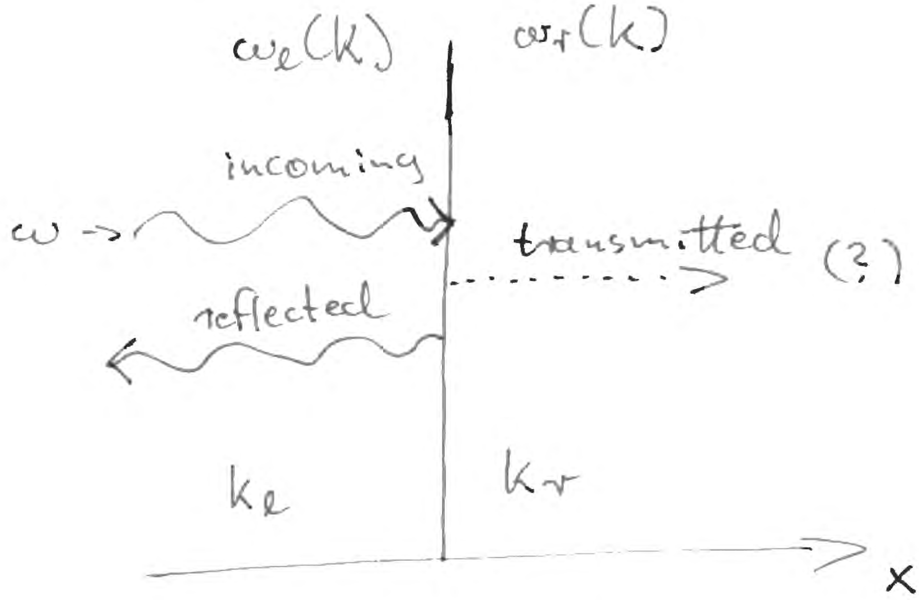
Condensed Matter Physics , HS 2011

Worksheet 5, solutions

19.



incoming wave $\propto$ $e^{ik_\ell x}$

reflected wave $\propto$ $r \cdot e^{-ik_\ell x}$

transmitted wave $\propto$ $t \cdot e^{ik_r x}$

$$\omega_\ell = \omega_r = \omega$$

$s(x)$, $\frac{\partial s}{\partial x}$ continuous

$$\Rightarrow t = \frac{2k_\ell}{k_\ell + k_r} \qquad r = \frac{k_\ell - k_r}{k_\ell + k_r}$$

$$\omega^2(k) = \omega_{Max}^2 (1 - \cos ka) = 2\omega_{Max}^2 \cdot \sin^2 \frac{ka}{2}$$

Ansatz for k_r: $k_r = k_1 + i \cdot k_2$

$$\Rightarrow \cos(k \cdot a) = \cos(k_1 a + i k_2 a)$$
$$= \cos(k_1 a) \cdot \cosh(k_2 a) - i \sin(k_1 a) \sinh(k_2 a)$$

Set $\omega^2 \geq 0$ (ω should be real !)

$$\Rightarrow \quad \sin(k_1 a)\cdot \sinh(k_2 a) = 0$$

$$\Leftrightarrow \quad \bullet \; k_2 = 0$$

$$\bullet \; k_1 = \frac{\pi}{a}\cdot l \quad ; \; l \in \mathbb{Z}$$

$$\Rightarrow \quad \cos(k_1 a + i k_2 a) = \pm 1 \cdot \cosh(k_2 a) \quad (k_2 \in \mathbb{R})$$

$$\omega^2 \underset{\substack{\uparrow \\ k_1 = \frac{\pi}{a}\ (l=1)}}{=} 4\omega_{Max}^2 \left(1 + \cosh(k_2 a)\right)$$

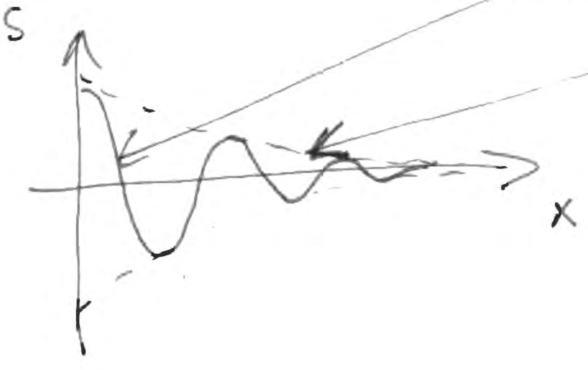
$$\omega\left(\frac{\pi}{a} \pm i k_2\right) = 2\cdot\sqrt{2}\,\omega_{Max}\sqrt{\frac{1+\cosh(k_2 a)}{\sqrt{2}}}$$

$$= 2\sqrt{2}\,\omega_{Max}\cosh\left(k_2 \cdot \frac{a}{2}\right)$$

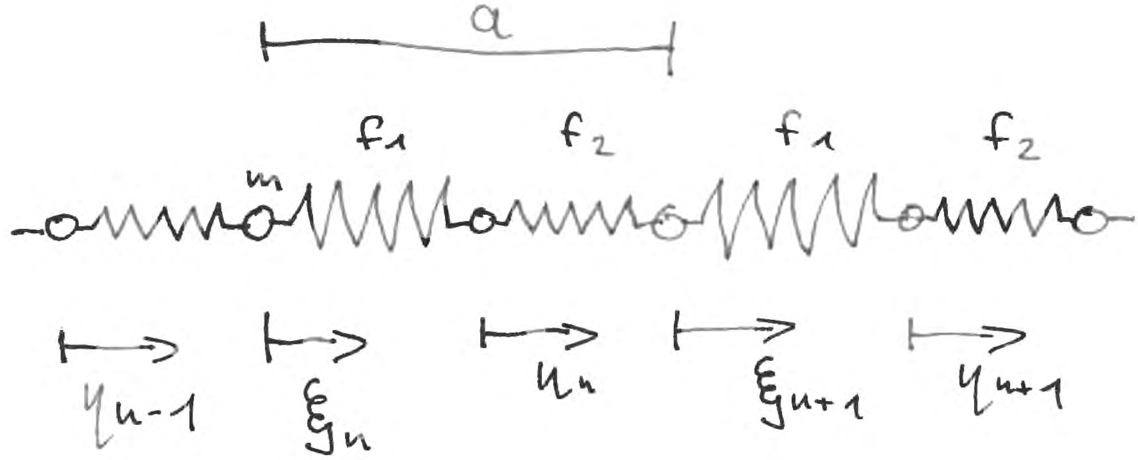
$$k_r = \frac{\pi}{a} \pm i\cdot k_2, \quad s_r \propto e^{i k_r x} = e^{i\frac{\pi}{a}x}\cdot e^{-k_2 x}$$

oscillation

exponential damping



20.



a) chose ξ_n, η_n, so that $f_1 > f_2$

$$m\cdot\ddot{\xi}_n = -f_1\xi_n - f_2\xi_n + f_2\eta_{n-1} + f_1\eta_n$$

$$= f_1(\eta_n - \xi_n) + f_2(\eta_{n-1} - \xi_n) \qquad (1)$$

$$m\cdot\ddot{\eta} = f_2(\xi_{n+1} - \eta_n) + f_1(\xi_n - \eta_n) \qquad (2)$$

Ansatz: $\xi_n = A\cdot e^{i(kna-\omega t)}$ $\qquad \eta_n = B e^{i(kna-\omega t)}$

-> into (1), (2):

$$\begin{cases} (-i\omega)^2\cdot mA = f_1(B-A) + f_2(Be^{-ika} - A) \\ (-i\omega)^2\cdot mB = f_2(Ae^{ika} - B) + f_1(A-B) \end{cases}$$

$$\begin{cases} (-m\omega^2 + f_1 + f_2)A - (f_2e^{-ika} + f_1)B = 0 \\ (-f_2e^{ika} - f_1)A + (-m\omega^2 + f_1 + f_2)B = 0 \end{cases}$$

$$\begin{cases} \left(-\omega^2 + \frac{f_1}{m} + \frac{f_2}{m}\right)A + \left(-\frac{f_2}{m}e^{-ika} - \frac{f_1}{m}\right)B = 0 \\ \left(-\frac{f_2}{m}e^{ika} - \frac{f_1}{m}\right)A + \left(-\omega^2 + \frac{f_1}{m} + \frac{f_2}{m}\right)B = 0 \end{cases}$$

set $\frac{f_1}{m} := \omega_1^2$, $\frac{f_2}{m} = \omega_2^2$

$$\underbrace{\begin{pmatrix} (-\omega^2+\omega_1^2+\omega_2^2) & -(\omega_2^2 e^{-ika}+\omega_1^2) \\ -(\omega_2^2 e^{ika}+\omega_1^2) & (-\omega^2+\omega_1^2+\omega_2^2) \end{pmatrix}}\begin{pmatrix} A \\ B \end{pmatrix} = 0$$

nontrivial solution, if det( ) = 0

$$(-\omega^2+\omega_1^2+\omega_2^2)^2 - (\omega_2^2 e^{ika}+\omega_1^2)(\omega_2^2 e^{-ika}+\omega_1^2) = 0$$

$$\omega^4 - 2\omega^2(\omega_1^2+\omega_2^2) + (\omega_1^2+\omega_2^2)^2 - \omega_2^4 - \omega_1^2\omega_2^2\underbrace{\left(e^{ika}+e^{-ika}\right)}_{2\cdot\cos(ka)} = 0$$

$$\omega^4 - 2\omega^2(\omega_1^2+\omega_2^2) + 2\omega_1^2\omega_2^2\,(1-\cos(ka)) = 0$$

$$\Rightarrow \quad (\omega^2)_\pm = \frac{2(\omega_1^2+\omega_2^2) \pm \sqrt{4(\omega_1^2+\omega_2^2) - 8\omega_1^2\omega_2^2(1-\cos ka)}}{2}$$

$$\boxed{(\omega^2)_\pm = (\omega_1^2+\omega_2^2) \pm \sqrt{\omega_1^4 + 2\cos(ka)\,\omega_1^2\omega_2^2 + \omega_2^4}}$$

$k=0$:

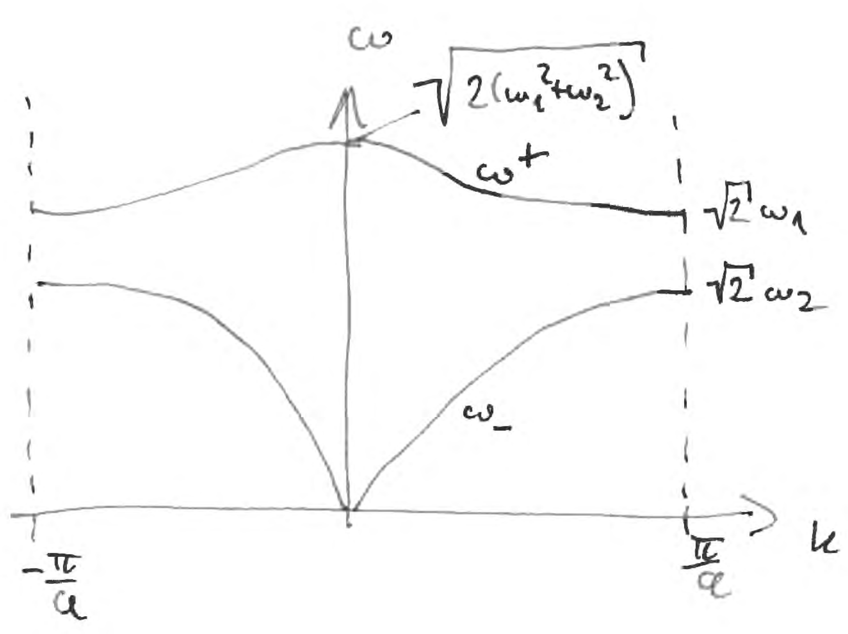
$(\omega^2)_+ = 2(\omega_1^2+\omega_2^2)$

$(\omega^2)_- = 0$

$k=\frac{\pi}{a}$:

$(\omega^2)_+ = 2\omega_1^2$

$(\omega^2)_- = 2\omega_2^2$



$\underline{k \simeq 0:}$

$$(\omega^2)_\pm = (\omega_1^2+\omega_2^2) \pm \sqrt{\omega_1^4 + 2\cos(ka)\,\omega_1^2\omega_2^2 + \omega_2^4}$$

$$\simeq (\omega_1^2+\omega_2^2) \pm \sqrt{\omega_1^4 + 2\left(1 - \frac{(ka)^2}{2}\right)\omega_1^2\omega_2^2 + \omega_2^4}$$

$$= (\omega_1^2+\omega_2^2) \pm \sqrt{(\omega_1^4+\omega_2^4) + 2\omega_1^2\omega_2^2 - (ka)^2\omega_1^2\omega_2^2}$$

$$= (\omega_1^2+\omega_2^2) \pm \sqrt{(\omega_1^2+\omega_2^2)^2 - (ka)^2\,\omega_1^2\omega_2^2}$$

$$= (\omega_1^2+\omega_2^2) \pm \sqrt{1 - (ka)^2 \frac{\omega_1^2\omega_2^2}{(\omega_1^2+\omega_2^2)^2}}$$

$$\times (\omega_1^2+\omega_2^2)$$

$$\Rightarrow \quad \omega_+^2 \simeq 2(\omega_1^2+\omega_2^2) - \frac{(ka)^2}{2}\frac{\omega_1^2\omega_2^2}{(\omega_1^2+\omega_2^2)}$$

$$\omega_-^2 \simeq \frac{(ka)^2}{2}\frac{\omega_1^2\omega_2^2}{\omega_1^2+\omega_2^2}$$

$\rightarrow$ for $ka \ll 1$: $\omega_- \propto k$

Amplitudes:

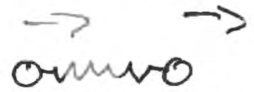
use e.g. from first equation of motion:

$$(-\omega^2+\omega_1^2+\omega_2^2)A - (\omega_2^2 e^{-ika} + \omega_1^2)B = 0$$

$k=0$:

$\omega_-^2 = 0 \quad \Rightarrow \quad (\omega_1^2+\omega_2^2)A - (\omega_1^2+\omega_2^2)B = 0$

$\Rightarrow \quad A = B$



in-phase movement

("acoustic phonon")

$\omega_+^2 = 2(\omega_1^2+\omega_2^2) \quad \Rightarrow \quad -(\omega_1^2+\omega_2^2)A - (\omega_1^2+\omega_2^2)B = 0$

$\Rightarrow \quad A = -B$

out of phase movement

("optical phonon")

$k=\frac{\pi}{a}$:

$\omega_-^2 = 2\omega_2^2 \quad \Rightarrow \quad (\omega_1^2-\omega_2^2)A - (\omega_1^2-\omega_2^2)B = 0$

$\Rightarrow \quad A = B$

$\omega_+^2 = 2\omega_1^2 \quad \Rightarrow \quad -(\omega_1^2+\omega_2^2)A - (\omega_1^2-\omega_2^2)B = 0$

$\Rightarrow \quad A = -B$

phase velocity $v_\phi = \dfrac{\omega}{k}$

$$v_\phi^{\pm} = \frac{\sqrt{(\omega_1^2+\omega_2^2) \pm \sqrt{\omega_1^4 + 2\cos(ka)\,\omega_1^2\omega_2^2 + \omega_2^4}}}{k}$$

$ka \ll 1$:

$$v_\phi^{+} \simeq \sqrt{\frac{2(\omega_1^2+\omega_2^2)}{k^2} - \frac{a^2}{2}\,\frac{\omega_1^2\omega_2^2}{\omega_1^2+\omega_2^2}}$$

$$v_\phi^{-} \simeq \frac{a^2}{2}\,\frac{\omega_1^2\omega_2^2}{\omega_1^2+\omega_2^2} = \text{const.}$$

$k = \frac{\pi}{a}$: $$v_\phi^{+} = \sqrt{2}\,\frac{\omega_1}{k} = \sqrt{2}\,\frac{a\omega_1}{\pi}$$

$$v_\phi^{-} = \sqrt{2}\,\frac{a\omega_2}{\pi}$$

group velocity $v_{gr} = \dfrac{\partial\omega}{\partial k}$

$$\frac{\partial\omega}{\partial k} = \frac{\partial\omega}{\partial f(\omega)}\cdot\frac{\partial f(\omega)}{\partial k} = \frac{1}{\frac{\partial f(\omega)}{\partial\omega}}\cdot\frac{\partial f(\omega)}{\partial k} \underset{f(\omega)=\omega^2}{=} \frac{1}{2\omega}\cdot\frac{\partial f(\omega)}{\partial k}$$

$$\Rightarrow v_{gr}^{\pm} = \frac{1}{2\sqrt{(\omega_1^2+\omega_2^2) \pm \sqrt{\omega_1^4 + 2\cos(ka)\,\omega_1^2\omega_2^2+\omega_2^4}}}\cdot\frac{\pm a\omega_1^2\omega_2^2\cdot(-2)\sin(ka)}{2\sqrt{\omega_1^4+2\cos(ka)\,\omega_1^2\omega_2^2+\omega_2^4}}$$

$$= \frac{\mp\frac{a}{2}\,\omega_1^2\omega_2^2\cdot\sin(ka)}{\sqrt{(\omega_1^2+\omega_2^2)\sqrt{\omega_1^4+2\omega_1^2\omega_2^2\cos(ka)+\omega_2^4} \pm (\omega_1^4+2\omega_1^2\omega_2^2\cos(ka)+\omega_2^4)}}$$

$k \to 0$: $v_{gr}^{+} = 0$; $v_{gr}^{-} \simeq \sqrt{\frac{\omega_1^2\omega_2^2}{\omega_1^2+\omega_2^2}}\cdot\frac{a}{\sqrt{2}}$; $k = \frac{\pi}{a}$: $v_{gr}^{+} = v_{gr}^{-} = 0$

b) $f_1 = f_2 = f \quad \Rightarrow \quad \omega_1^2 = \omega_2^2 = \omega'^2$

$$\Rightarrow \quad (\omega^2)_\pm = 2\omega'^2 \pm \omega'^2 \sqrt{2 + 2\cdot\cos(ka)}$$

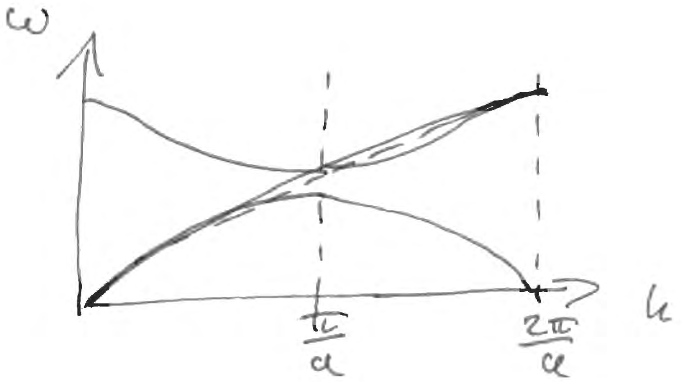
$$= \omega'^2 \left(2 \pm \sqrt{2(1+\cos(ka))}\right)$$

$$\overset{\uparrow}{=} \quad \omega'^2 \left(2 \pm \sqrt{2\cdot 2\cos^2\left(\tfrac{ka}{2}\right)}\right.$$

$1+\cos(ka) = 2\cos^2\left(\frac{ka}{2}\right)$

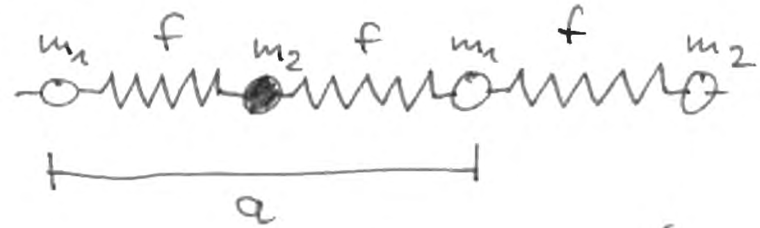
$$= 2\omega'^2 \left(1 \pm \cos\frac{ka}{2}\right)$$

$$\Rightarrow \quad \omega_\pm = \omega' \sqrt{2\left(1 \pm \cos\left(\tfrac{ka}{2}\right)\right)}$$



$\rightarrow$ linear chain with $f_1 = f_2$,
$m_1 = m_2$

c) lecture :



$$\omega_1 = \frac{f}{m_1}, \quad \omega_2 = \frac{f}{m_2} \quad ; \quad (m_1 < m_2)$$

$\rightarrow$ gives identical dispersion relation

but: amplitude relations will be different in general

Problem 20 (d)

When $m_1 = m_2 =$ m

$$\omega^2 = \frac{f_1 + f_2}{M}(2 \pm \sqrt{2 + 2cos(ka)})$$

this dispersion relation is shown as in Figure 1, where for the first Brillouin zone for the diatomic chain is ka $\in$ [-π, π]. In terms of the new lattice constant a' = a/2, the dispersion relation is then:

$$\omega^2 = \frac{f_1 + f_2}{M}(1 \pm cos(ka')), ka' \in [-\pi/2, \pi/2]$$

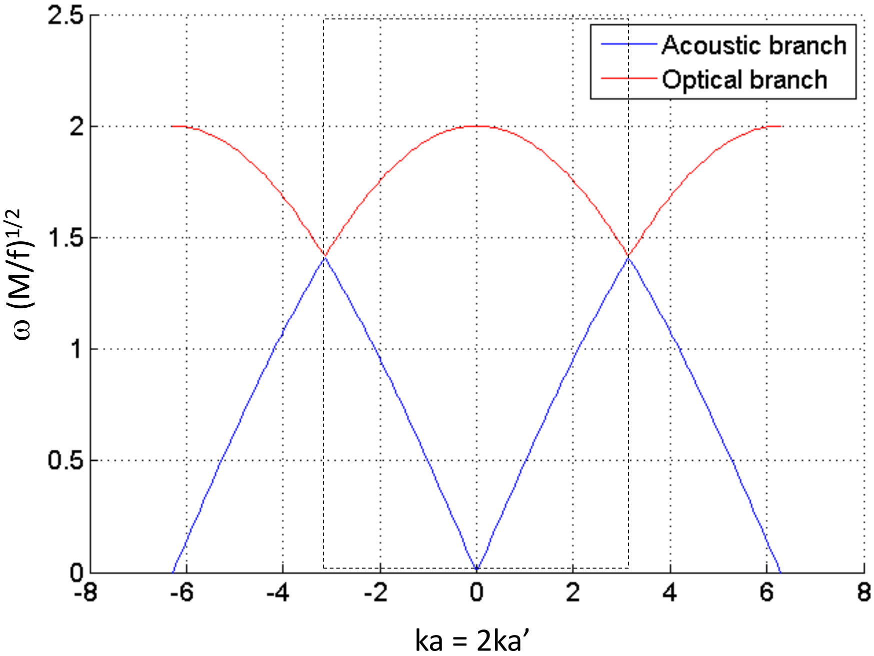


Figure 1:
The dispersion relation for the diatomic linear chain when $m_1 = m_2 =$ m. Dashed rectangular area gives the Brillouin zone for the diatomic chain.

For the optical branch, consider the part with $ka' \in$ [-π/2, 0], then:

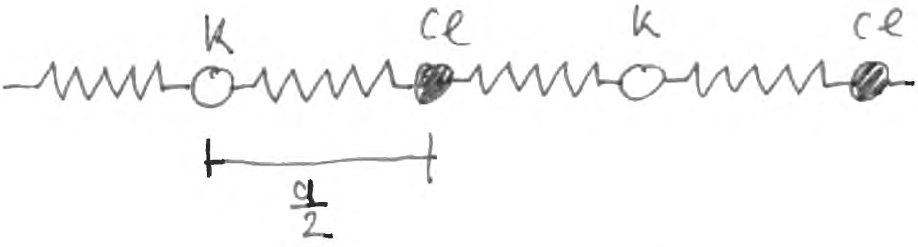
$$\omega^2 = \frac{f_1 + f_2}{M}(1 + cos(ka')) = \frac{f_1 + f_2}{M}(1 - cos(ka' + \pi))$$

notice that $ka' + \pi \in [\pi/2, \pi]$, above expession indicates that the optical branch in dispersion relation for the diatomic chain in [-π/2, 0] is equivalent to the acoustic branch in [π/2, π].

Similarly, the optical branch in dispersion relation for the diatomic chain in [0, π/2] is equvalent to the acoustic branch in [-π, -π/2]. Thus, instead of describing the dispersion relation with both optical and acoustic branch in $ka' \in$ [-π/2, π/2], it is equivalent to just consider the acoustic branch in $ka' \in$ [-π, π], which is just the dispersion relation for the monatomic chain. Therefore, when setting $m_1 = m_2 =$ m, the dispersion relation for monatomic chain is recovered.

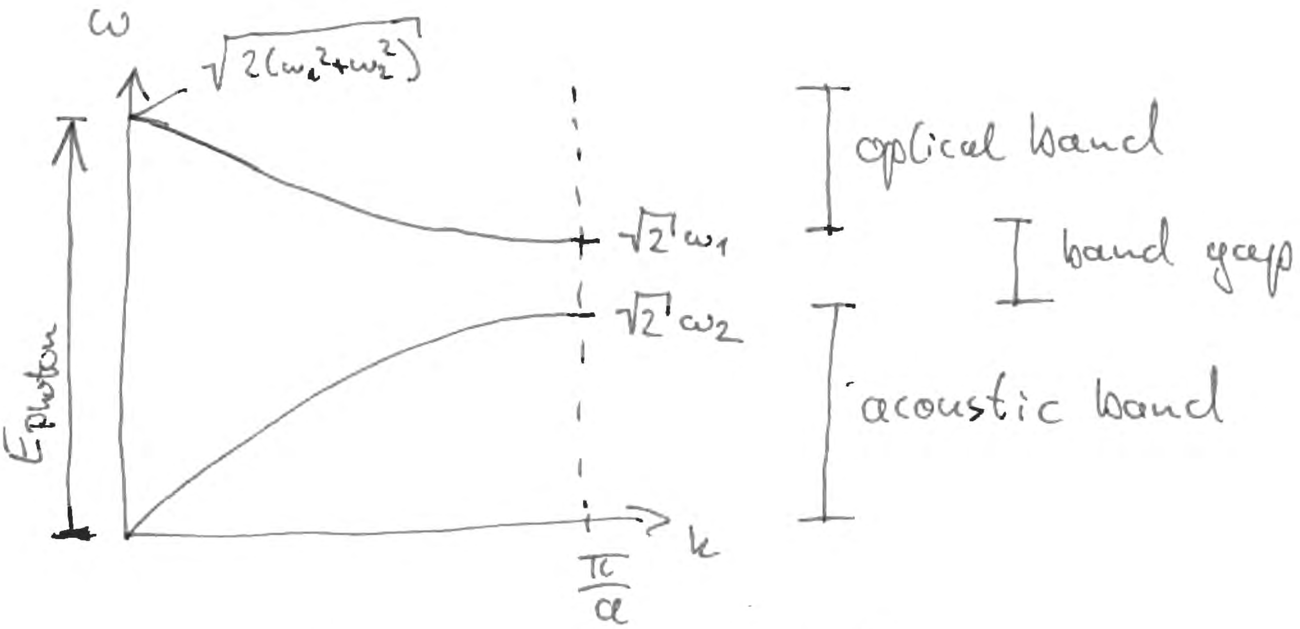
21. linear KCl - chain :

$\frac{a}{2} = 3{,}1\ \text{Å} = 3{,}1 \cdot 10^{-10}\,\text{m}$; $f = 8{,}8\,\frac{\text{N}}{\text{m}}$; $m_K = 39\,u$; $m_{Cl} = 35{,}5\,u$



$\omega_1^2 = \frac{f}{m_{Cl}}$; $\omega_2^2 = \frac{f}{m_K}$

$$(\omega^2)_\pm = (\omega_1^2 + \omega_2^2) \pm \sqrt{\omega_1^4 + 2\cos(ka)\,\omega_1^2\omega_2^2 + \omega_2^4}$$



a) bandwidth of acoustic band :

$$\Delta E_{ac} = \hbar \cdot \sqrt{2}\,\omega_2 = 1{,}73 \cdot 10^{-21}\,\text{J} = 10{,}8\,\text{meV}$$

bandwidth of optical band :

$$\Delta E_{opt} = \hbar\left(\sqrt{2(\omega_1^2+\omega_2^2)} - \sqrt{2}\,\omega_1\right)$$

$$= 6{,}94 \cdot 10^{-22}\,\text{J} = 4{,}33\,\text{meV}$$

$$E_{gap} = \hbar\left(\sqrt{2}\,\omega_1 - \sqrt{2}\,\omega_2\right)$$

$$= 0{,}834 \cdot 10^{-22}\,\text{J} = 0{,}520\,\text{meV}$$

b) optical excitation of an optical phonon at $k \simeq 0$:

$$E_{Phonon} = \hbar \cdot \sqrt{2(\omega_1^2+\omega_2^2)}$$

$$E_{Photon} = h \cdot \nu_{Photon} = \frac{h \cdot c}{\lambda_{photon}}$$

$$E_{Phonon} = E_{Photon}$$

$$\hbar \sqrt{2(\omega_1^2+\omega_2^2)} = \frac{h \cdot c}{\lambda_{Photon}}$$

$$\Rightarrow \lambda_{Photon} = \frac{2\pi \cdot c}{\sqrt{2(\omega_1^2+\omega_2^2)}} = 79{,}2\ \mu m$$

Far infrared radiation !

22. Phonon density of states

given: linear chain, periodic boundary conditions:

$$s(x+N\cdot a) \stackrel{!}{=} s(x)$$

Ansatz: $s(x) = A\cdot e^{i(kx-\omega t)}$

$$\to A\cdot e^{i[k(x+Na)-\omega t]} = A\cdot e^{i(kx-\omega t)}\cdot e^{ikNa} \stackrel{!}{=} A e^{i(kx-\omega t)}$$

$$\Rightarrow e^{ikNa} = 1 \iff k = \frac{2\pi}{aN}\cdot n,$$

$n = -N, \dots, 0, \dots, +N$.

$\to$ one possible k-state per intervall $\Delta k = \frac{2\pi}{aN}$ in k-space (states are uniformly distributed)

$$\Rightarrow g_k = \frac{1}{\Delta k} = \frac{1}{\frac{2\pi}{aN}} = \frac{aN}{2\pi}$$ density of states in k-space

2-dimensions:

$$\vec{s}_{n_x+N, n_y+N} = \begin{pmatrix} A_x e^{i[k_x(x+Na)-\omega t]} \\ A_y e^{i[k_y(y+Na)-\omega t]} \end{pmatrix} \stackrel{!}{=} \begin{pmatrix} A_x e^{i(k_x x-\omega t)} \\ A_y e^{i(k_y y-\omega t)} \end{pmatrix}$$

$$\Rightarrow \left.\begin{matrix} e^{ik_x Na} = 1 \\ e^{ik_y Na} = 1 \end{matrix}\right\} \Rightarrow k_{x/y} = \frac{2\pi}{Na}\cdot n_{x/y}$$

$n_{x/y} = -N, \dots, 0, \dots + N$

$\rightarrow$ one k-state per area $\left(\frac{2\pi}{Na}\right)^2$ in k-space

$$\Rightarrow \rho_k^{2D} = \left(\frac{Na}{2\pi}\right)^2$$

$\rightarrow$ density of state in frequency / energy space ?

strategy: calculate $\rho_k \rightarrow N(k) \rightarrow N(\omega) \rightarrow \rho_\omega(\omega)$

$$\underline{2D:} \quad N(k) = \int_0^k \rho_{k'}^{2D}\, d^2k' = \left(\frac{Na}{2\pi}\right)^2 \int_0^k d^2k' = \left(\frac{Na}{2\pi}\right)^2 \cdot k^2 \pi$$

assume linear dispersion: $\omega = c \cdot k$

$$\Rightarrow N(\omega) = \left(\frac{Na}{2\pi}\right)^2 \cdot \left(\frac{\omega}{c}\right)^2 \cdot \pi$$

$$\Rightarrow \rho_\omega^{2D}(\omega) = \frac{\partial N(\omega)}{\partial \omega} = \frac{(Na)^2}{2\pi c^2} \cdot \omega$$

$$\underline{3D:} \quad \rho_k^{3D} = \left(\frac{Na}{2\pi}\right)^3$$ (proof is analogous to 2D case)

$$\rightarrow N(k) = \int_0^k \rho_{k'}^{3D}\, d^3k' = \left(\frac{Na}{2\pi}\right)^3 \int_0^k d^3k' = \left(\frac{Na}{2\pi}\right)^3 \frac{4\pi}{3} k^3$$

$$N(\omega) = \frac{4\pi}{3} \left(\frac{Na}{2\pi}\right)^3 \cdot \left(\frac{\omega}{c}\right)^3$$

$$\Rightarrow \rho_\omega^{3D}(\omega) = \frac{dN(\omega)}{d\omega} = \frac{(Na)^3}{2\pi^2 c^3} \cdot \omega^2$$

$\underline{1D}$: see Worksheet 6 next week