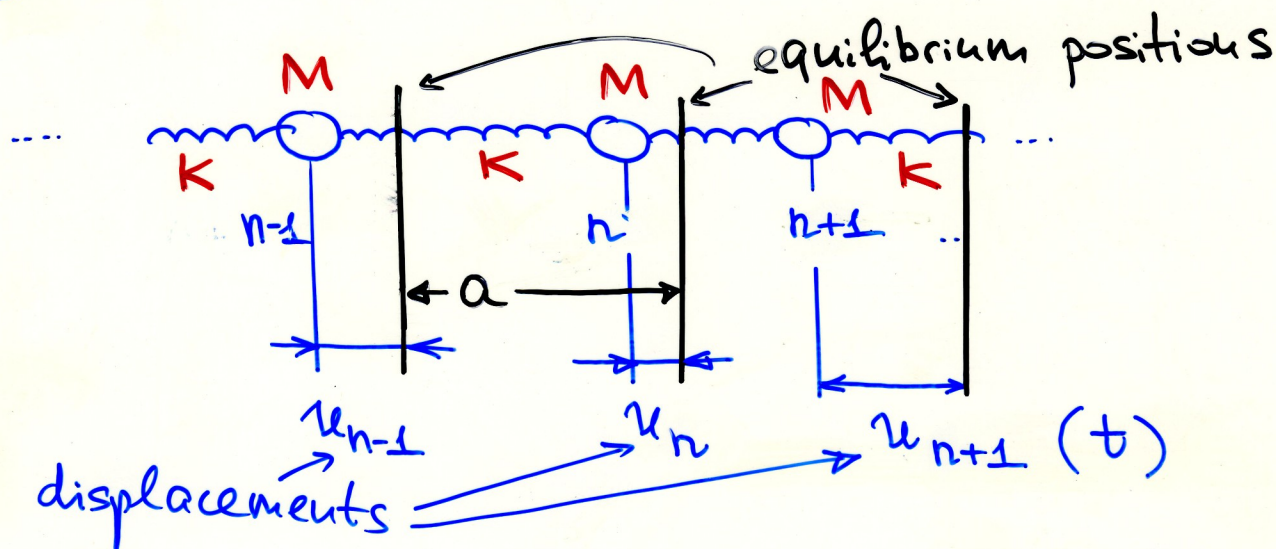


Normal Modes of Harmonic Lattices

① 1D monatomic chain



$$M\ddot{u}_n = -K(u_n - u_{n-1}) + K(u_{n+1} - u_n)$$

Normal Modes $u_n(t) \sim e^{i\omega t} \psi_n$

dispersion relations
 $u \sim e^{ikx - i\omega t} : \omega = \omega(k)$

$$x \leftrightarrow na$$

$$e^{ikna - i\omega t}$$

$$u_n(t) \sim e$$

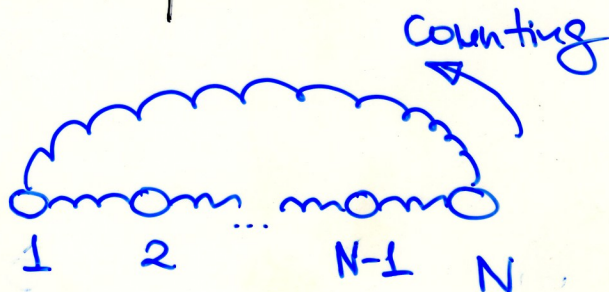
look for solutions in the form
of normal modes

Boundary conditions? (BC)

when number of atoms $N \gg 1$
few modes are affected by
specific BC $\Rightarrow$ choose simplest

Born - von Karman BC: periodic

$$\begin{aligned} u_N &= u_0 \\ u_{N+1} &= u_1 \\ u_{N+2} &= u_2 \end{aligned}$$



Periodicity.

$$e^{ik \cdot na} = e^{ik \cdot (n+N)a}$$

$$e^{ikNa} = 1$$

$k \rightarrow$ quantized
into
discrete

$$k_m = \frac{2\pi}{a} \cdot \frac{m}{N}$$

$$m = 0, \pm 1, \pm 2, \dots$$

$$m \rightarrow m+N$$

$$k_m \rightarrow k_m + \frac{2\pi}{a}$$

$$e^{i(k_m + \frac{2\pi}{a}) \cdot na} = e^{ik_m na}$$

$\forall n$

m and $m+N$ are equivalent

$\Rightarrow \exists$ N non-equivalent
wave vectors k_m

A usual convenient choice $m=0, \pm 1, \dots, \pm \frac{N}{2}$.

$$-\frac{\pi}{a} \leq k_m = \frac{2\pi}{a} \cdot \frac{m}{N} \leq \frac{\pi}{a}$$

The first Brillouin Zone

$$\frac{\pi}{a} \leq k \leq \frac{\pi}{a} \quad N \text{ non-equivalent wave vectors}$$

N - number of atoms (cells)
in a crystal

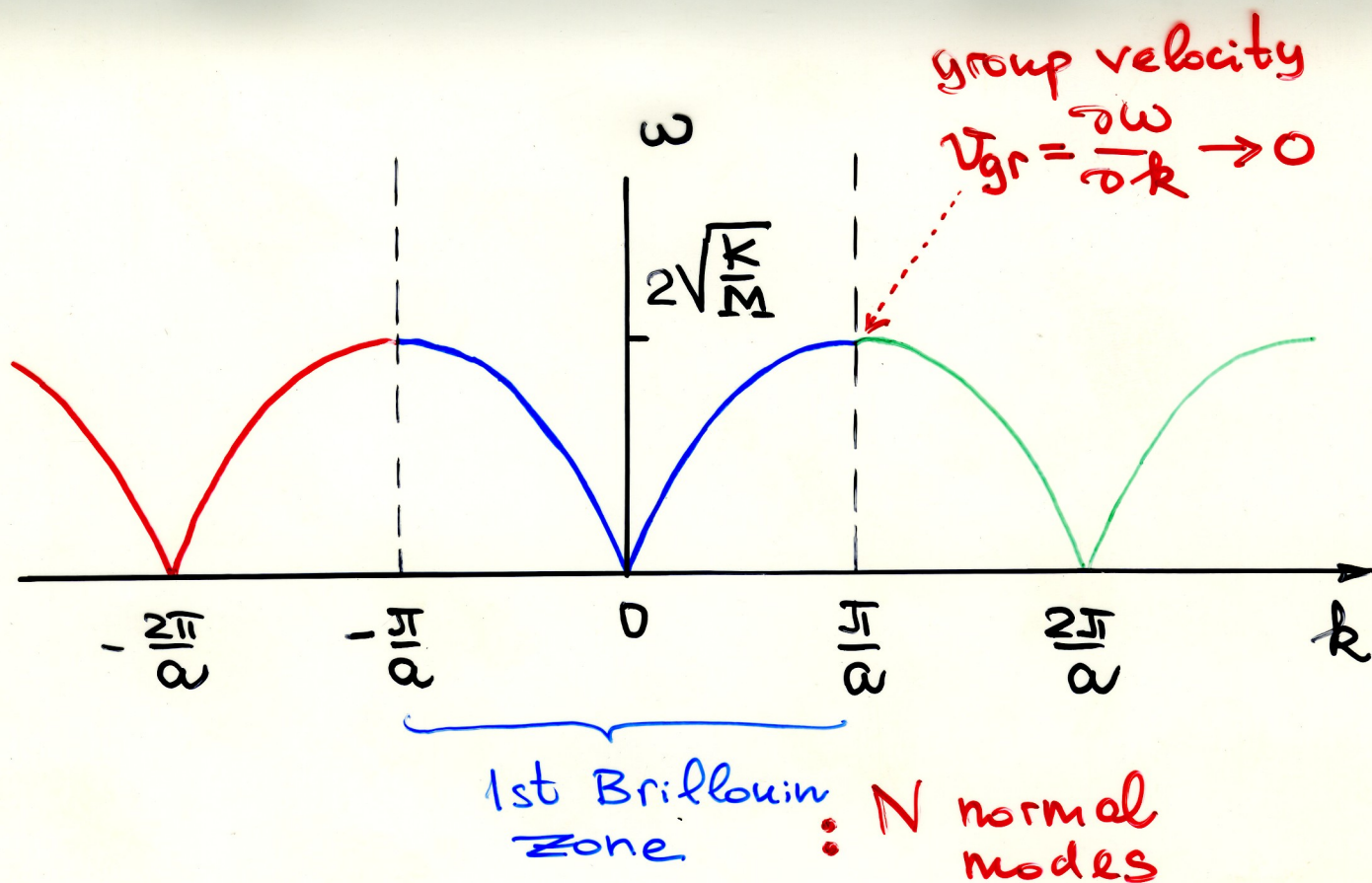
$$-M\omega^2 = -K(1 - e^{ika}) + K(e^{ika} - 1)$$

$$\omega^2 = \frac{2K}{M} \left(1 - \frac{1}{2} [e^{ika} + e^{-ika}] \right)$$

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

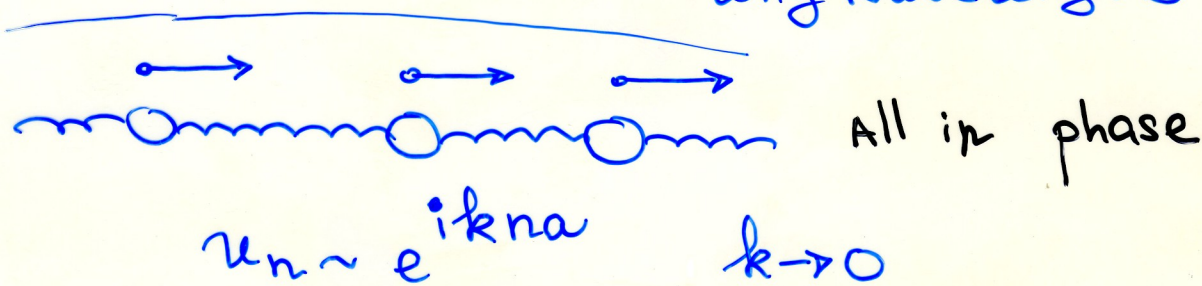
$$\omega = \omega(k) = 2\sqrt{\frac{K}{M}} \left| \sin \frac{ka}{2} \right|$$

dispersion relation

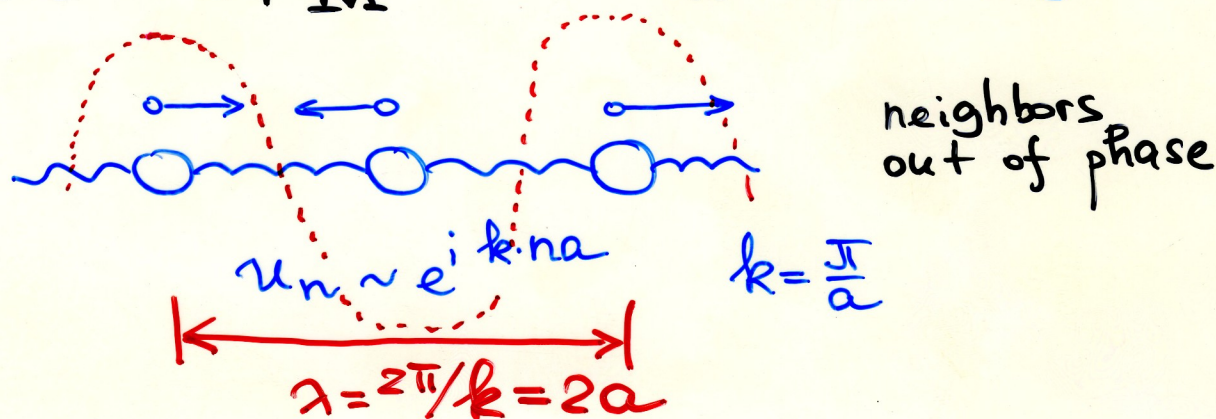


$$\omega(k) = \sqrt{\frac{K}{M}} ka \sim k \quad ka \ll 1 \quad \lambda \gg a$$

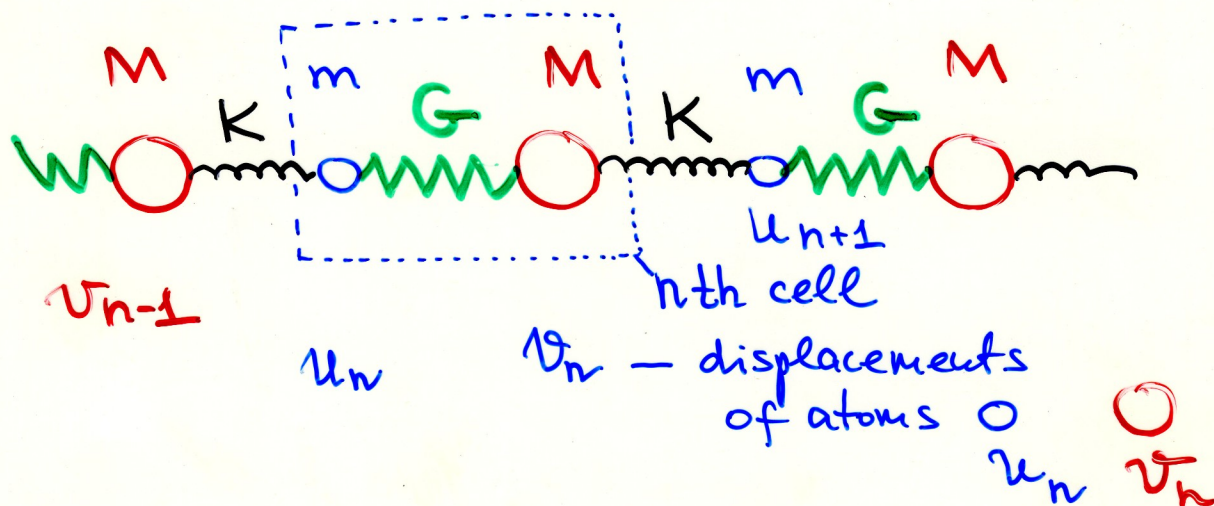
long wavelengths



$$\omega(k) = 2\sqrt{\frac{K}{M}} \quad k = \frac{\pi}{a} \quad \text{Zone Boundary}$$



② 1D chain with a basis



$$\begin{cases} m\ddot{u}_n = -K(u_n - v_{n-1}) + G(v_n - u_n) \\ M\ddot{v}_n = -G(v_n - u_n) + K(u_{n+1} - v_n) \end{cases}$$

Normal modes $u_n = \epsilon_1 \exp(ikna - i\omega t)$ ✓
 $v_n = \epsilon_2 \exp(ikna - i\omega t)$ ✓

$$\begin{cases} -\epsilon_1 m \omega^2 = -K(\epsilon_1 - \epsilon_2 e^{-ika}) + G(\epsilon_2 - \epsilon_1) \\ -\epsilon_2 M \omega^2 = -G(\epsilon_2 - \epsilon_1) + K(\epsilon_1 e^{ika} - \epsilon_2) \end{cases}$$

$$\begin{cases} \epsilon_1 [m\omega^2 - (K+G)] + \epsilon_2 [K e^{-ika} + G] = 0 \\ \epsilon_1 [K e^{ika} + G] + \epsilon_2 [M\omega^2 - (K+G)] = 0 \end{cases}$$

$$\exists \text{ non-trivial solution} \iff \det = 0$$

$$[m\omega^2 - (K+G)][M\omega^2 - (K+G)] = \underbrace{[K e^{-ika} + G] \cdot [K e^{ika} + G]}$$

$$\begin{aligned} \text{Rhs} &= K^2 + G^2 + KG(e^{ika} + e^{-ika}) \\ &= K^2 + G^2 + 2KG \cos ka \end{aligned}$$

$$\begin{aligned} mM\omega^4 - (m+M)(K+G)\omega^2 + (K+G)^2 &= \\ &= K^2 + G^2 + 2KG \cos ka \end{aligned}$$

$$\boxed{\omega^4 - \frac{m+M}{mM} (K+G)\omega^2 = \frac{2KG}{mM} (\cos ka - 1)}$$

determines two solutions

$$\text{for } \omega^2 = \omega^2(k) [\geq 0 \text{ !}]$$

$$\begin{aligned} \omega^2(k) &= \omega^2(-k) \\ \omega(k) &= \omega(-k) \end{aligned}$$

$$\frac{m+M}{mM} (K+G) \equiv 2\Omega^2 \quad \frac{K}{m} \equiv \omega_1^2 \quad \frac{G}{M} \equiv \omega_2^2$$

$$\omega^4 - 2\Omega^2 \omega^2 = -2\omega_1^2 \omega_2^2 (1 - \cos ka)$$

$$\omega_{\pm}^2 = \Omega^2 \pm \sqrt{\Omega^4 - 2\omega_1^2 \omega_2^2 (1 - \cos ka)}$$

$$\omega_{\pm}^2 \geq 0 \quad \text{Yes}$$

Let's analyze in detail

a case $m=M$ $K \neq G$

$$2\Omega^2 = \frac{2M}{M^2} (K+G)$$

$$\boxed{\Omega^2 = \frac{K+G}{M}}$$

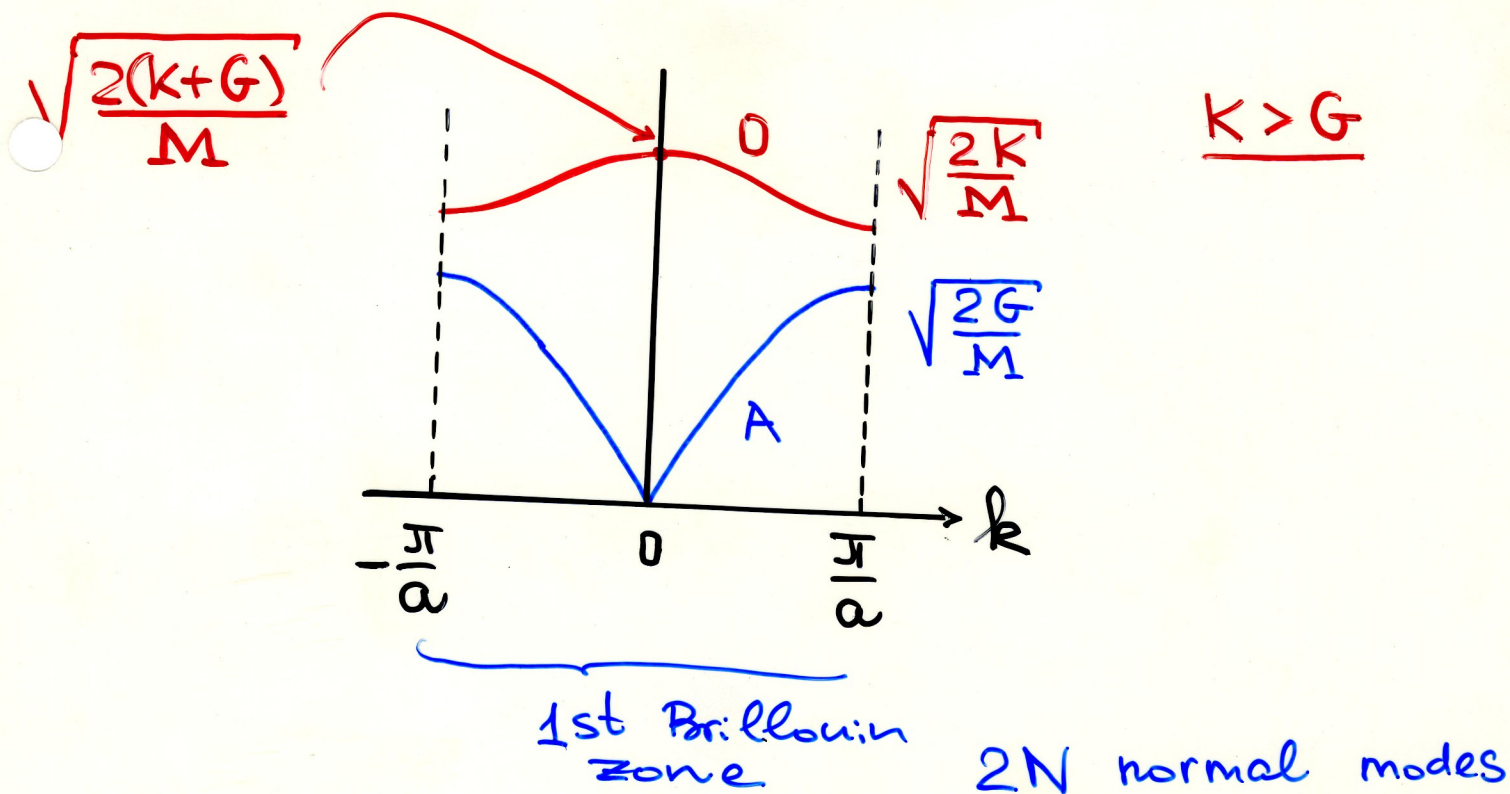
$$\omega_{\pm}^2 = \frac{K+G}{M} \pm \sqrt{\left(\frac{K+G}{M}\right)^2 - 2 \frac{KG}{M^2} (1 - \cos ka)}$$

$$\omega_{\pm}^2 = \frac{K+G}{M} \pm \sqrt{\frac{K^2}{M^2} + \frac{G^2}{M^2} + 2 \frac{KG}{M^2} \cos ka}$$

two branches of excitations:

ω_+ optical branch $\equiv \omega_o$

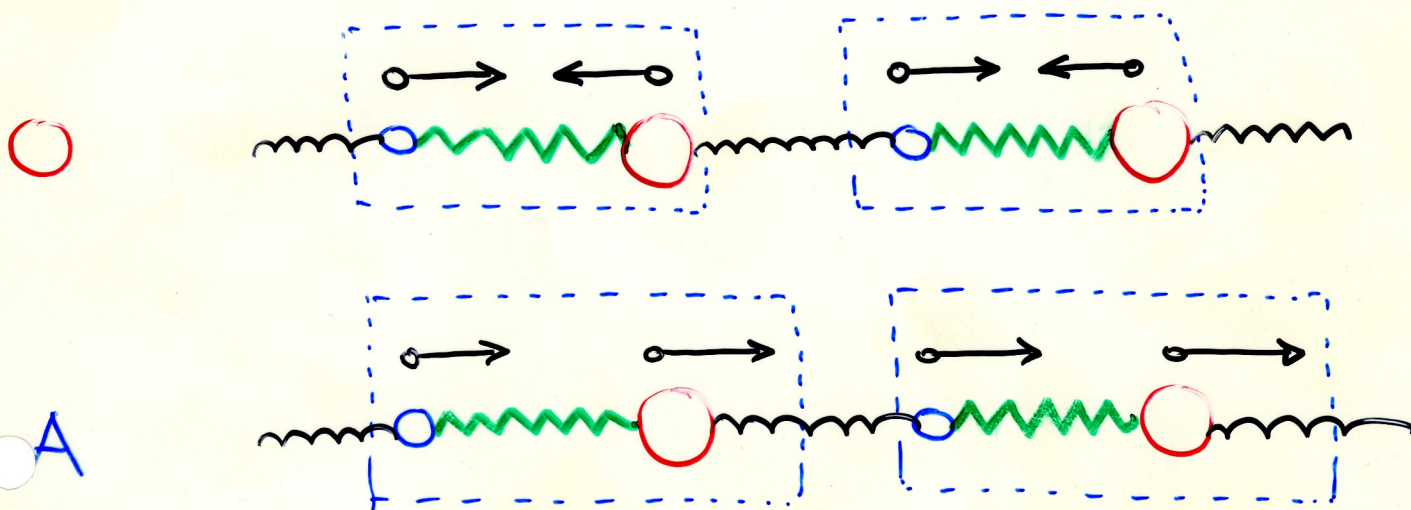
ω_- acoustic branch $\equiv \omega_a$



Long wavelengths $ka \ll 1$, $\lambda = \frac{2\pi}{k} \gg a$

$$\omega_O = \sqrt{\frac{2(K+G)}{M}} - O(k^2)$$

$$\omega_A = \sqrt{\frac{KG}{2M(K+G)}} \cdot ka$$



Short wavelengths $ka = \pi$, $\lambda = \frac{2\pi}{k} = 2a$

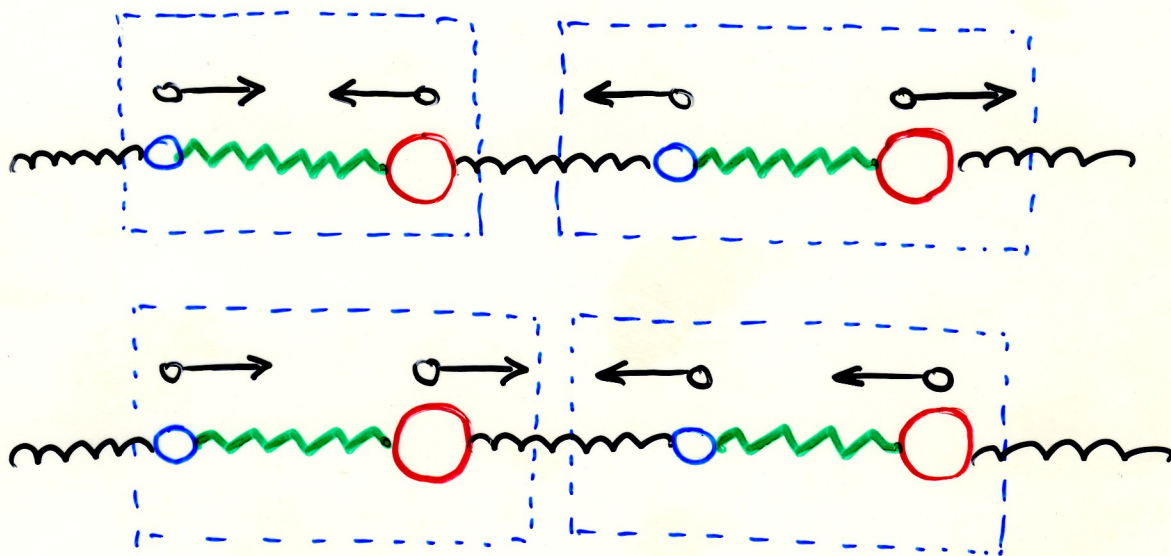
$$\omega_o (k = \frac{\pi}{a}) = \sqrt{\frac{2 \max(K, G)}{M}}$$

$$\omega_A (k = \frac{\pi}{a}) = \sqrt{\frac{2 \min(K, G)}{M}}$$

$$\frac{E_2}{E_1} = \frac{0}{A} \frac{K + G e^{ika}}{|K + G e^{ika}|} = \mp 1$$

ratio of amplitudes

$ka = \pi$
 $ka = 0$

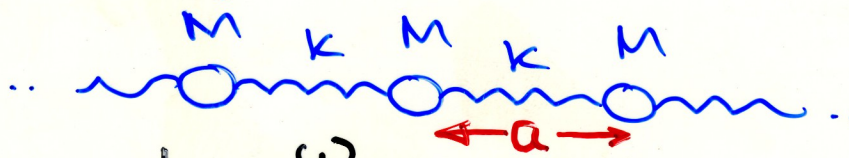


ω_A in phase inside cell ($E_1 = E_2$);
cells are out of phase $e^{ik \cdot a} = -1$

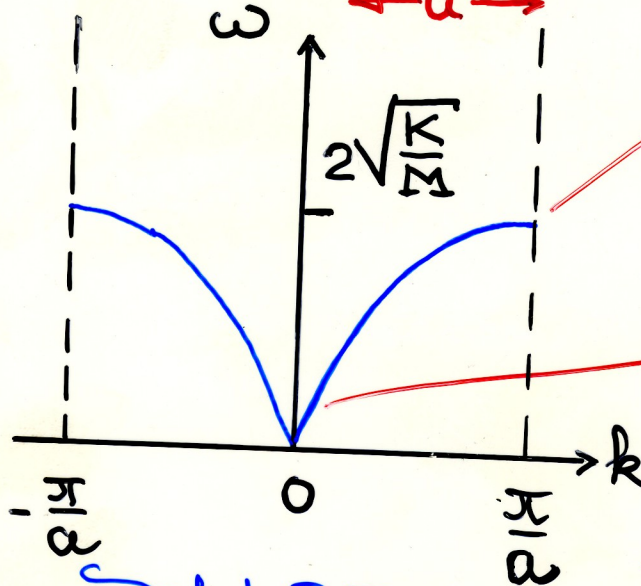
ω_o out of phase inside cell ($E_1 = -E_2$)

Normal Modes of Harmonic Crystals II

1D longitudinal



I



$$v_{gr} = \left. \frac{\partial \omega}{\partial k} \right|_{k=\frac{\pi}{2a}} = 0$$

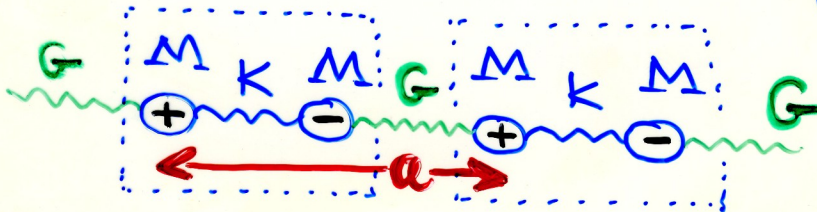
$$\omega(k) \approx \sqrt{\frac{K}{M}} ka \sim k$$

of atoms in a crystal

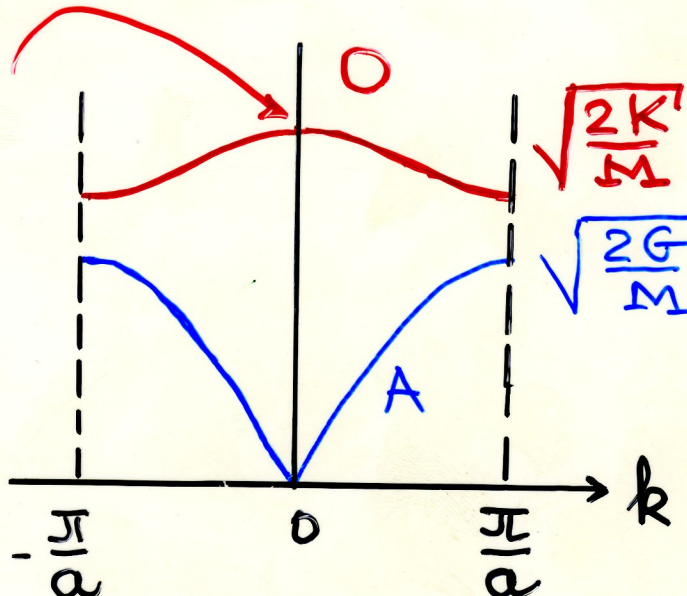
N acoustic modes

$k \in [-\frac{\pi}{a}, \frac{\pi}{a}]$, $k_m = \frac{2\pi}{a} \cdot \frac{m}{N}$ non-equivalent N values

II



$$\sqrt{\frac{2(K+G)}{M}}$$



$$K > G$$

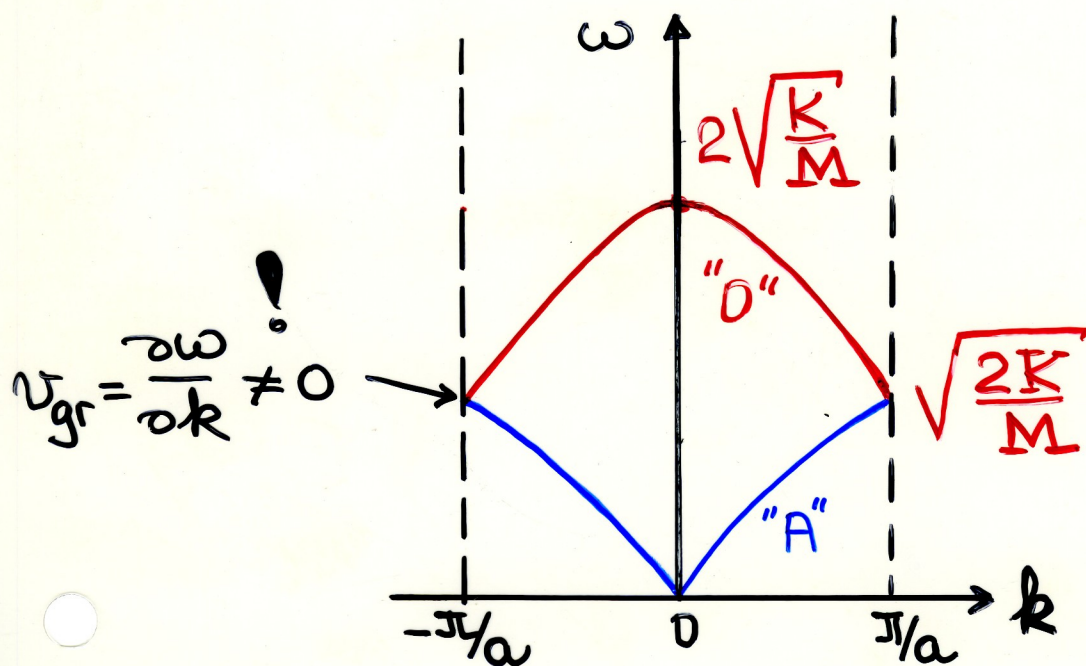
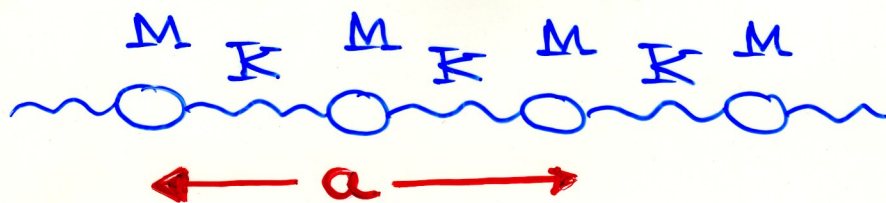
N acoustic modes

N optical modes

$$\vec{d} = e \vec{r}_{+-} e^{-i\omega t}$$

dipoles

Consider the limiting case $K = G$



$$\omega_{\pm}^2 = \frac{2K}{M} \pm \sqrt{2 \frac{K^2}{M^2} (1 + \cos ka)}$$

$$\omega_{\pm}^2 = \frac{2K}{M} \left\{ 1 \pm \sqrt{\frac{1 + \cos ka}{2}} \right\}$$

$$\omega_{\pm}^2 = \frac{2K}{M} \left\{ 1 \pm \cos \frac{ka}{2} \right\} \quad -\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$$

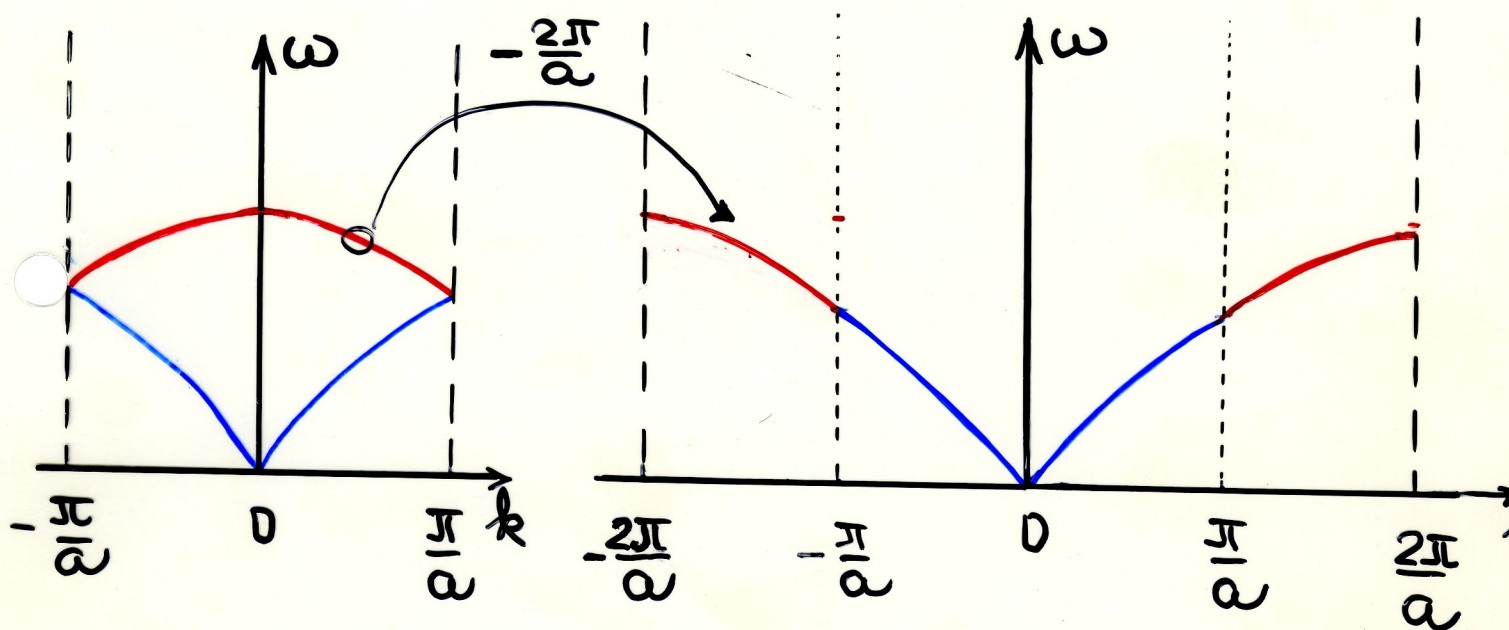
$$\boxed{\begin{aligned} \omega_{+} &= 2\sqrt{\frac{K}{M}} \cos \frac{ka}{4} && \text{"O"} \\ \omega_{-} &= 2\sqrt{\frac{K}{M}} \sin \frac{ka}{4} && \text{"A"} \end{aligned}}$$

We treated monatomic chain of period $\frac{a}{2}$ as diatomic of period a

$$\frac{a}{2} \rightarrow 1^{\text{st}} \text{ BZ } -\frac{2\pi}{a} \leq k \leq \frac{2\pi}{a}$$

$$a \rightarrow 1^{\text{st}} \text{ BZ } -\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$$

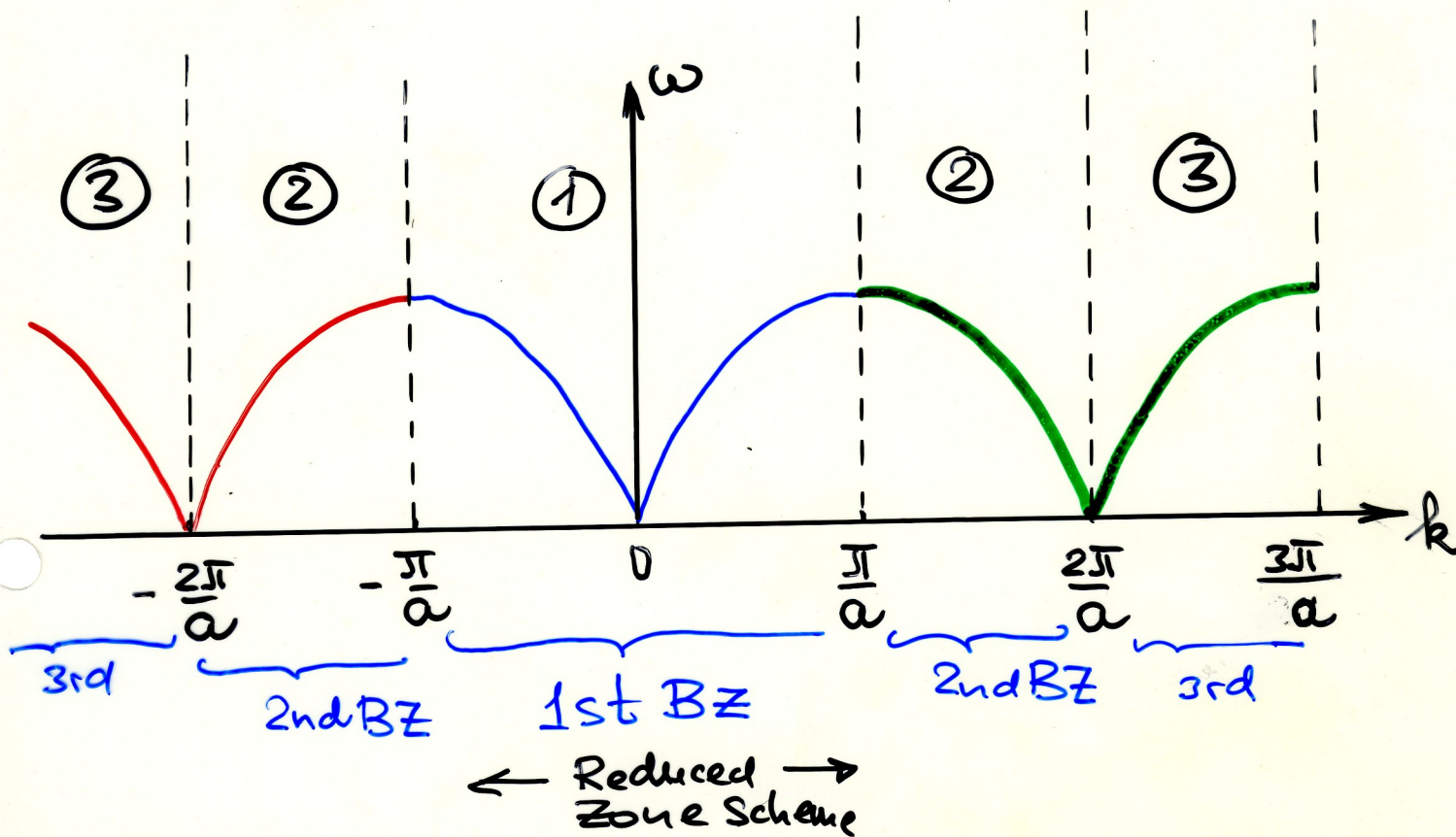
↓
we halved the size of BZ!



k and $k' = k + \frac{2\pi}{a} \cdot m$ equivalent $m = \pm 1, \pm 2, \dots$

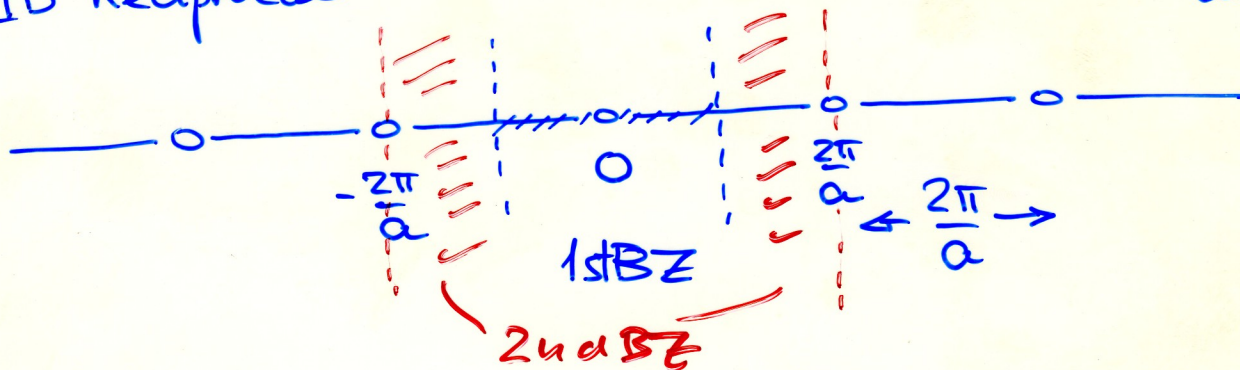
displacements are the same $u_n \sim e^{ik'na} = e^{i(k + \frac{2\pi}{a} \cdot m)na} = e^{ikna}$

$\Rightarrow$ we can translate portions of $\omega_{\pm}(k)$ to higher BZones

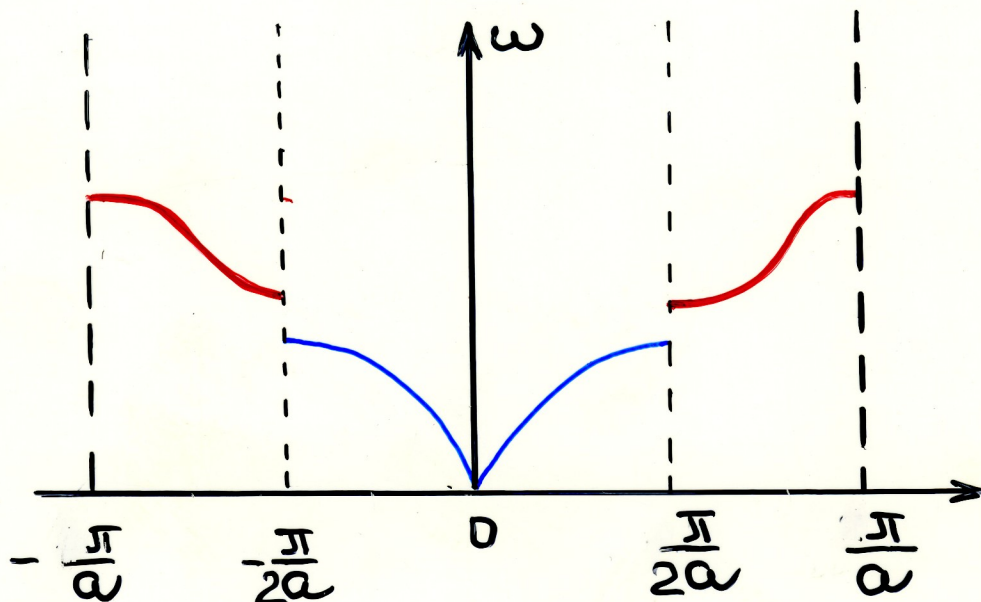


... ← Repeated Zone Scheme → ...

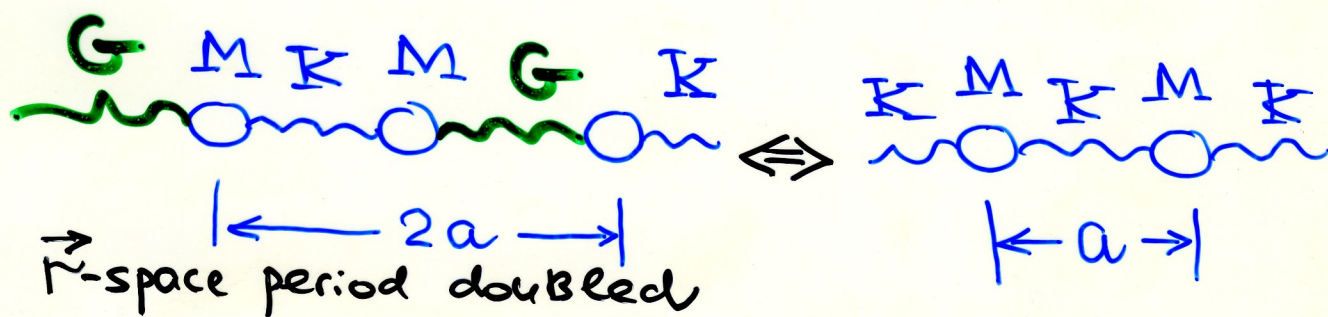
1D Reciprocal lattice // k -space // $\vec{b} = \frac{2\pi}{a} \hat{x}$



Another interpretation of results
for diatomic chains:



Diatomic chain as a limiting case $G \rightarrow K$
of monatomic chain:



1st BZ: $\pm \frac{\pi}{2a}$

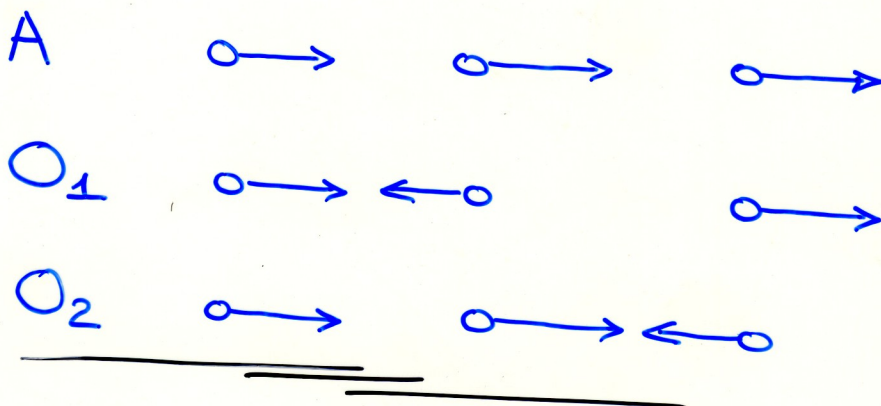
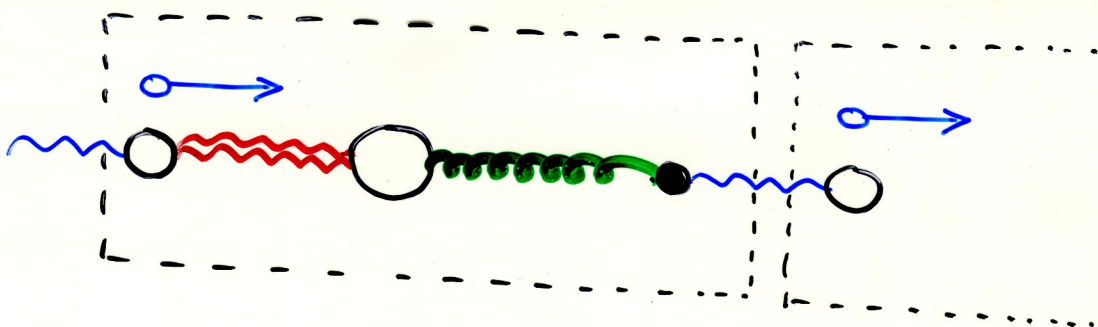
1st BZ: $\pm \frac{\pi}{a}$

k -space period halved

- new zone boundaries
- at which gaps open !

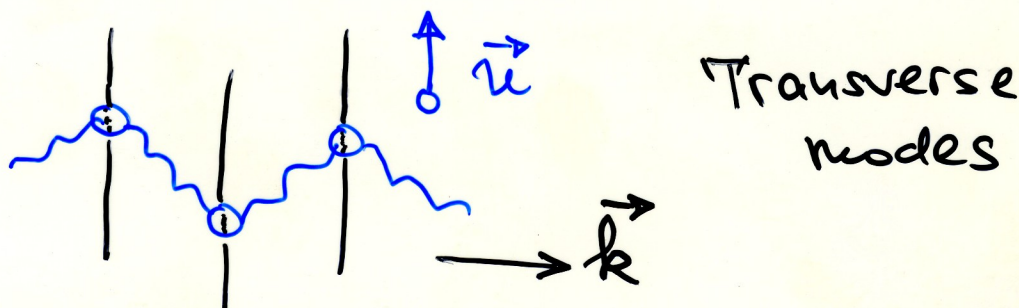
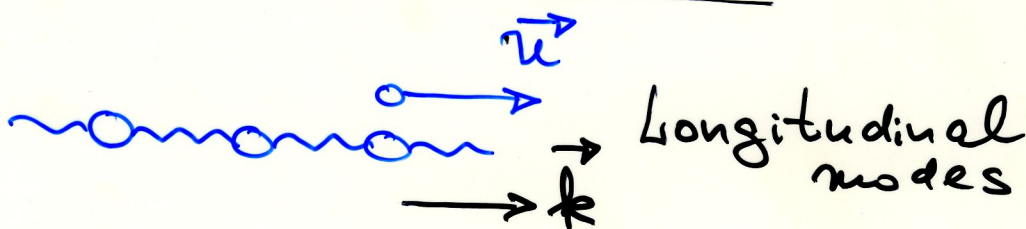
$$ka \ll 1$$

$$\lambda \gg a$$



p atoms per unit cell

1D	1 Acoustic mode	$p-1$ Optical modes
2D	2 — —	$2(p-1)$ — —
3D	3 — —	$3(p-1)$ — —



Normal modes of monatomic 3D crystal

$$\boxed{A_\mu B_\mu = \sum_{\mu=1}^3 A_\mu B_\mu} \quad U^{\text{harm}} = \frac{1}{2} \sum_{\vec{R}, \vec{R}'} D_{\mu\nu}(\vec{R}-\vec{R}') u_\mu(\vec{R}) u_\nu(\vec{R}') \quad \mu, \nu = x, y, z$$

$$M \ddot{u}_\mu(\vec{R}) = - \frac{\partial U^{\text{harm}}}{\partial u_\mu(\vec{R})} = - \sum_{\vec{R}'} D_{\mu\nu}(\vec{R}-\vec{R}') u_\nu(\vec{R}')$$

matrix $D_{\mu\nu}(\vec{R}) = \hat{D}(\vec{R})$
 ↓ reflects symmetries of the crystal

We consider single BL: inversion symmetry

$$\textcircled{1} \quad \begin{aligned} D_{\mu\nu}(\vec{R}) &= D_{\mu\nu}(-\vec{R}) \\ \hat{D}(\vec{R}) &= \hat{D}(-\vec{R}) \end{aligned}$$

$$\textcircled{2} \quad \begin{aligned} D_{\mu\nu}(\vec{R}) &= D_{\nu\mu}(-\vec{R}) & \hat{D}^T(\vec{R}) &= \hat{D}(-\vec{R}) \\ & & \text{T: transposed matrix} & \end{aligned}$$

can be chosen symmetric: consider terms coming from $\sum_{\vec{R}, \vec{R}'}$

$$\begin{aligned} & \frac{1}{2} \left\{ D_{\mu\nu}(\vec{R}-\vec{R}') u_\mu(\vec{R}) u_\nu(\vec{R}') + \right. \\ & \quad \left. + D_{\nu\mu}(\vec{R}'-\vec{R}) u_\nu(\vec{R}') u_\mu(\vec{R}) \right\} = \\ & = \frac{1}{2} \left[D_{\mu\nu}(\vec{R}-\vec{R}') + D_{\nu\mu}(\vec{R}'-\vec{R}) \right] u_\mu(\vec{R}) u_\nu(\vec{R}') \end{aligned}$$

a new "symmetric"

$$\begin{aligned} D_{\mu\nu}(\vec{R}-\vec{R}') &= \\ &= D_{\nu\mu}(\vec{R}'-\vec{R}) \end{aligned}$$

$$\textcircled{3} \quad \sum_{\vec{R}} D_{\mu\nu}(\vec{R}) = 0$$

$$\vec{u}(\vec{r}) = \vec{d} = \text{const}$$

$$U^{\text{harm}} = \frac{1}{2} \sum_{\vec{R}, \vec{R}'} D_{\mu\nu}(\vec{R} - \vec{R}') d_\mu d_\nu$$

$$\{\vec{R}, \vec{R}'\} \rightarrow \left\{ \frac{1}{2}(\vec{R} + \vec{R}'), \vec{R} - \vec{R}' \right\}$$

$\vec{R}_1 \qquad \qquad \vec{R}_2$

$$U^{\text{harm}} = \frac{1}{2} \sum_{\vec{R}_1} \left(\sum_{\vec{R}_2} D_{\mu\nu}(\vec{R}_2) \right) d_\mu d_\nu$$

$$= \frac{1}{2} N \left(\sum_{\vec{R}_2} D_{\mu\nu}(\vec{R}_2) \right) d_\mu d_\nu = 0$$

$\forall \vec{d}$

$$\Rightarrow \boxed{\sum_{\vec{R}} D_{\mu\nu}(\vec{R}) = 0}$$

$$\textcircled{3} \quad \boxed{\sum_{\vec{R}} \hat{D}(\vec{R}) = 0}$$

$$\textcircled{2} \quad \boxed{\hat{D}(\vec{R}) = \hat{D}^T(-\vec{R})}$$

$$\textcircled{1} \quad \boxed{\hat{D}(\vec{R}) = \hat{D}(-\vec{R})}$$

$$(\hat{A}^T)_{\mu\nu} = A_{\nu\mu}$$

$$\hat{D}^T(\vec{R}) = \hat{D}(-\vec{R})$$

$$(\hat{D}^T)^T = \hat{D}$$

Equation of motion

$$M \ddot{\vec{u}}(\vec{R}; t) = - \sum_{\vec{R}'} \hat{D}(\vec{R} - \vec{R}') \vec{u}(\vec{R}'; t)$$

We seek solutions in the form of simple plane waves

$$\vec{u}(\vec{R}; t) = \vec{E} \cdot \exp\{i \vec{k} \cdot \vec{R} - i \omega t\}$$

polarization vector
// to be determined together with $\omega = \omega(\vec{k})$

Born-von Karman periodic boundary cond.

$$\vec{u}(\vec{R} + N_i \vec{a}_i) = \vec{u}(\vec{R}) \quad i=1,2,3$$

$$N_1 N_2 N_3 = N \quad \text{total \# of cells}$$

Allowed wave vectors $\vec{k}$ are discretized:

$$\vec{k} = \frac{n_1}{N_1} \vec{b}_1 + \frac{n_2}{N_2} \vec{b}_2 + \frac{n_3}{N_3} \vec{b}_3$$

RL primitive vectors

$$\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$$

n_i integer

$\vec{k}$ and $\vec{k} + \vec{K}$ equivalent
 $\equiv_{RL}$

$$M\ddot{\vec{u}} = - \sum_{\vec{R}'} \hat{D}(\vec{R}-\vec{R}') \vec{u}(\vec{R}')$$

$$\vec{u} = \vec{E} \exp \{ i(\vec{k} \cdot \vec{R} - \omega t) \}$$

$$M\omega^2 \vec{E} = \sum_{\vec{R}'} \hat{D}(\vec{R}-\vec{R}') e^{-i\vec{k} \cdot (\vec{R}-\vec{R}')} \vec{E}$$

$$\boxed{M\omega^2 \vec{E} = \hat{D}(\vec{k}) \vec{E}} \quad \begin{matrix} \hat{D}(\vec{k}) \\ \text{three-dimensional} \\ \text{eigenvalue} \\ \text{equation} \end{matrix}$$

determines $\vec{E}, \omega$ || $\vec{E}_s = \vec{E}_s(\vec{k})$ eigenvectors of $\hat{D}(\vec{k}) \vec{E}_s = \lambda_s \vec{E}_s(\vec{k})$

$\lambda_s = \lambda_s(\vec{k})$ eigenvalues

① $\hat{D}(\vec{k})$ symmetric $D_{\mu\nu}(\vec{k}) = D_{\nu\mu}(\vec{k})$

② $\hat{D}(\vec{k})$ real

$$\begin{aligned} \hat{D}(\vec{k})^* &= \left(\sum_{\vec{R}} e^{-i\vec{k} \cdot \vec{R}} \hat{D}(\vec{R}) \right)^* = \\ &= \sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} \hat{D}(\vec{R}) = \sum_{\vec{R}'} e^{-i\vec{k} \cdot \vec{R}'} \hat{D}(-\vec{R}') = \hat{D}(\vec{k}) \end{aligned}$$

inversion
symmetry

$$\hat{D}(-\vec{R}') = \hat{D}(\vec{R}')$$

$$D_{\mu\nu}^*(\vec{k}) = D_{\mu\nu}(\vec{k}) \quad \text{real}$$

$$D_{\mu\nu}(\vec{k}) = D_{\nu\mu}(\vec{k}) \quad \text{symmetric}$$

$$\left[D_{\mu\nu}^*(\vec{k}) = D_{\nu\mu}(\vec{k}) \quad \text{Hermitian} \right]$$

$$\hat{D}^* = \hat{D}^T$$

$$\hat{D}^{T*} = \hat{D}$$

For $\forall$ fixed $\vec{k}$ ↓ real eigenvalues

$$\hat{D}(\vec{k}) \vec{E}_s(\vec{k}) = \lambda_s(\vec{k}) \vec{E}_s(\vec{k})$$

$s = 1, 2, 3$

three orthogonal
eigenvectors

$$\vec{E}_s(\vec{k}) \cdot \vec{E}_{s'}(\vec{k}) = \delta_{ss'}$$

Eigenmodes $\equiv$ Normal modes

$$M\omega^2 \vec{E} = \hat{D} \vec{E} = \lambda_s \vec{E}$$

$$\omega_s = \sqrt{\frac{\lambda_s}{M}} = \omega_s(\vec{k}) \quad \text{Real!}$$

$$\lambda_s \geq 0$$

Physically: from the stability
of a crystal



$$\text{If } \lambda_s < 0 \Rightarrow \omega_s \sim \sqrt{\lambda_s} : \text{Im}\omega_s \neq 0$$

$$u \sim \exp(-i \cdot i \text{Im}\omega_s \cdot t)$$

Do we have acoustic modes?

$$|\vec{k}|a \ll 1: \omega_s(\vec{k}) \simeq c_s(\vec{k}) \cdot |\vec{k}|$$

speed of sound $\rightarrow$
propagating along $\vec{k}$

Behavior of $\hat{D}(\vec{k})$ at $|\vec{k}| \rightarrow 0$:

$$\hat{D}(\vec{k}) = \sum_{\vec{R}} e^{-i\vec{k} \cdot \vec{R}} \hat{D}(\vec{R}) =$$

$$= \sum_{\vec{R}} \left\{ \underbrace{\hat{D}(\vec{R})}_{\emptyset} - i\vec{k} \cdot \vec{R} \underbrace{\hat{D}(\vec{R})}_{\text{odd}} - \frac{1}{2}(\vec{k} \cdot \vec{R})^2 \underbrace{\hat{D}(\vec{R})}_{\text{even}} + \dots \right\}$$

$\vec{R} \rightarrow -\vec{R} \Rightarrow \phi$

$$\hat{D}(\vec{k}) \simeq -\frac{k^2}{2} \cdot \sum_{\vec{R}} \left(\frac{\vec{k} \cdot \vec{R}}{k} \right)^2 \hat{D}(\vec{R})$$

$$\hat{D}(\vec{k}) = -\frac{1}{2}k^2 \cdot \hat{\mathcal{D}}\left(\frac{\vec{k}}{k}\right) : \text{depends on direction of } \vec{k} \text{ only}$$

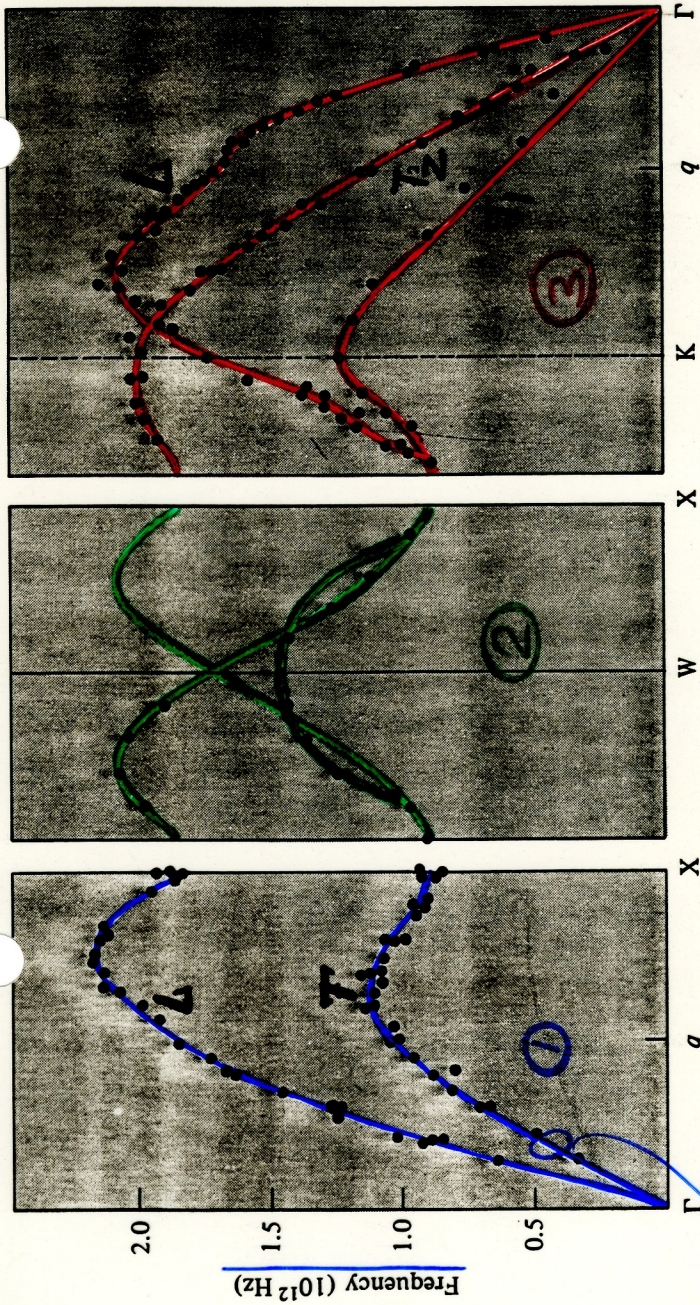
$$M\omega_s^2 \vec{E}_s(\vec{k}) = -\frac{1}{2}k^2 \hat{\mathcal{D}}\left(\frac{\vec{k}}{k}\right) \vec{E}_s(\vec{k})$$

$$c_s^2(\vec{k}) \vec{E}_s = -\frac{1}{2M} \hat{\mathcal{D}} \vec{E}_s$$

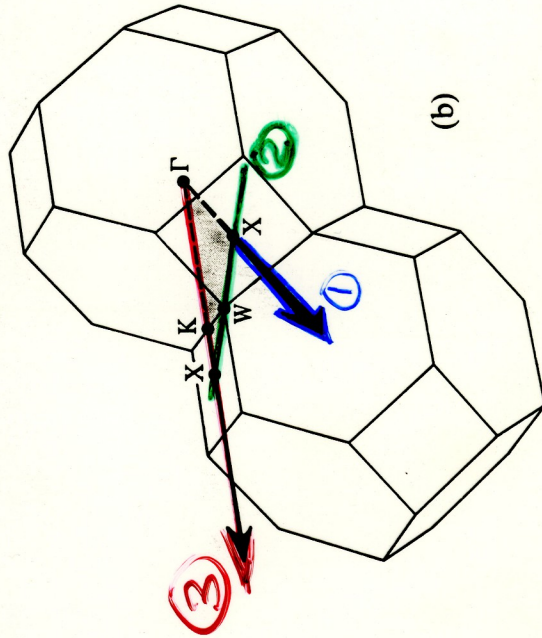
Longitudinal
modes
 $\vec{E} \parallel \vec{k}$

Transverse
modes
 $\vec{E} \perp \vec{k}$

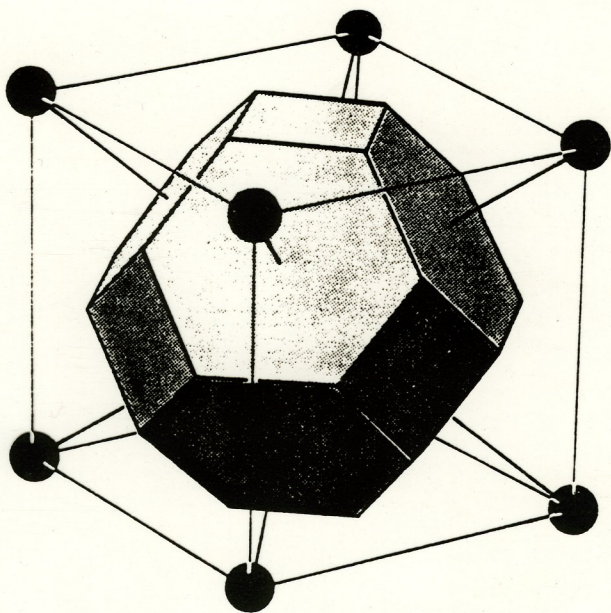
In crystals
only along
high-symmetry
directions.
(ANISOTROPY
 $\Rightarrow$ no pure T or L
modes)



Phonon dispersions $\omega_s(\vec{k})$



Pb [FCC] $\longrightarrow$ RL BCC

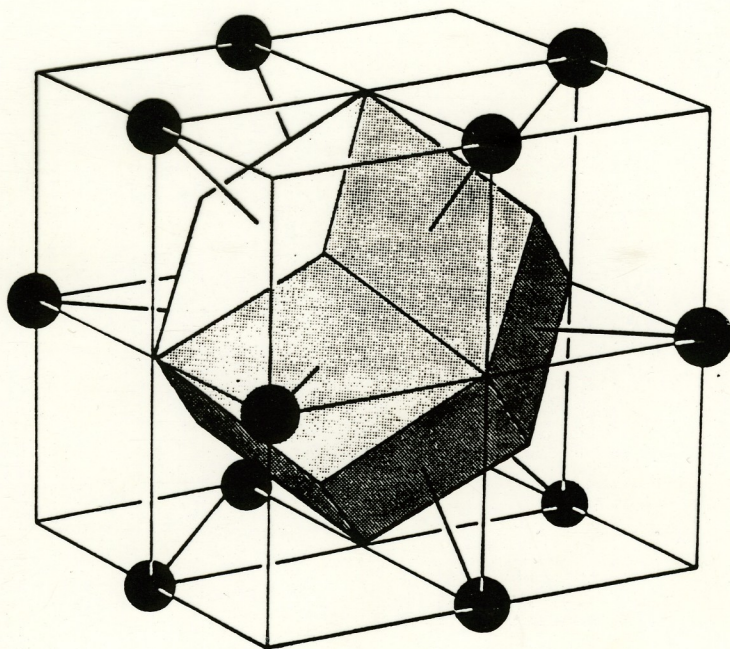


truncated octahedron
(hexagons + squares)

Wigner-Seitz cell
for BCC ($\vec{r}$ -space)
lattice const. a

First Brillouin
Zone for FCC
($\vec{k}$ -space)

$$\frac{4\pi}{a}$$



rhombic dodecahedron

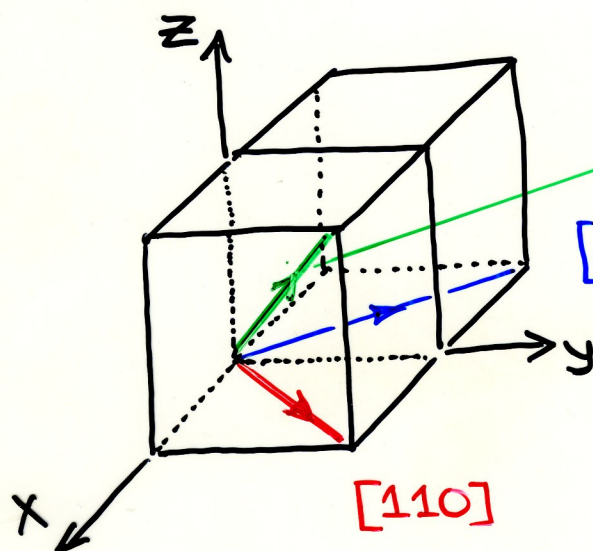
Wigner-Seitz cell
for FCC ($\vec{r}$ -space)
lattice const. a

First Brillouin
Zone for BCC
($\vec{k}$ -space)

$$\frac{4\pi}{a}$$

Directions in crystals

- Miller indices: defined using RL vectors $\vec{K}$ (hkl) parenthesis
- We can directly specify directions in the direct RL [n₁ n₂ n₃] Brackets



Body diagonal: [111]

$$[-1\ 1\ 0] = [\bar{1}\ 1\ 0]$$

Generally:
a lattice point $n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$
lies in the direction $[n_1 n_2 n_3]$

All Directions equivalent by virtue of the crystal symmetry: ⟨n₁ n₂ n₃⟩

Example for cubic crystals:

$$[110] \quad [\bar{1}10] \quad [\bar{1}\bar{1}0] \quad [1\bar{1}0]$$

$$[101] \quad [10\bar{1}] \quad [\bar{1}01] \quad [\bar{1}0\bar{1}]$$

$$\langle 110 \rangle$$

In cubic crystals the direction $[hkl]$ is perpendicular to a plane (hkl)

Normal modes of a 3D lattice with a Basis

p-atom Basis

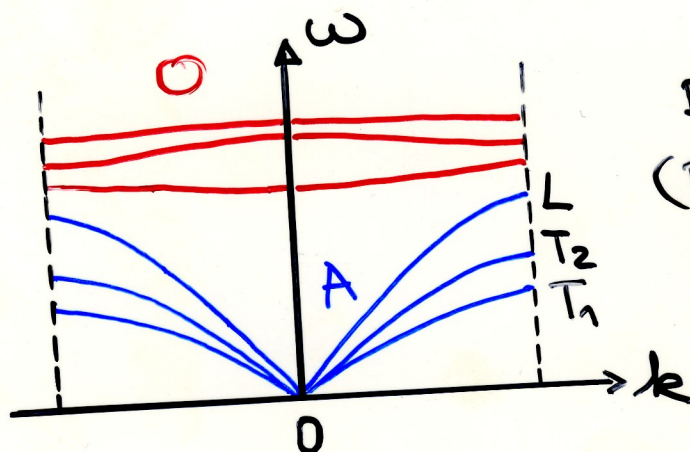
for each $\vec{k}$ 3p normal modes $\omega_s(\vec{k})$
 $s=1, \dots, 3p$

$$\omega_s(\vec{k} + \vec{K}) = \omega_s(\vec{k})$$

/ $\vec{K}$ vector

$\omega_s(\vec{k})$: periodicity of a RL

3 Acoustic modes, $3(p-1)$ Optical Modes



Diatomic
($p=2$)
lattice

Usually $\omega_L > \omega_T$

But when anisotropy present
there are no pure L or T modes
in general // except high-symmetry
directions in cubic crystals //