

GUÍA 7:

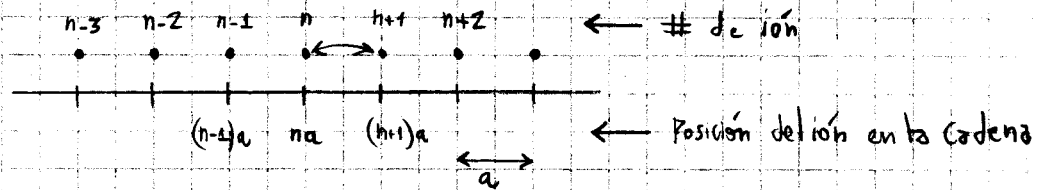
Dinámica de Redes

NOVA*

FECHA

1.

Cadena 1D



Consideramos interacción a primeras vecinos (de intensidad K)

$$U^{\text{harm}} = \frac{1}{2} K \sum_n [U(na) - U((n+1)a)]^2, \quad K = \frac{d^2 \phi(x)}{dx^2}$$

Ahora aplicamos las ecuaciones de Newton en el sitio 'n' situado en (na)

$$M \ddot{u}(na) = - \frac{\partial U^{\text{harm}}}{\partial u(na)} = - \frac{K}{\cancel{2}} \cdot \cancel{2} (U(na) - U((n+1)a))$$

masa de las iones

$$M \ddot{u} = -K \{ U(na) - U((n+1)a) + U(na) - U((n-1)a) \}$$

$$M \ddot{u} = -K [2U(na) - U((n-1)a) - U((n+1)a)]$$

Planteo las condiciones de contorno

$$\begin{cases} U((N+1)a) = U(a) & (\text{Cuando se termina vuelve a empezar}) \\ U(0) = U(Na) & (\text{EL 1erº es igual al último}) \end{cases}$$

Pensamos en ondas planas:

$$u(na, t) \propto e^{i(kna - \omega t)}$$

$$\begin{aligned} \dot{u}(na, t) &\propto e^{i(kna - \omega t)} (-i\omega) = -i\omega e^{i(kna - \omega t)} \\ \ddot{u}(na, t) &\propto e^{i(kna - \omega t)} (-i\omega)^2 = -\omega^2 e^{i(kna - \omega t)} \end{aligned}$$

$$-M\omega^2 e^{i(kna - \omega t)} = -K [2e^{i(kna - \omega t)} - e^{i(k(n-1)a - \omega t)} - e^{i(k(n+1)a - \omega t)}]$$

$$-M\omega^2 = -K [2 - e^{-ika} - e^{ika}]$$

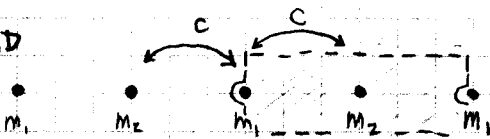
$$-M\omega^2 = -K [2 - 2\cos(ka)]$$

$$\omega^2 = \frac{2K}{M} [1 - \cos(ka)]$$

$$\boxed{\omega = \sqrt{\frac{2K}{M} (1 - \cos[ka])}}$$

Esta es la relación de dispersión pedida. Aquí k es discreto de las c.c.

2. Cadena 1D



Interacción a primeras vecinos C

# Ion	$n-1$	n	$n+1$	$n+2$
Posición (celda)	$(n-1)a$	na	$(n+1)a$	

base $\left\{ \begin{array}{l} \vec{0} \\ \vec{a} = a\hat{x} \end{array} \right.$

$$a) \quad U^{\text{harm}} = \frac{C}{2} \sum_n [U_1(na) - U_2(na)]^2 + \frac{C}{2} \sum_n [U_1(na) - U_2((n-1)a)]^2$$

Hemos contado una sola vez cada interacción.

$$\begin{cases} U_1 = U_1^0 e^{i(kna - \omega t)} \\ U_2 = U_2^0 e^{i(kna - \omega t)} \end{cases}$$

Cada ión oscila torno a su posición de equilibrio

$$m_1 \ddot{U}_1 = -m_1 U_1^0 \omega^2 e^{i(kna - \omega t)} = -\frac{C}{a} [U_1(na) - U_2(na) - U_2((n-1)a)]$$

$$= -C [2U_1(na) - U_2(na) - U_2((n-1)a)]$$

$$= -C [2U_1^0 e^{i(kna - \omega t)} - U_2^0 e^{i(kna - \omega t)} - U_2^0 e^{i(k(n-1)a - \omega t)}]$$

$$\cancel{m_1} U_1^0 \omega^2 = \cancel{C} [2U_1^0 - U_2^0 - U_2^0 e^{-i(ka)}]$$

$$m_2 \ddot{U}_2 = -m_2 U_2^0 \omega^2 e^{i(kna - \omega t)} = +\frac{C}{a} [U_1(na) - U_2(na)] + \frac{C}{a} [U_1((n+1)a) - U_2(na)]$$

$$= C [-2U_2(na) + U_1(na) + U_1((n+1)a)]$$

$$-m_2 U_2^0 \omega^2 = C [-2U_2^0 + U_1^0 + U_1^0 e^{i(ka)}]$$

$$\begin{cases} m_1 U_1^0 \omega^2 = C 2U_1^0 - C U_2^0 - C U_2^0 e^{-i(ka)} \\ m_2 U_2^0 \omega^2 = C 2U_2^0 - C U_1^0 - C U_1^0 e^{i(ka)} \end{cases}$$

$$\begin{cases} U_1^0 (m_1 \omega^2 - 2C) + U_2^0 (C + C e^{-i(ka)}) = 0 \\ U_2^0 (m_2 \omega^2 - 2C) + U_1^0 (C + C e^{i(ka)}) = 0 \end{cases}$$

$$\begin{pmatrix} m_1 \omega^2 - 2C & C(1 + e^{-i(ka)}) \\ C(1 + e^{i(ka)}) & m_2 \omega^2 - 2C \end{pmatrix} \begin{pmatrix} U_1^0 \\ U_2^0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$(m_1 \omega^2 + 2C)(m_2 \omega^2 + 2C) - C^2 (1 + e^{-i(ka)})(1 + e^{i(ka)}) = 0$$

$$m_1 m_2 \omega^4 + 4C^2 - m_1 \omega^2 2C - 2(1 + \cos ka) C^2 = 0$$

$$-m_2 \omega^2 2C$$

$$m_1 m_2 \omega^4 + (m_1 + m_2) 2C \omega^2 - Z(1 + \cos ka) C^2 + 4C^2 = 0$$

define $Z = \omega^2$

$$Z^2 - \underbrace{\left(\frac{m_1 + m_2}{m_1 m_2}\right)}_{\mu} 2C Z - \frac{Z(1 + \cos(ka)) C^2}{m_1 m_2} + \frac{4C^2}{m_1 m_2} = 0$$

$$\mu = \frac{m_1 + m_2}{m_1 m_2}$$

$$\downarrow = \frac{2C}{\mu} Z$$

$$Z = \left(\frac{+2C}{\mu} \pm \sqrt{\frac{4C^2}{\mu^2} - 4 \left(\frac{-Z(1 + \cos[ka]) C^2}{m_1 m_2} + \frac{4C^2}{m_1 m_2} \right)} \right) \frac{1}{2}$$

$$\omega^2 = \frac{C}{\mu} \pm \sqrt{\frac{C^2}{\mu^2} - \frac{C^2}{\mu^2} \left(\frac{-Z(1 + \cos(ka))}{(m_1 m_2)} + \frac{4\mu^2}{m_1 m_2} \right)}$$

$$\omega^2 = \frac{C}{\mu} \left(1 \pm \sqrt{1 - \frac{\mu^2}{(m_1 m_2)} [Z - Z \cos(ka) + 4]} \right)$$

$$\omega^2 = \frac{C}{\mu} \left(1 \pm \sqrt{1 - \frac{Z \mu^2}{m_1 m_2} (1 - \cos[ka])} \right)$$

↑ óptica
↓ acústica

b)

En $k = \pi/a$ es $\begin{cases} \cos(\pi) = -1 \\ e^{-i\pi} = e^{i\pi} = -1 \end{cases} \Rightarrow \omega^2 = \frac{C}{\mu} \left[1 \pm \sqrt{1 - \frac{4\mu^2}{m_1 m_2}} \right]$

$$\omega_A = \sqrt{\frac{C}{\mu}} \left(1 + \sqrt{1 - \frac{4\mu^2}{m_1 m_2}} \right)^{1/2}$$

$$\omega_B = \sqrt{\frac{C}{\mu}} \left(1 - \sqrt{1 - \frac{4\mu^2}{m_1 m_2}} \right)^{1/2}$$

$$1 - \frac{4\mu^2}{m_1 m_2} = 1 - \frac{4(m_1 + m_2)^2}{(m_1 m_2)^2} = \frac{m_1^2 + m_2^2 + 2m_1 m_2 - 4m_1 m_2}{(m_1 + m_2)^2} = \left(\frac{m_1 - m_2}{m_1 + m_2} \right)^2$$

NOTA
 $\sqrt{\left(\frac{m_1 - m_2}{m_1 + m_2}\right)^2} = \left| \frac{m_1 - m_2}{m_1 + m_2} \right|$
 Suponemos $m_1 > m_2$ pero es similar con $m_2 > m_1$

$$\omega_+^2 = \frac{C}{\mu} \left(1 + \frac{m_1 - m_2}{m_1 + m_2} \right) = \frac{C}{\mu} \left(\frac{2m_1}{m_1 + m_2} \right) = \frac{C}{\mu} \frac{2m_1}{m_1 + m_2}$$

$$\omega_-^2 = \frac{C}{\mu} \left(1 - \frac{m_1 - m_2}{m_1 + m_2} \right) = \frac{C}{\mu} \left(\frac{2m_2}{m_1 + m_2} \right) = \frac{C}{\mu} \frac{2m_2}{m_1 + m_2}$$

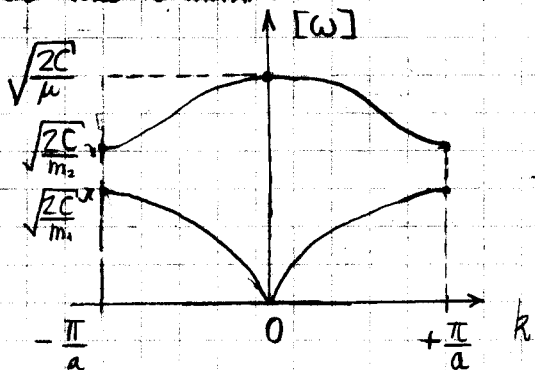
$$\Rightarrow * \omega_+ = \omega \rightarrow \omega = \sqrt{\frac{2C}{m_2}}$$

$$U_1^0 \left(\frac{m_1}{m_2} ZC - ZC \right) = 0 \rightarrow \begin{cases} U_2^0 \propto \text{cte} \\ U_1^0 = 0 \end{cases}$$

$$* \omega_- = \omega \rightarrow \omega = \sqrt{\frac{2C}{m_1}}$$

$$U_2^0 \left(\frac{m_2}{m_1} ZC - ZC \right) = 0 \rightarrow \begin{cases} U_2^0 = 0 \\ U_1^0 \propto \text{cte} \end{cases}$$

En el borde de zona tenemos a un tipo de ion oscilando, y el otro inmóvil. El cociente U_1^0/U_2^0 será nulo o infinito



NOTA
Al hacer supuesto $m_1 \gg m_2$ resulta $\frac{1}{m_1} < \frac{1}{m_2}$ lo cual define que curva se halla por encima
▲ viene de la nota anterior

c)

$$m_1 \gg m_2 \rightarrow 1 \gg \frac{m_2}{m_1} \rightarrow \frac{\mu^2}{m_1 \cdot m_2} = \frac{m_1 \cdot m_2}{(m_1 + m_2)^2} = \frac{m_2}{m_1 \left(1 + \frac{m_2}{m_1}\right)^2} = \frac{m_2}{m_1} \left(1 - 2\frac{m_2}{m_1}\right) \approx \frac{m_2}{m_1}$$

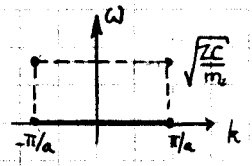
$$\mu = \frac{m_1 \cdot m_2}{m_1 + m_2} = \frac{m_2}{\left(1 + \frac{m_2}{m_1}\right)}$$

$$\mu \approx m_2 \cdot \left(1 - \frac{m_2}{m_1}\right)$$

$$\mu \approx m_2 - \frac{m_2^2}{m_1} \rightarrow \mu \approx m_2$$

$$\omega^2 = \frac{C}{m_2} \left(1 + \frac{m_2}{m_1}\right) \left(1 \pm \sqrt{1 - 2\frac{m_2}{m_1} [1 - \cos(ka)]}\right) \leftarrow \text{No veo expresión fácil de analizar}$$

Si $m_1 \rightarrow \infty \Rightarrow \omega^2 \approx \frac{C}{m_2} (1 + 1) = \omega_+^2 = \frac{2C}{m_2}$ (óptica)
 $\omega_-^2 = 0$ (acústica)



$\rightarrow U_1^0 = 0, U_2^0 = 0$ salvo en $k = \pi/a$ donde $U_2^0 = \text{cte.}$
 \rightarrow se mueven todos en bloque

d) En el caso de igualdad valdrán:

$$\mu = \frac{m_1 \cdot m_2}{m_1 + m_2} = \frac{m^2}{2m} = \frac{m}{2} \rightarrow \frac{\mu^2}{m^2} = \frac{m^2}{4m^2}$$

$$\omega^2(k) = \frac{2C}{m} \left(1 \pm \sqrt{1 - \frac{2}{4} [1 - \cos(ka)]}\right)$$

$$\omega^2(k=0) = \frac{2C}{m} (1 \pm 1) \rightarrow \sqrt{\frac{4C}{m}} = \omega \text{ óptica}$$

$$\rightarrow 0 = \omega \text{ acústica}$$

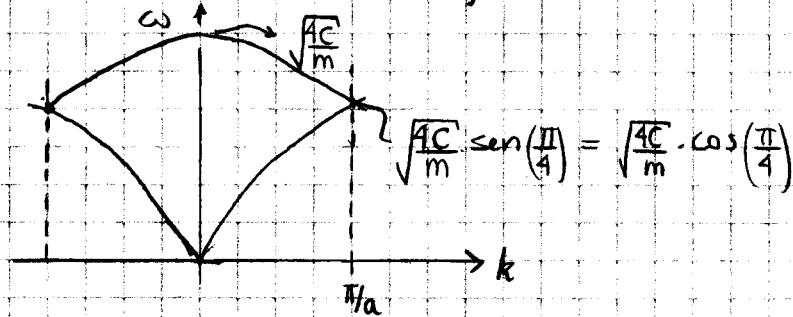
$$\left[1 \pm \sqrt{1 - \frac{1}{2} + \frac{1}{2} \cos(ka)}\right]$$

$$\boxed{\omega^2(k) = \frac{2C}{m} \left[1 \pm \cos\left(\frac{ka}{2}\right)\right]} \text{ donde } \begin{cases} - \text{ corresp. acústica} \\ + \text{ corresp. óptica} \end{cases}$$

Vemos que coincide con lo obtenido para la cadena monoatómica en el caso en que tomamos el signo (-); es decir la rama acústica.

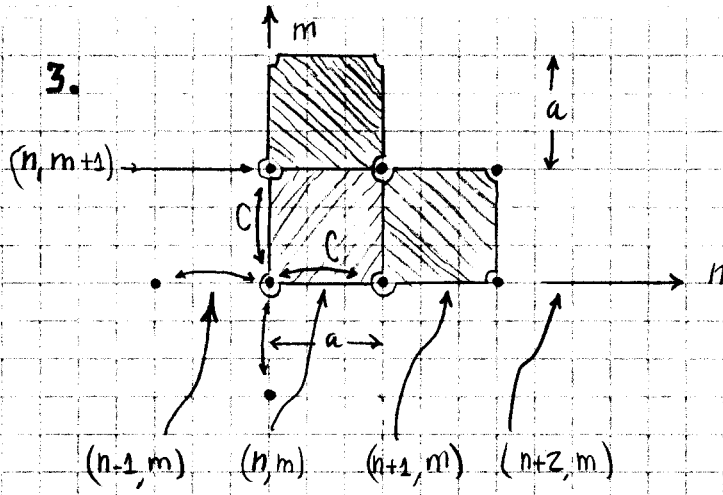
$$\omega_{AC}^2 = \frac{2C}{m} \left(1 - \cos \left[\frac{ka}{2} \right] \right) = \frac{2C}{m} \cdot 2 \sin^2 \left(\frac{ka}{4} \right)$$

$$\omega_{OP}^2 = \frac{2C}{m} \left(1 + \cos \left[\frac{ka}{2} \right] \right) = \frac{2C}{m} \cdot 2 \cos^2 \left(\frac{ka}{4} \right)$$



Con $m_1 = m_2$ las ramas ópticas y acústicas se hallan degeneradas en el borde de zona.

3.



Red cuadrada plana (2D)
monatómica de parámetro
a.

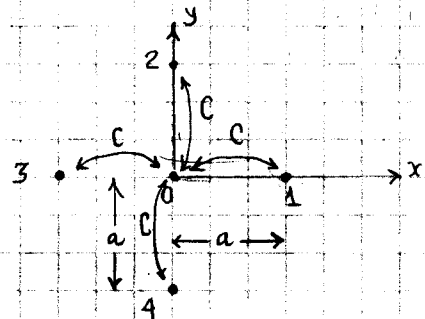
Interacción C a primeros
vecinos

$$U = \vec{U}^{(n)} \cdot e^{i(\vec{k} \cdot \vec{R}_n - \omega t)}$$

$$U^{harm} = \frac{1}{2} \left(\frac{1}{2} \right) \sum_n \sum_m C \left\{ [U(na, ma) - U((n+1)a, ma)]^2 + [U(na, ma) - U((n-1)a, ma)]^2 \right. \\ \left. + [U(na, ma) - U(na, (m+1)a)]^2 + [U(na, ma) - U(na, (m-1)a)]^2 \right\}$$

$$U^{harm} = \frac{1}{2} \sum_n \sum_m C \left\{ [u(na, ma) - u((n+1)a, ma)]^2 + [u(na, ma) - u(na, (m+1)a)]^2 \right\}$$

a) Para el armado de la matriz se redefinirán los primeros vecinos:



$$\phi = -\frac{e^2}{r} = -\frac{e^2}{\sqrt{x^2 + y^2}}$$

$$C \equiv \left. \frac{\partial \phi}{\partial r^2} \right|_{r_0} = e^2 \left. \frac{\partial}{\partial r^2} (-r^{-1}) \right|_{r_0} = \left. -\frac{e^2}{r^3} \right|_{r_0} = -\frac{2e^2}{r_0^3} = -\frac{2e^2}{a^3} = C$$

$$\vec{D}^{p1} = \begin{pmatrix} -C & 0 \\ 0 & 0 \end{pmatrix}$$

$$\vec{D}^{p2} = \begin{pmatrix} 0 & 0 \\ 0 & -C \end{pmatrix}$$

$$\vec{D}^{p3} = \begin{pmatrix} -C & 0 \\ 0 & 0 \end{pmatrix}$$

$$\vec{D}^{p4} = \begin{pmatrix} 0 & 0 \\ 0 & -C \end{pmatrix}$$

$$\vec{D}^{p0} = \begin{pmatrix} 2C & 0 \\ 0 & 2C \end{pmatrix}$$

$$E_i^{p1} = \hat{x}$$

$$\vec{D}_y^{pn} = -\chi^{pn} E_i E_j$$

$$\frac{\partial \phi}{\partial x} = -e^2 \frac{1}{\partial x} \left(\frac{1}{(x^2 + y^2)^{3/2}} \right) = -e^2 \left(-\frac{3}{2} \right) \frac{x}{(x^2 + y^2)^{5/2}}$$

$$\frac{\partial \phi}{\partial y \partial x} = -\frac{e^2 3xy}{(x^2 + y^2)^{5/2}}$$

$$\frac{\partial \phi}{\partial x^2} = \frac{\partial}{\partial x} \left[x (x^2 + y^2)^{-3/2} \right] (e^2) = -e^2 \left[(x^2 + y^2)^{-3/2} - x (x^2 + y^2)^{-5/2} \cdot 2x \right]$$

$$\frac{\partial \phi}{\partial x^2} = -e^2 \left(\frac{y^2 - 2x^2}{(x^2 + y^2)^{5/2}} \right)$$

$$\frac{\partial \phi}{\partial y^2} = -e^2 \left(\frac{x^2 - 2y^2}{(x^2 + y^2)^{5/2}} \right)$$

$$\left. \frac{\partial \phi}{\partial x^2} \right|_{x=0} = -e^2 \left(\frac{2a^2}{a^5} \right) = \frac{2e^2}{a^3}$$

$$\vec{D}(\vec{k}) = \sum_{\vec{R}_n} \vec{D}(\vec{R}_n) \cdot e^{i\vec{k} \cdot \vec{R}_n} ; \text{ con } \vec{R}_n = \vec{0}; (a,0); (-a,0); (0,a); (0,-a)$$

$$\Rightarrow \vec{D}(\vec{k}) = \begin{pmatrix} -C & 0 \\ 0 & 0 \end{pmatrix} e^{ik_x a} + \begin{pmatrix} -C & 0 \\ 0 & 0 \end{pmatrix} e^{-ik_x a} + \begin{pmatrix} 2C & 0 \\ 0 & 2C \end{pmatrix} \\ + \begin{pmatrix} 0 & 0 \\ 0 & -C \end{pmatrix} e^{ik_y a} + \begin{pmatrix} 0 & 0 \\ 0 & -C \end{pmatrix} e^{-ik_y a}$$

$$\boxed{\vec{D}(\vec{k}) = \begin{pmatrix} -C & 0 \\ 0 & 0 \end{pmatrix} 2 \cos(k_x a) + \begin{pmatrix} 0 & 0 \\ 0 & -C \end{pmatrix} 2 \cos(k_y a) + \begin{pmatrix} 2C & 0 \\ 0 & 2C \end{pmatrix}}$$

b)

$$M\omega^2 \vec{u} = \vec{D}(\vec{k}) \vec{u} \rightarrow$$

$$\det [M\omega^2 - \vec{D}(\vec{k})] = 0 \rightarrow$$

$$\begin{bmatrix} M\omega^2 + 2C [\cos(k_x a) - 1] & 0 \\ 0 & M\omega^2 + 2C [\cos(k_y a) - 1] \end{bmatrix}$$

$$\begin{bmatrix} M\omega^2 - 2C 2 \sin^2\left(\frac{k_x a}{2}\right) & 0 \\ 0 & M\omega^2 - 2C 2 \sin^2\left(\frac{k_y a}{2}\right) \end{bmatrix}$$

$$\left[M\omega^2 - 4C \sin^2\left(\frac{k_x a}{2}\right) \right] \left[M\omega^2 - 4C \sin^2\left(\frac{k_y a}{2}\right) \right]$$

$$M^2 \omega^4 - M\omega^2 4C \sin^2\left(\frac{k_x a}{2}\right) - M\omega^2 4C \sin^2\left(\frac{k_y a}{2}\right) + 16C^2 \sin^2\left(\frac{k_x a}{2}\right) \sin^2\left(\frac{k_y a}{2}\right) = 0$$

$$M^2 \omega^4 - \omega^2 M 4C \left[\sin^2\left(\frac{k_x a}{2}\right) + \sin^2\left(\frac{k_y a}{2}\right) \right] + 16C^2 \sin^2\left(\frac{k_x a}{2}\right) \sin^2\left(\frac{k_y a}{2}\right) = 0$$

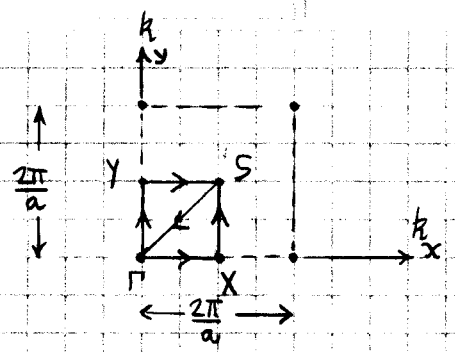
$$\omega^2 = \frac{4CM [\sin^2(X) + \sin^2(Y)]}{2M^2} \mp \frac{\sqrt{4^2 C^2 M^2 [\sin^2(X) + \sin^2(Y)]^2 - 4M^2 16C^2 \sin^2(X) \sin^2(Y)}}{2M^2}$$

$$\frac{2C}{M} (\sin^2 X + \sin^2 Y) \mp \frac{1}{2M^2} \sqrt{16C^2 M^2 [\sin^4 X + \sin^4 Y + 2 \sin^2 X \sin^2 Y - 4 \sin^2 X \sin^2 Y]}$$

$$\omega^2(k) = \frac{2C}{M} (\sin^2 X + \sin^2 Y) \mp \frac{4CM}{2M^2} (\sin^2 X - \sin^2 Y) \quad \text{con } X \equiv k_x a/2 \\ Y \equiv k_y a/2$$

$$\omega^2(k) = \frac{2C}{M} [\sin^2 X + \sin^2 Y \mp (\sin^2 X - \sin^2 Y)]$$

$$\omega_-^2(k) = \frac{2C}{M} 2 \sin^2\left(\frac{k_y a}{2}\right) ; \quad \omega_+^2(k) = \frac{2C}{M} 2 \sin^2\left(\frac{k_x a}{2}\right)$$



$\Gamma \rightarrow X \rightarrow S \rightarrow Y \rightarrow S$: recorda

$(\frac{\pi}{a}, 0) \quad (\frac{\pi}{a}, \frac{\pi}{a}) \quad (0, \frac{\pi}{a})$

* $\Gamma \rightarrow X$: $\omega_{+}^2(k) = \frac{2C}{M} \left[\sin^2\left(\frac{k_x a}{2}\right) \right]$

* $X \rightarrow S$: $\omega_{+}^2 = \frac{2C}{M} [1 + 1]$
 $\omega_{-}^2 = \frac{2C}{M} \left[2 \sin^2\left(\frac{k_y a}{2}\right) \right]$

* $S \rightarrow \Gamma$: $\omega_{+}^2 = \frac{2C}{M} \left[2 \sin^2\left(\frac{k a}{\sqrt{2} \cdot 2}\right) \right]$ $\omega_{-}^2 = \frac{2C}{M} \left[2 \sin^2\left(\frac{k a}{\sqrt{2} \cdot 2}\right) \right]$

$k_x = \frac{k}{\sqrt{2}}$
 $k_y = \frac{k}{\sqrt{2}}$

* $\Gamma \rightarrow Y$: $\omega_{-}^2 = \frac{2C}{M} \left[2 \sin^2\left(\frac{k_y a}{2}\right) \right]$

* $Y \rightarrow S$: $\omega_{+}^2 = \frac{2C}{M} \left[2 \sin^2\left(\frac{k_x a}{2}\right) \right]$

$\omega_{-}^2 = \frac{2C}{M} [2]$

$2\left(\frac{\pi}{a}\right)^2 = \frac{2\pi^2}{a^2}$

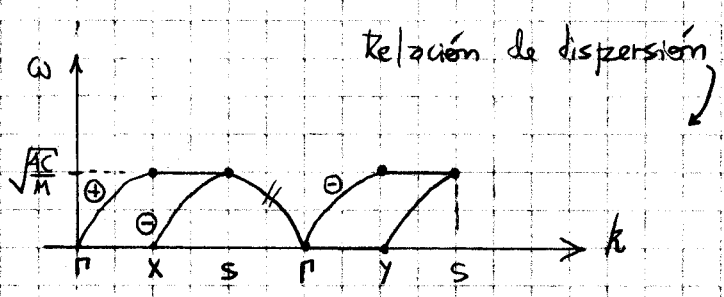
Ahora evaluamos los autovectores correspondientes:

$\left[M\omega_{-}^2 - 4C \sin^2\left(\frac{k_y a}{2}\right) \right] u_x^{(0)} = 0$

$\omega_{-}(k) \rightarrow \vec{u}_{(0)} \propto \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$\left[\sin^2\left(\frac{k_y a}{2}\right) - \sin^2\left(\frac{k_x a}{2}\right) \right] u_x^{(1)} = 0 \rightarrow$

$\omega_{+}(k) \rightarrow \vec{u}_{(1)} \propto \begin{pmatrix} 1 \\ 0 \end{pmatrix}$



Relación de dispersión

Desde $\Gamma \rightarrow X$ el modo de ω_{+} es el longitudinal y el de ω_{-} el transversal