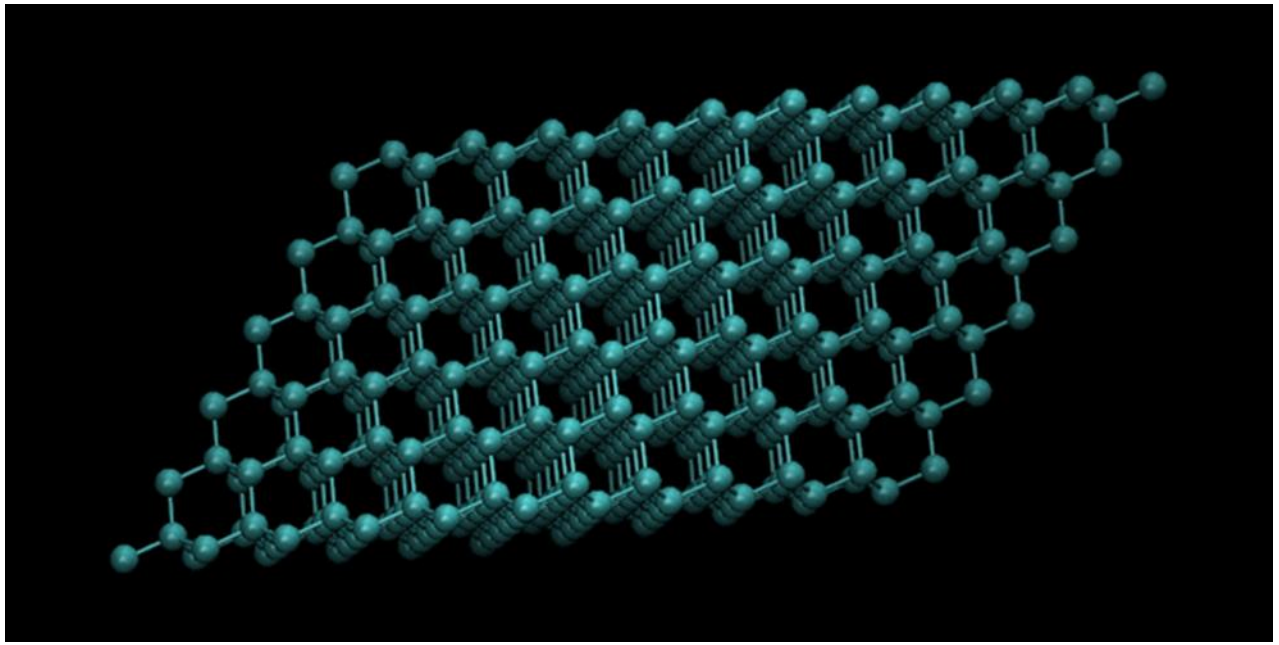
Crystal vibrations - Phonons

see, for instance, Kittel Chapter 4

[animated slide shown in the class]



So far, we have been considering atoms fixed at a given position in the crystal

However, atoms/ions have their own dynamics and they move from such equilibrium positions

TODAY GOAL: Describe crystal vibrations, i.e. collective motion of atoms/ions

1D chain

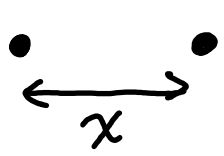
Transverse Acoustical Mode:

Longitudinal Acoustical Mode:

We will start looking at the vibrations of 1D chain

[animated slide. shown in the class]

Potential between neighboring atoms



2 neighboring atoms

1D

Potential : Taylor expansion

$$V(x) \simeq V(x_{eq}) + \frac{c}{2}(x-x_{eq})^2 - \frac{c}{3}(x-x_{eq})^3 + \dots$$

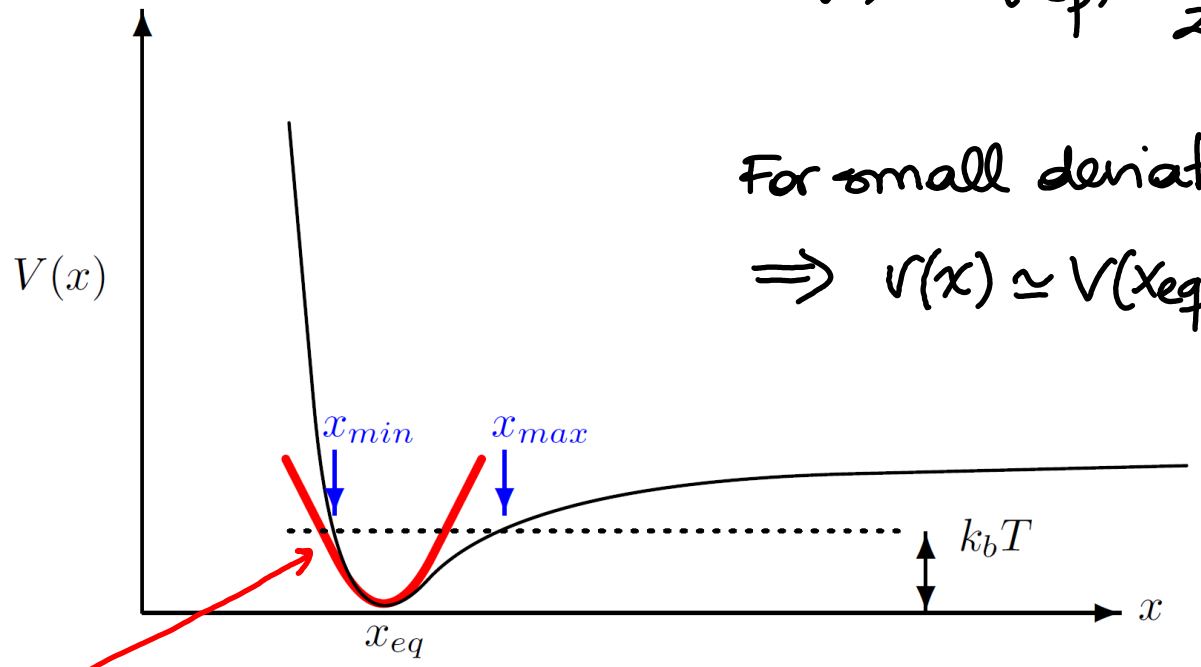
For small deviations

$$\Rightarrow V(x) \simeq V(x_{eq}) + \frac{c}{2}(x-x_{eq})^2$$

↑ potential is quadratic

Equivalent to Hook's Law

$F = c\delta x$



quadratic approximation*

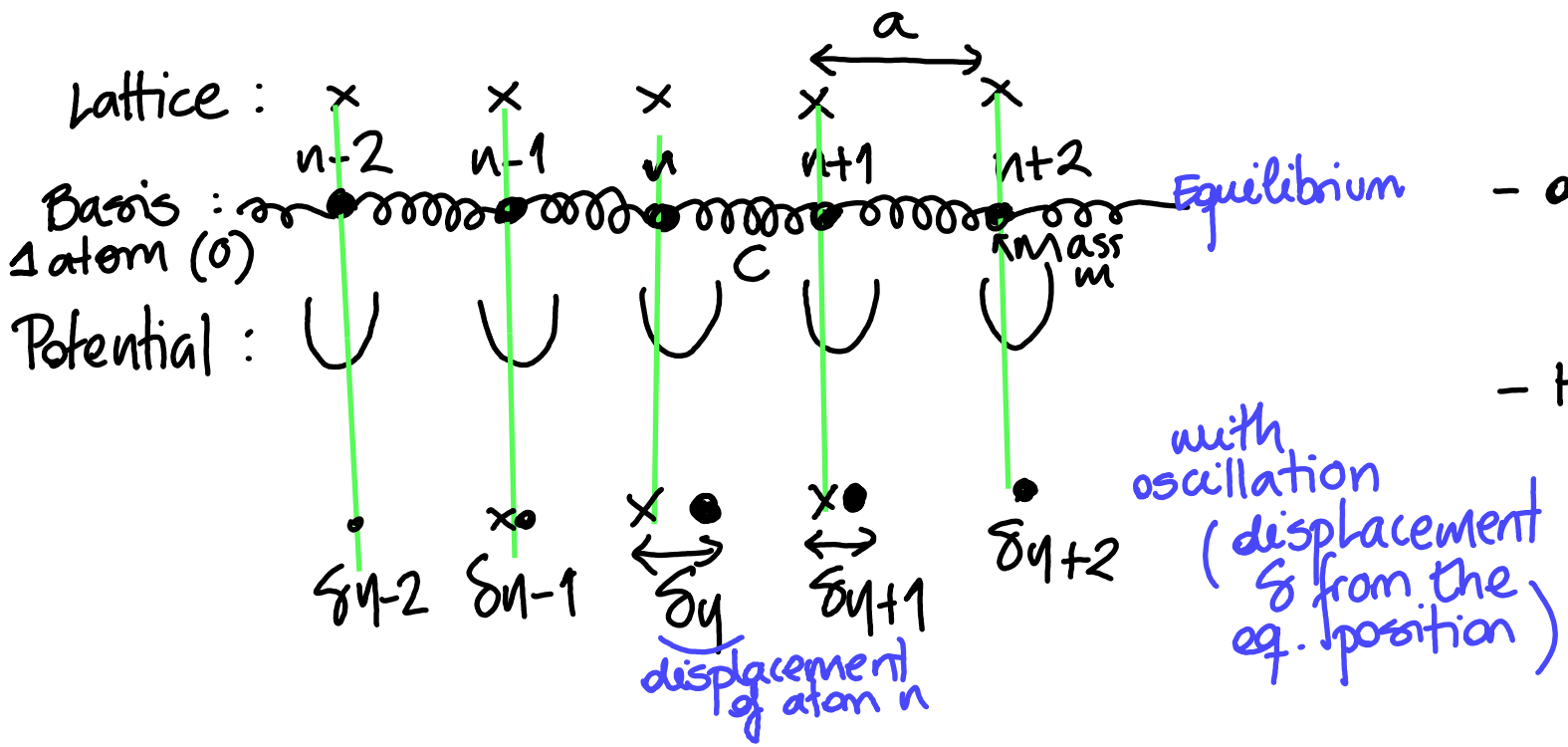
Equilibrium position

* at finite T, system oscillate between x_{min} and x_{max}

Notice that $\frac{x_{min}+x_{max}}{2} > x_{eq} \Rightarrow$ system expands (orders higher than 2nd required to capture it)

Vibrations of 1D monoatomic chain (I)

We want to find NORMAL MODE(S) = collective oscillation where all particles move at the same frequency.



- atoms restricted to move in a Line (Longitudinal vibration)

- Harmonic approximation "crystal as atoms interconnected by elastic springs"

$$\Rightarrow F_n = C(\delta_{n+1} - \delta_n) + C(\delta_{n-1} - \delta_n)$$

$$= C\{\delta_{n+1} + \delta_{n-1} - 2\delta_n\} = M\frac{d^2\delta_n}{dt}$$

Force in atom n comes from the difference in displacement between this atom n and the neighbors (n+1, n-1)

Newton 2nd law

$\Rightarrow$ we must find the displacements δ_n which are solution of this equation

Vibrations of 1D monoatomic chain (II)

Ansatz: $\boxed{\delta_n = \text{plane wave} = A e^{-i\omega t + iKx_n}} = \boxed{A e^{-i\omega t + iKna}}$

x_n: eq. position of the n-th atom, $x_n = n \cdot a$

let's test it:

$$M \frac{d^2\delta_n}{dt^2} = C\{\delta_{n+1} + \delta_{n-1} - 2\delta_n\}$$

$$-M \cdot \omega^2 \cdot \delta_n = C A e^{-i\omega t}\{e^{iK(n+1)a} + e^{iK(n-1)a} - 2e^{iKna}\}$$

$$= C\delta_n\{\underbrace{e^{iKa} + e^{-iKa}}_{=2\cos Ka} - 2\}$$

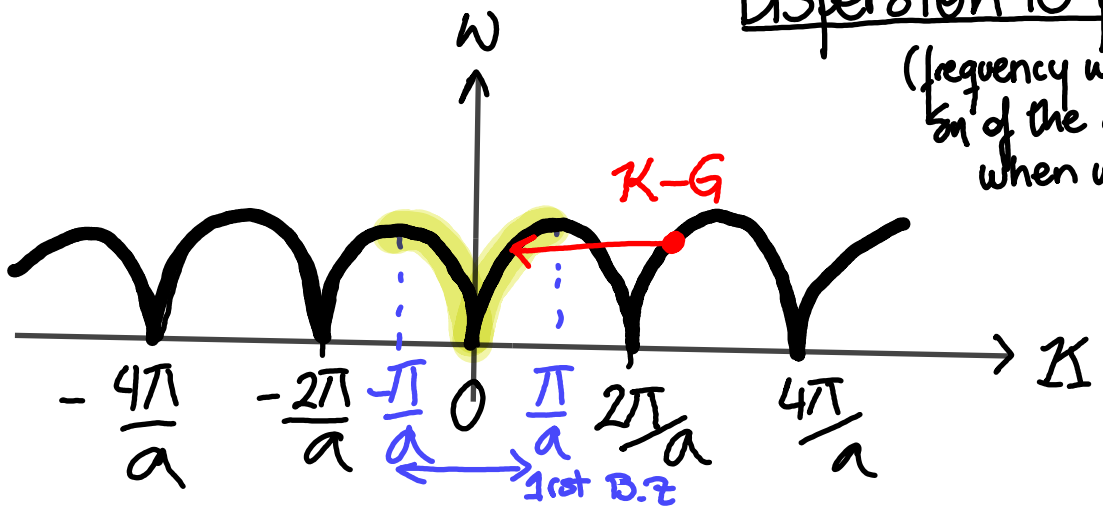
$$= C\delta_n(2\cos Ka - 2)$$

$$\omega^2 = \frac{2C}{M}[1 - \cos Ka] = \frac{4C}{M}\sin^2\frac{Ka}{2} \longrightarrow \boxed{\omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{1}{2}Ka\right|}$$

Dispersion Relation
(= relationship between frequency of vibration ω and wavevector K)

Range of significant K

$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\frac{Ka}{2}\right|$$



Dispersion is periodic in K!

(frequency ω and displacement s_n of the atoms do not change when we change $K \to K + \frac{2\pi}{a}$)

Reciprocal Lattice vector G

Range of significant K:

2 consecutive atoms: $\frac{s_{n+1}}{s_n} = \frac{A e^{-i\omega t + iK(n+1)a}}{A e^{-i\omega t + iKna}} = e^{iKa}$

displacement

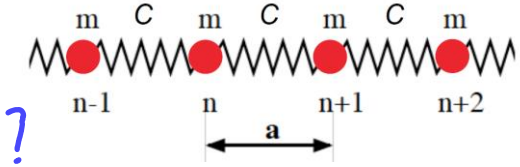
range $-\pi < Ka < \pi$ covers all range of independent K.

$$\boxed{-\frac{\pi}{a} < K < \frac{\pi}{a}}$$

1rst Brillouin zone!

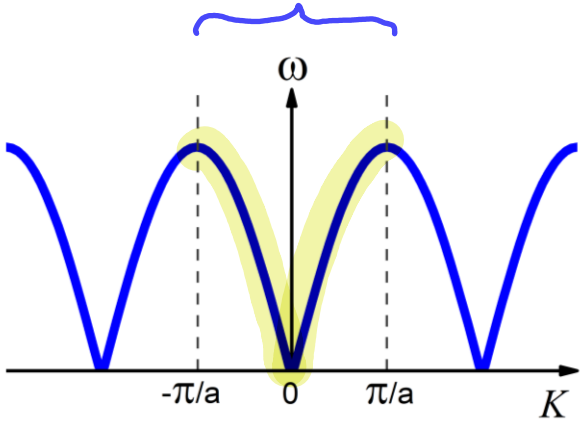
the 1rst. B.Z. covers all information about Lattice motion (again, special role of B.Z.!)

Aliasing of waves



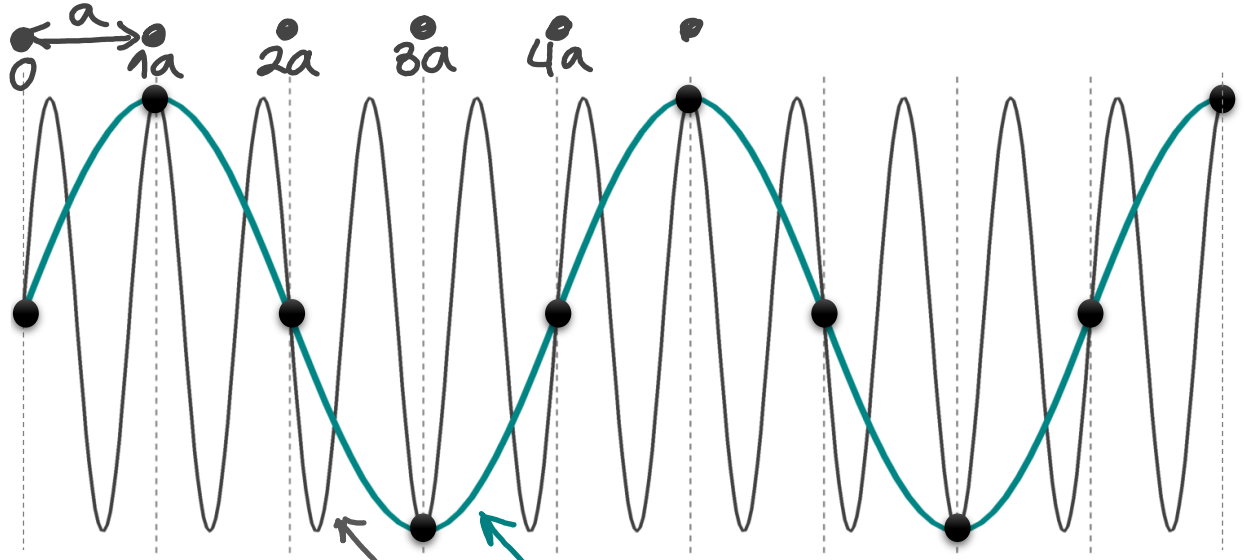
1rst B.Z. contains all info ⇒ wavevector K describes the same wave as wavevector $K+G$. What does it mean?

" given $\lambda = \frac{2\pi}{G}$, which λ we chose $\frac{2\pi}{K}$ or $\frac{2\pi}{K+G}$?"



Equil.

Oscill.



$\lambda_1 = 4a \Rightarrow K_1 = \frac{1}{4}\frac{2\pi}{a}$

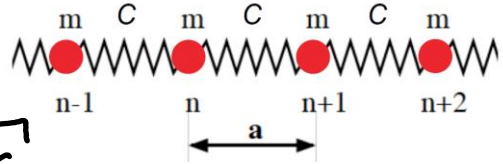
$5\lambda_2 = 4a \Rightarrow K_2 = \frac{5}{4}\frac{2\pi}{a}$

$K_2 = K_1 + \underbrace{\frac{2\pi}{a}}_{G}$

⇒ the point is to realize that K and $K+G$ are only equivalent at the lattice points $\delta_n = na$

Both waves are equivalent: they take the same values at lattice points and do not coincide at all other points

Dispersion relation



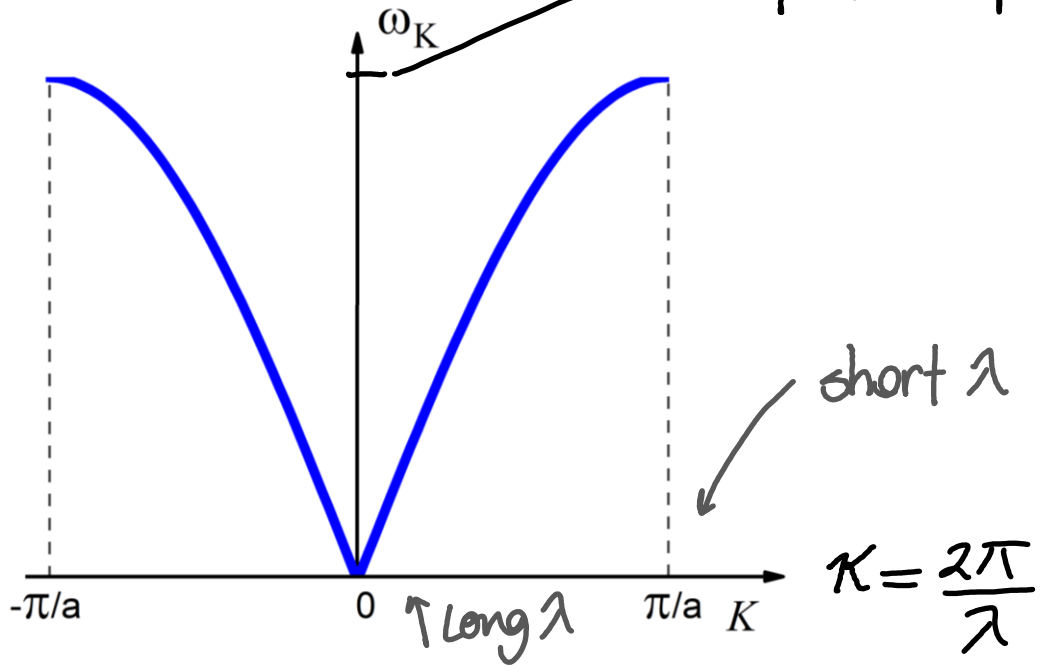
$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\frac{Ka}{2}\right|$$

max freq. $\omega = \sqrt{\frac{4C}{m}}$

ξ_n

$\xi_n = Ae^{i(Kna-\omega t)}$

↑ displacement



$K = \frac{2\pi}{\lambda}$

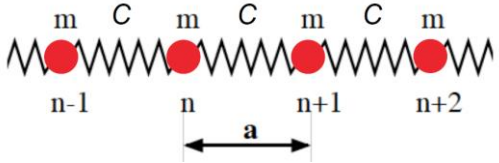
Frequency is symmetric with respect K : $\omega(K) = \omega(-K)$

it corresponds to waves travelling left → right and right → left

since these two directions are equivalent in the crystal, ω is the same

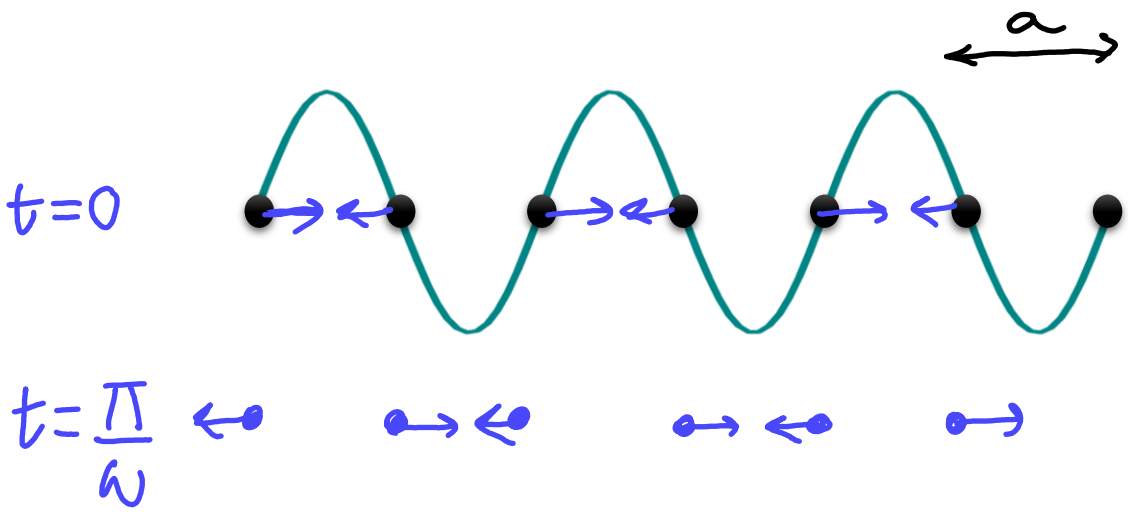
Dispersion relation

shortest λ supported by the crystal



Short wavelengths $\Rightarrow$ i.e. $\lambda = 2a$

$$\kappa = \frac{2\pi}{\lambda} = \frac{\pi}{a}$$ ← zone boundary!



$$u_n = A e^{i(-\omega t + \kappa n a)}$$

$$= A e^{i(-\omega t + \pi n)}$$

$$= A e^{-i\omega t} (-1)^n$$

neigh. atoms oscillate in opposite directions

$\Rightarrow$ At zone boundaries, solutions represent standing waves

see next slide

@ $\kappa = \pm \pi/a \Rightarrow v_g = 0$ ("dispersion $\omega(K)$ is flat") $\Rightarrow$ the transmission of energy is zero; any wave is diffracted if κ is at the zone boundary

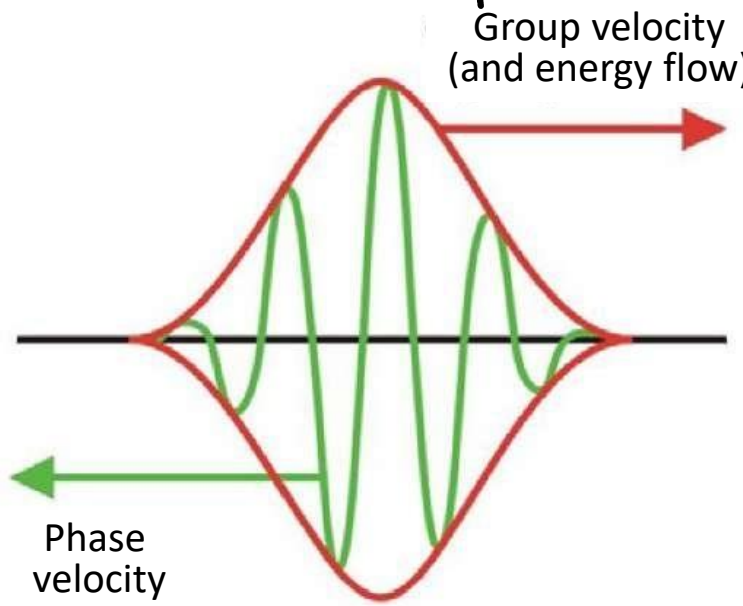
Phase and group velocity

$v_g = \frac{dw}{dK} = \text{grad}_K w_K \Rightarrow v_g = \sqrt{\frac{ca^2}{M}} \cos\frac{Ka}{2}$

(slope of $w(K)$)

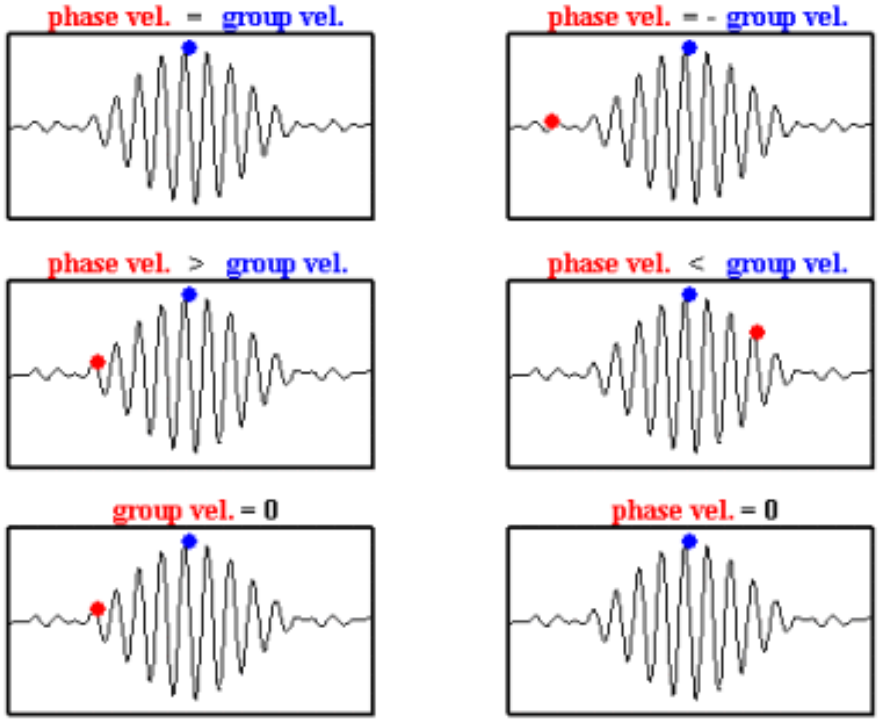
@ $K = \pm\frac{\pi}{a} \Rightarrow v_g = 0$

v of propagation of the wave packet



$v_p = \frac{w}{K}$

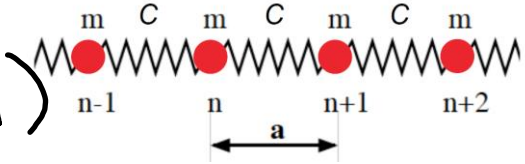
[velocity of propagation of the plane wave]



isvr

http://resource.isvr.soton.ac.uk/spcg/tutorial/tutorial/Tutorial_files/Web-further-dispersive.htm

Dispersion relation



compared to interatomic distances ($\sim 5\text{Å}$)

Long wavelengths (small K)

$\Rightarrow \lambda \sim 20\text{m} - 20\text{m}$

$$\omega = \sqrt{\frac{4C}{m}}\left|\sin\frac{Ka}{2}\right|$$

$\Rightarrow \lambda \gg a$

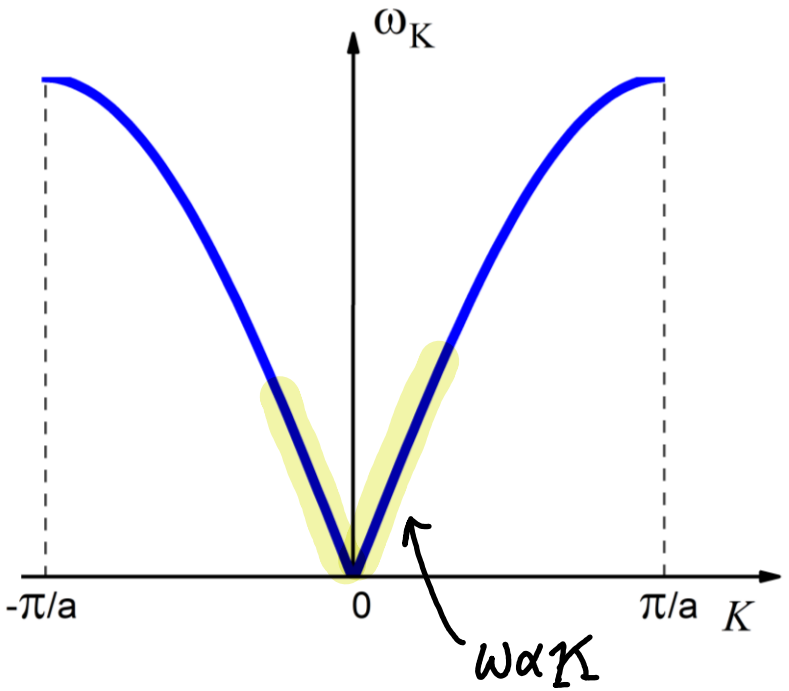
$\Rightarrow Ka \ll 1$

for small x

$$\sin x \simeq x - \frac{x^3}{3!} - \frac{x^5}{5!} \cdots$$

in this limit,

$$\omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{Ka}{2}\right| \simeq \sqrt{\frac{4C}{M}}\left(\frac{1}{2}Ka\right) = \sqrt{\frac{C}{M}}Ka$$



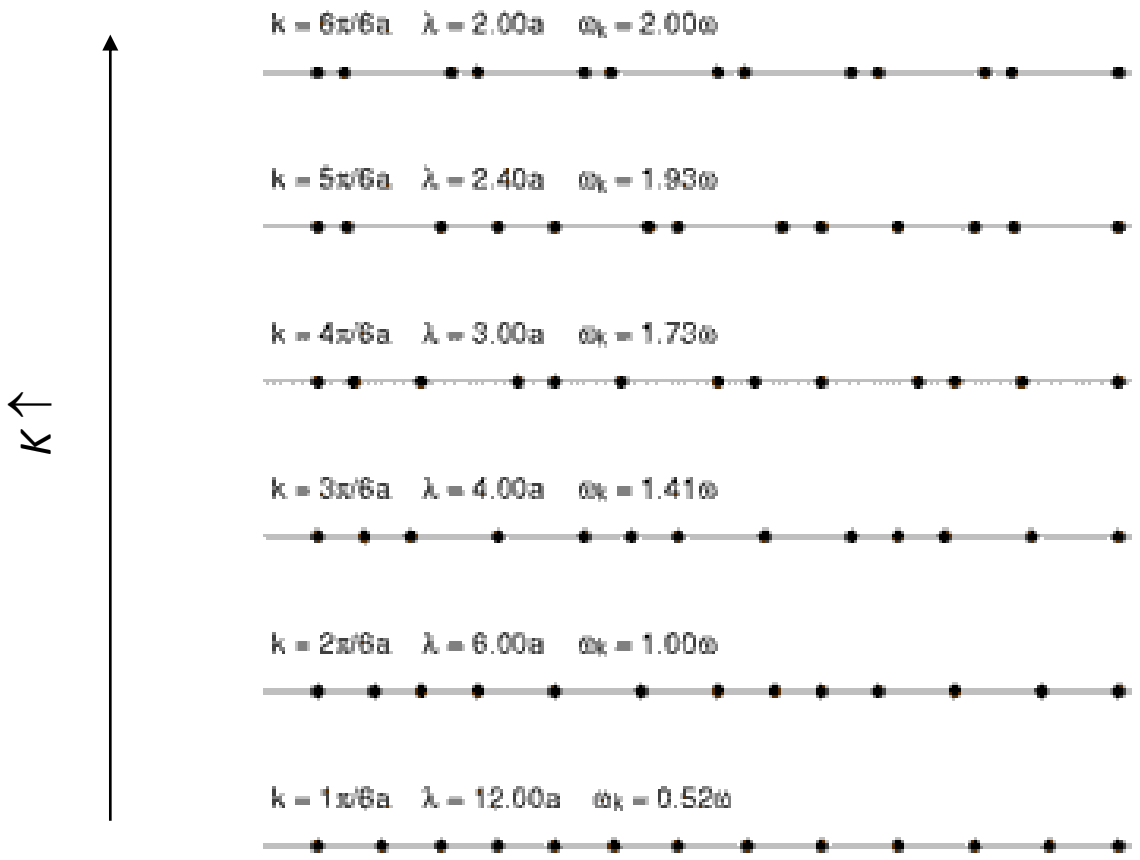
For very Large λ, $\boxed{\omega \propto K}$

In this regime, the velocity is independent of ω

$$v_p = \frac{\omega}{K} = \sqrt{\frac{C}{M}}a$$

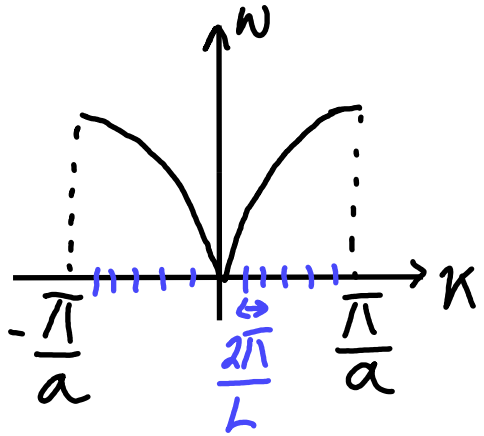
→ vibration is an elastic wave

1D monoatomic chain

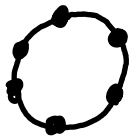


see, for instance, wikipedia animation for Phonons

Normal modes: how many K?



* N masses in a row
* Assume <u>periodic boundary conditions</u> : $\delta_{n+N} = \delta_n$

in 1D  length $L = Na$

$$\delta_{n+N} = \delta_n$$

$$e^{i(-\omega t + K(n+N)a)} = e^{-i(\omega t + Kna)}$$

$$e^{iKNa} = 1 \Rightarrow K \text{ must be of the type } K = \frac{2\pi}{Na} p = \frac{2\pi}{L} p$$

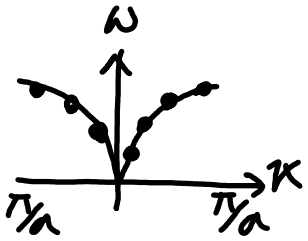
p: integer, $L = Na$

$\Rightarrow K$ is quantized

$$\underline{\text{Total number of modes}} = \frac{\text{Range of } K}{\text{spacing between neigh. } K} = \frac{2 \cdot \pi/a}{2\pi/Na} = \boxed{N}$$

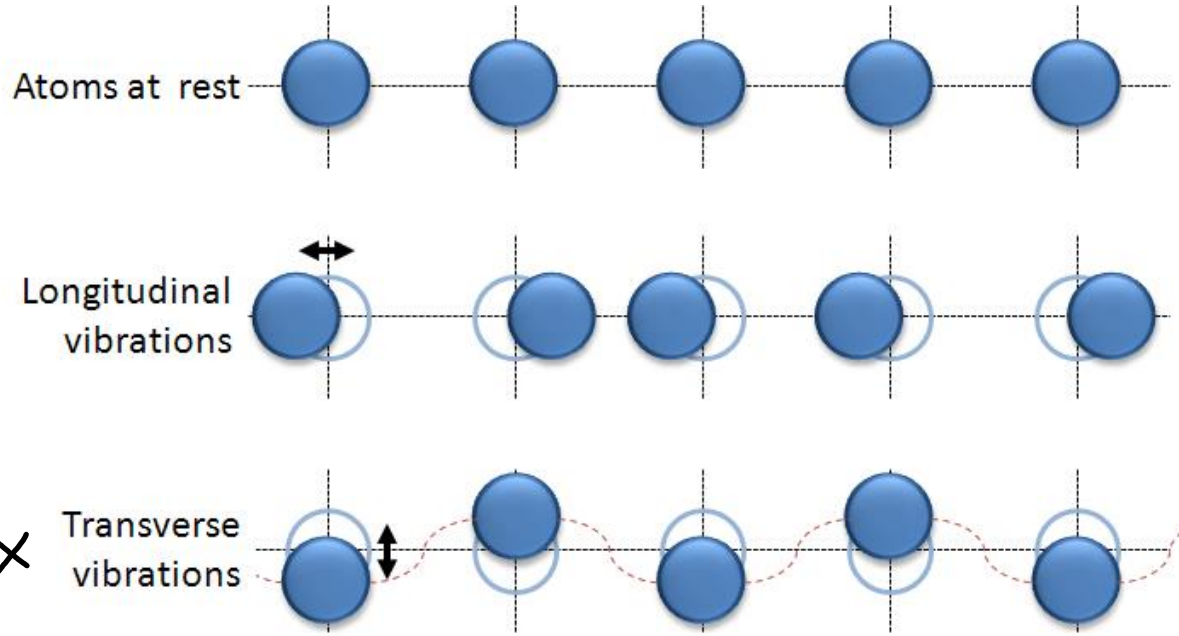
there is a normal mode per mass in the system

(remember: we are still dealing with 1D monoatomic chain)



Excitations in higher dimensions

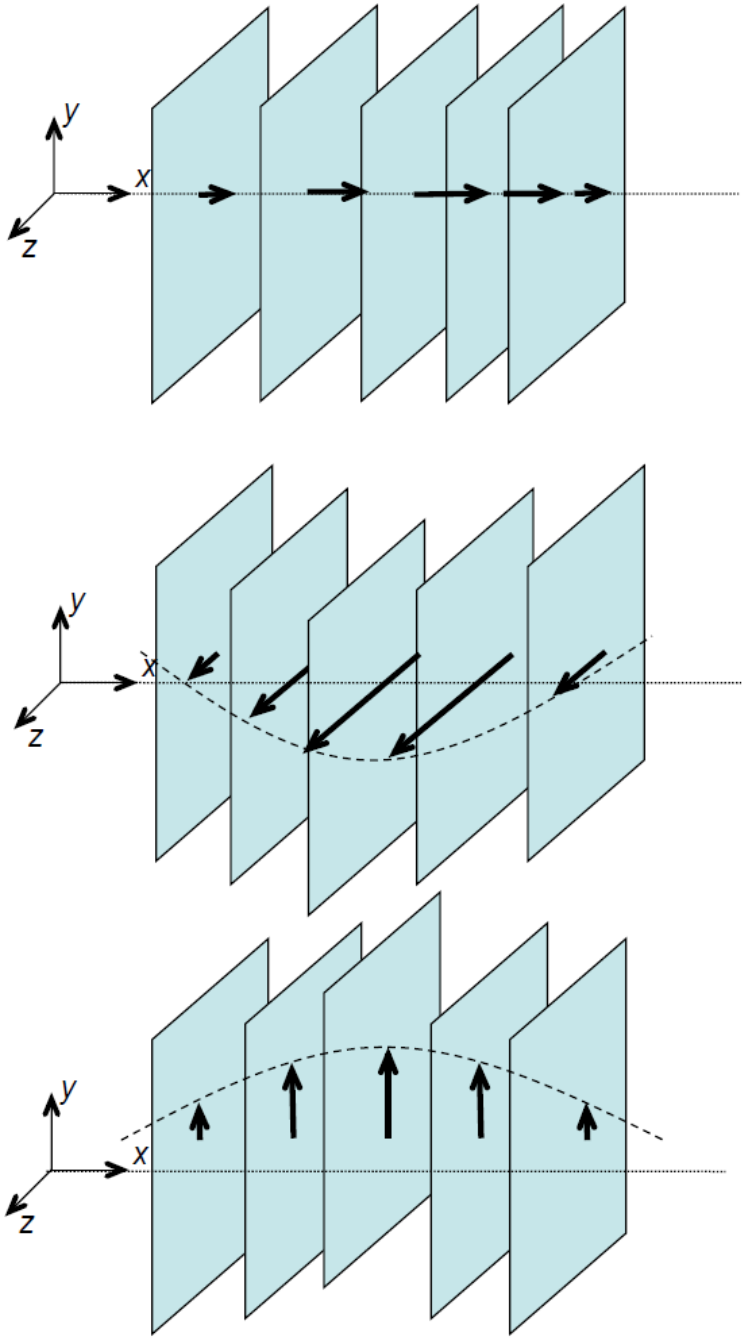
(monoatomic chain)



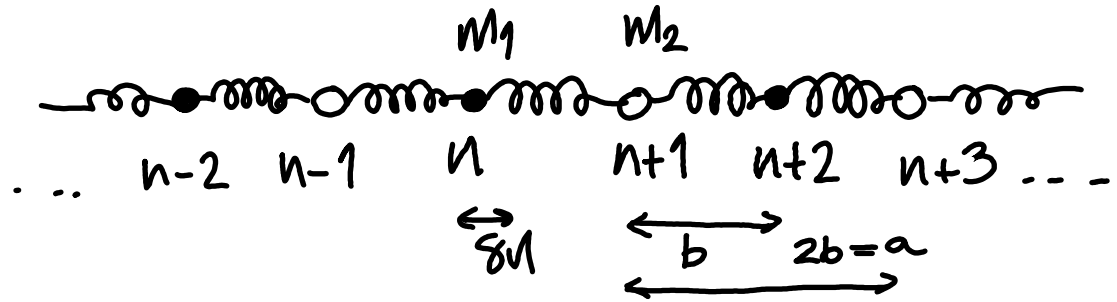
in 3D,

1 longitudinal mode
2 transverse modes
} ⇒ 3N

[3D monoatomic chain]



Vibrations of 1D diatomic chain



$$m_1 \frac{d^2\delta_n}{dt^2} = C(\delta_{n+1} + \delta_{n-1} - 2\delta_n)$$
$$m_2 \frac{d^2\delta_{n+1}}{dt^2} = C(\delta_{n+2} + \delta_n - 2\delta_{n+1})$$

Ansatz in matrix form

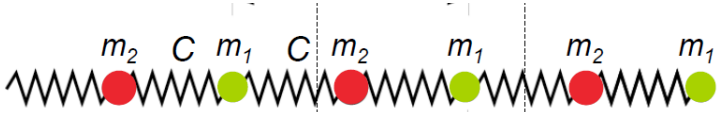
$$\begin{bmatrix} \delta_n \\ \delta_{n+1} \end{bmatrix} = \begin{bmatrix} A_1 e^{iKnb} \\ A_2 e^{iK(n+1)b} \end{bmatrix} e^{-i\omega t}$$

substituting Ansatz in the 2 equations of motion and solving the system of linear homogeneous eqs

Solution →

$$\omega^2 = C\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \pm \sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\sin^2 Kb}{m_1 m_2}}$$

Diatomic chain: dispersion relation



$$\omega^2 = C\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm C\sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\,sin^2 Ka}{m_1 m_2}}$$

2 solutions

$\Rightarrow$ there are <u>2 dispersion curves</u> for the diatomic chain : (depending on the sign)

* OPTICAL BRANCH (upper curve)
* ACOUSTIC BRANCH (lower curve)