_{ss}^2\left(2 + 2\cos ka\right) = 0$$

(1) [cont.]

$$\lambda(K) = \frac{e_B \pm \left[e_B^2 + 4V_{ss}^2 (2 + 2\cos Ka) \right]^{1/2}}{2}$$

$$= \frac{-3 \pm \left(9 + 8(1 + \cos Ka) \right)^{1/2}}{2}$$



$E_F \rightarrow K_F = \pi/2a \qquad e_+(K_F) = \dfrac{-3 + (9+8)^{1/2}}{2} = 0,56\ eV$

METÁLICO: el nivel de Fermi está en el medio de una banda → banda semi-llena.

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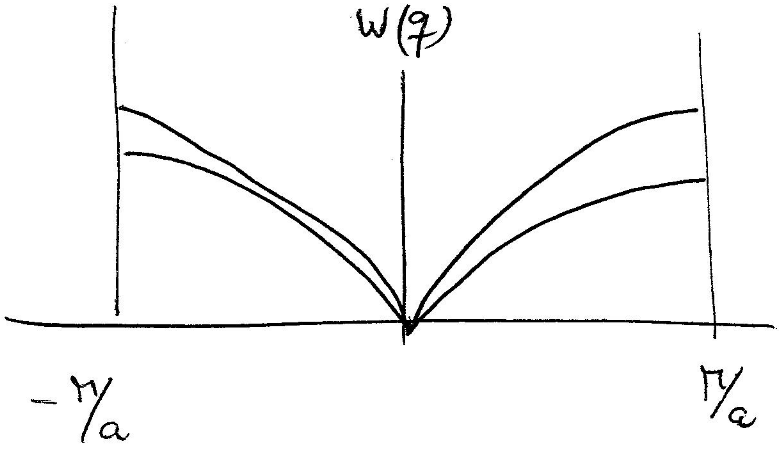
2

1 átomo por celda unidad → RAMAS ACÚSTICAS

movimiento en x, y → 2 RAMAS



$$E_p = \frac{1}{2}\sum_{m,n}\left(D^{xx}_{nm}\, x_n x_m + D^{yy}_{nm}\, y_n y_m\right)$$

Int. primeros vecinos:

$$E_p = \frac{1}{2}\sum_{n}\Big(D^{xx}_{nn}\, x_n x_n + D^{xx}_{n,n-1}\, x_n x_{n-1} + D_{n,n+1}\, x_n x_{n+1}$$
$$+ D^{yy}_{nn}\, y_n y_n + D^{yy}_{n,n-1}\, y_n y_{n-1} + D^{yy}_{n,n+1}\, y_n y_{n+1}\Big)$$

$$\sum_m D^{xx}_{nm} = 0 = D^{xx}_{nn} + D^{xx}_{n,n-1} + D^{xx}_{n,n+1} = D^{xx}_{nn} + 2C = 0$$

$$D^{xx}_{nn} = -2C \,;\quad D^{xx}_{n,n-1} = C$$

$$D^{yy}_{nn} = -2B \,;\quad D^{yy}_{n,n-1} = B$$

(2) [cont.]

$$E_P = \frac{1}{2}\sum_n C\left(x_n x_{n+1} + x_n x_{n-1} - 2 x_n x_n\right)$$
$$+ B\left(y_n y_{n+1} + y_n y_{n-1} - 2 y_n y_n\right)$$

$w(q)$: $\vec{F} = m\vec{a}$; $F_{nx} = -\dfrac{\partial E_p}{\partial x_n}$

$$F_{nx} = -\frac{1}{2}C\left(x_{n+1} + x_{n-1} + x_{n-1} + x_{n+1} - 4x_n\right)$$
$$= -C\left(x_{n+1} + x_{n-1} - 2x_n\right)$$

$$F_{ny} = -B\left(y_{n+1} + y_{n-1} - 2y_n\right)$$

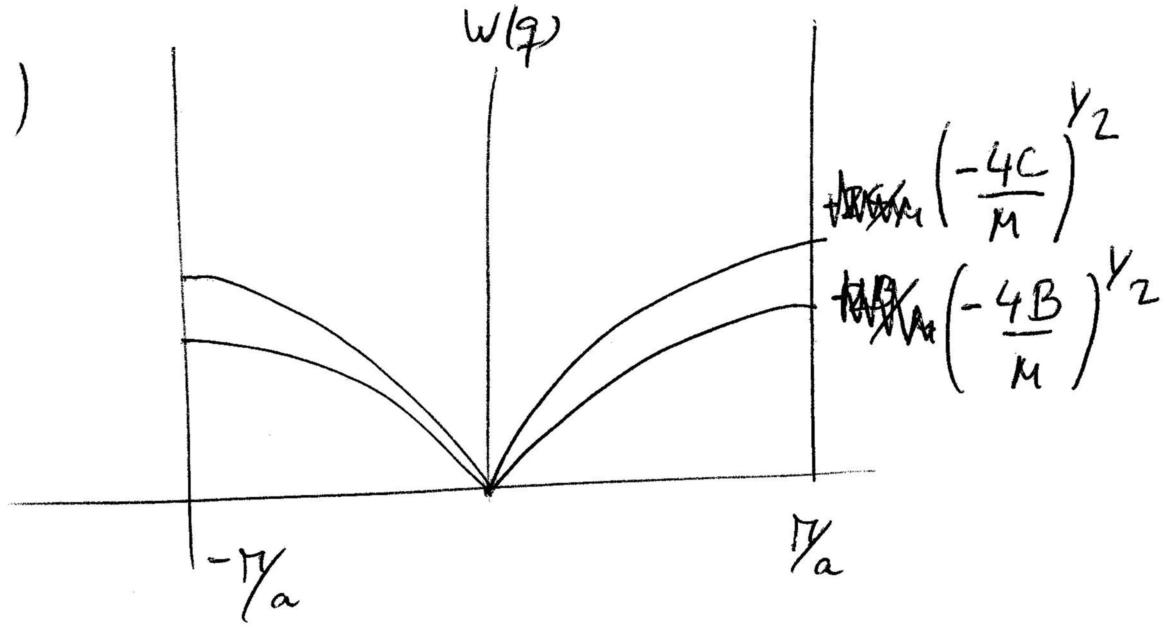
$x_m = x_0 e^{-i\omega t} e^{iqma}$; $\dfrac{d^2 x_m}{dt^2} = -\omega^2 x_0 e^{-i\omega t} e^{iqma}$

$$-M\omega^2 e^{-i\omega t} e^{iqma} x_0 = -x_0 e^{-i\omega t} e^{iqma} C\left(e^{iqa} + e^{-iqa} - 2\right)$$

$$\omega^2(q) = \frac{-C}{M}\left(2 - 2\cos(qa)\right) \rightarrow \omega_x$$

$$\omega^2(q) = \frac{-B}{M}\left(2 - 2\cos(qa)\right) \rightarrow \omega_y$$

(2 cont.)

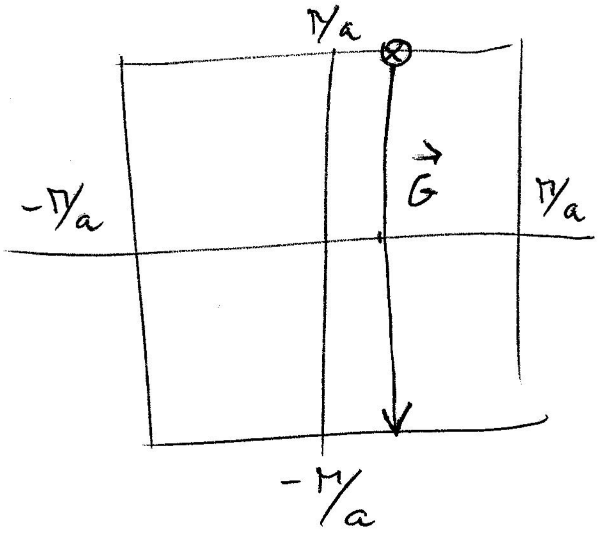


③ $$V(x,y) = \sum_{n,m} A_{n,m}\, e^{i\frac{2\pi}{a}(nx+my)}$$

electrones libres: $$e(\vec{k}) = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}\left(\frac{1}{16}+1\right)$$
$$= \frac{\hbar^2\pi^2}{2ma^2}\frac{17}{16}$$

electrones casi-libres: apertura de gaps: $E_g = 2\,|V(\vec{G})|$

$$\varepsilon(\vec{k}) \approx \varepsilon(\vec{k}-\vec{G}) \Rightarrow \vec{G} \equiv \left(0, -\frac{2\pi}{a}\right)$$



$$V(\vec{G}) = A_{0,\pm1}$$

$$e(\vec{k}) = \frac{\hbar^2\pi^2}{2ma^2}\frac{17}{16} \pm |A_{0,-1}|$$
$$\left(\pm\, |A_{0,1}|\right)$$

(4) Si $\rightarrow$ $m_{at} = 28$ u.m.a $= 28 \times 1{,}67 \times 10^{-31}$ Kg

$$\rho = 1730 \ \mathrm{Kg/m^3} = \frac{28 \times 1{,}67 \times 10^{-31}}{v} \Rightarrow v = 27 \times 10^{-30} \ \mathrm{m^3}$$

$$= 27 \ \mathring{A}^3$$

$$\frac{2\pi}{3} \mathring{A}^{-1} \rightarrow a = 3 \mathring{A} \longrightarrow$$

$$\vec{G} = 8\vec{g}_1 + 2\vec{g}_2 + 6\vec{g}_3$$

quitando factor común: $\vec{G}_0 = 4\vec{g}_1 + \vec{g}_2 + 3\vec{g}_3$

distancia entre planos: $d = \frac{2\pi}{|\vec{G}_0|} = \frac{3}{(26)^{1/2}} \mathring{A}$

$$|\vec{G}_0| = \frac{2\pi}{3}(16+1+9)^{1/2} \mathring{A}^{-1}$$

$v = A d$; $v \equiv$ volumen por átomo $\equiv 3^3 \mathring{A}^3 = 27 \mathring{A}^3$

$$A = \frac{27}{3}(26)^{1/2} = 9 \times (26)^{1/2} \mathring{A}^2 \equiv \underline{\underline{45{,}89 \mathring{A}^2}}$$