

# CMP Lecture 12

School of Physics  
The University of Sydney



## Perfect lattice

Bloch waves propagate freely without encountering any resistance

$$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k}\vec{r}}$$

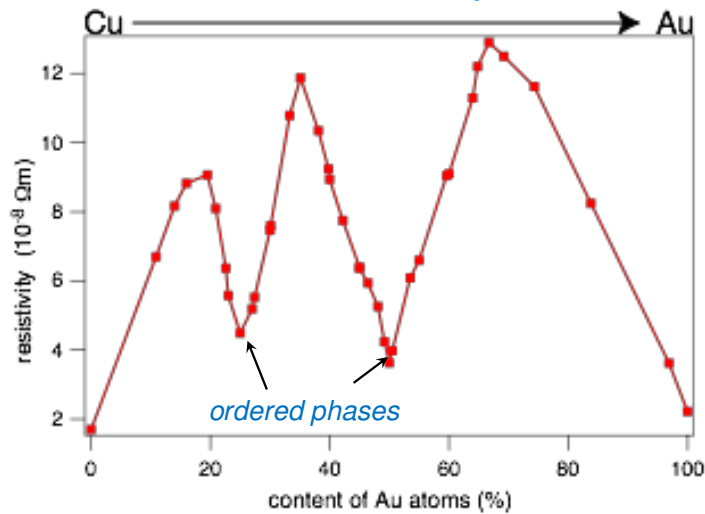
Causes of scattering / finite resistance:

- Any kind of deviation from the perfect lattice
- Point defects, extended defects, vacancies, substitutional atoms in the lattice....
- Thermal vibrations

give rise to relaxation time  $\tau$

*Updated picture compared to Drude*

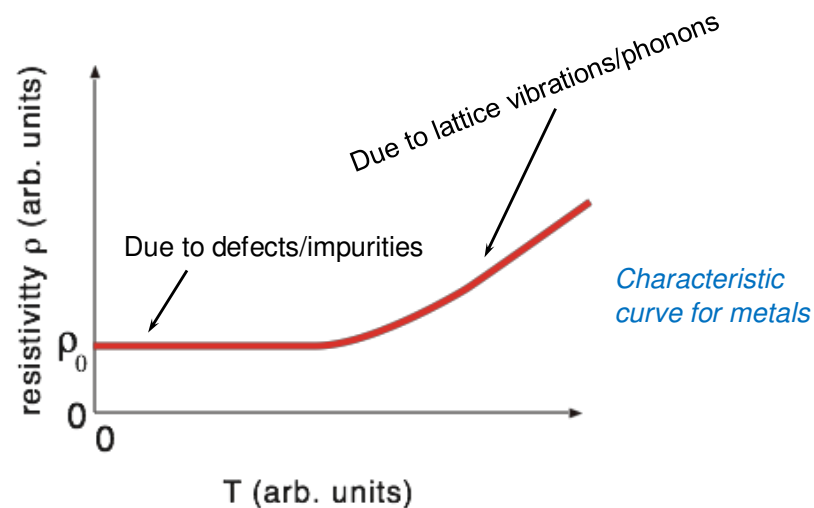
## Failures of the Drude model: electrical conductivity of an alloy



- Drude: the resistivity of an alloy should be between those of its components, or at least similar to them.
- But it can be much higher than that of either component.
- $Cu_3Au$  and  $CuAu$  form ordered alloys and show a minimum in the resistivity.

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## Temperature dependence of the resistivity



- At higher temperatures the resistivity (of a metal) increases because of stronger lattice vibrations / more phonons to scatter from.
- At low temperature the resistivity saturates because of the defects and impurities.

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## Modified Drude formula

mean free path by lattice imperfections

*Updated understanding*

$$\tau = \frac{\lambda}{v_t}$$

(average) velocity at the Fermi level

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## Modified Drude formula

electron density from  
partially filled bands

*Updated understanding*

conductivity

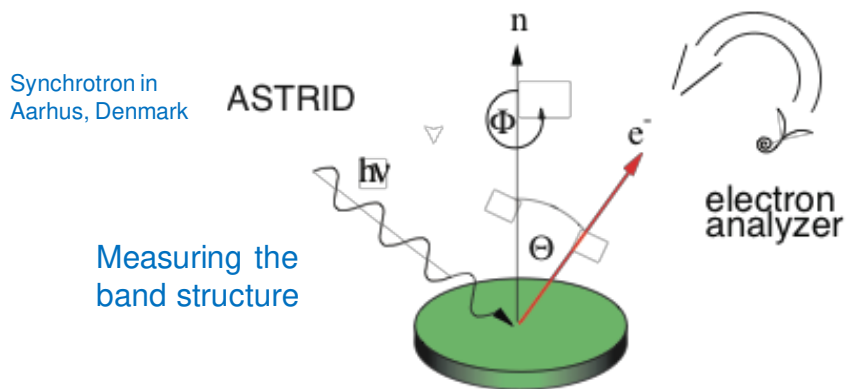
$$\sigma = \frac{n e^2 \tau}{m^*}$$

relaxation time

(average) effective mass of those electrons

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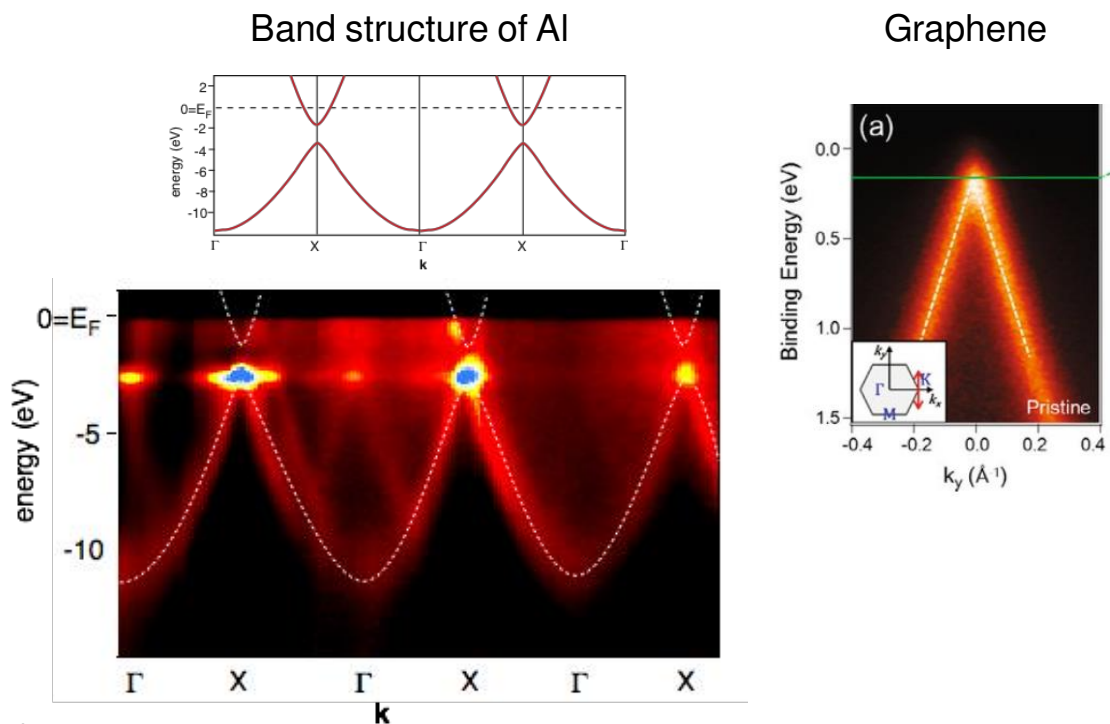
# Angle-resolved photoemission (ARPES) spectroscopy



- Measure the energy and emission angle of the photoemitted electrons outside the surface.
- Infer the energy and the  $k$ -vector inside the solid, i.e. the bands.

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## Angle-resolved photoemission (ARPES)



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# Revision

## Electrons in periodic potentials

- Define Bloch's theorem and discuss its consequences.
- How is the (average) velocity for an electron related to  $\epsilon_{\mathbf{k}}$ ?
- What is crystal momentum? How is it related to ordinary momentum?
- What is the basic assumption behind the "nearly free electron" approximation?
- Which electron states are most influenced by a weak periodic potential?
- Sketch the energy bands in a 1D metal in the extended, reduced, and repeated zone scheme according to (i) the free electron approximation, and (ii) the nearly free electron approximation.
- What is the basic idea behind the tight-binding method, and what can it be used for?
- Sketch how the energy levels change as atoms condense to form a crystalline solid.
- What is a metal-insulator transition?

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# Revision

## Band theory

- The Bloch theorem: the wave function for an electron in a periodic potential can be written in the form:  $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$  where  $u_{\mathbf{k}}(\mathbf{r})$  is a periodic function with the period of the lattice.
- The energy spectrum of electrons consists of a set of continuous *energy bands*, separated by regions with no allowed states – *gaps*.
- Function  $E(\mathbf{k})$  satisfies the symmetry properties of a crystal, in particular, the translational invariance:  $E(\mathbf{k}) = E(\mathbf{k} + \mathbf{G})$ .  
This allows considering the first Brillouin zone only.  
Also, inversion symmetry:  $E(\mathbf{k}) = E(-\mathbf{k})$ .
- Nearly free electron model – weak crystal potential. Electron behaves essentially as a free particle, except the wave vectors close to the boundaries of the zone. In these regions, energy gaps appear.

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# Revision

## Band theory

- Tight-binding model: strong crystal potential, weak overlap. The band width increases and electrons become more mobile (smaller effective mass) as the overlap between atomic wave functions increases.
- Concept of effective mass: in a periodic potential electron moves as in free space, but with different mass:

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} \quad i, j = x, y, z$$

- Physical origin of effective mass: crystal field.
- Metals: partially filled bands. Insulators: at 0 K the valence band is full, conduction band is empty. Semiconductors and semimetals.
- Perfectly periodic lattice: no scattering of electrons, velocity remains constant.
- Density of states: number of electronic states per unit energy range. Simple case:

$$D(E) = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2}\right)^{3/2} E^{1/2}$$

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## Normal modes and phonons

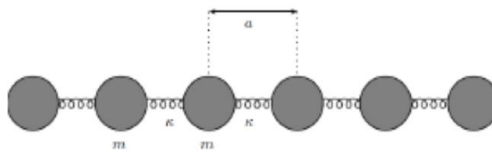
At finite temperatures atoms in a crystal vibrate

[http://lampx.tugraz.at/~hadley/ss1/phonons/phonon\\_script.php](http://lampx.tugraz.at/~hadley/ss1/phonons/phonon_script.php)

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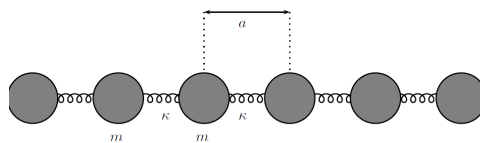
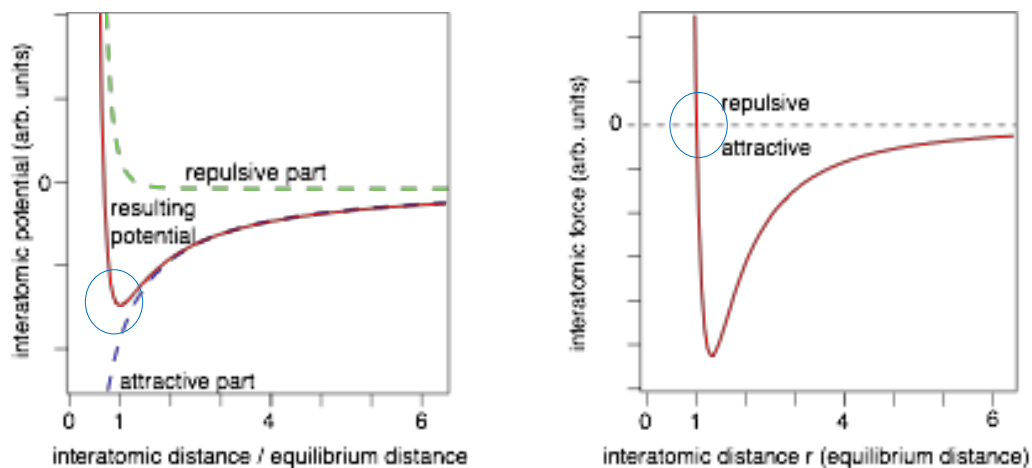
# Dispersion of one-dimensional chain

- We will study wavelike modes of vibration of a linear chain of classical masses in the harmonic approximation.
- Quantisation of the modes of vibration will then be undertaken – the quanta are **phonons**.
- We need this for transport properties such as electrical and thermal conductivity, specific heat, diffraction properties, to develop structural diagnostics based on spectroscopies and to understand phase changes.
- Our initial study is a linear chain based on the harmonic approximation.



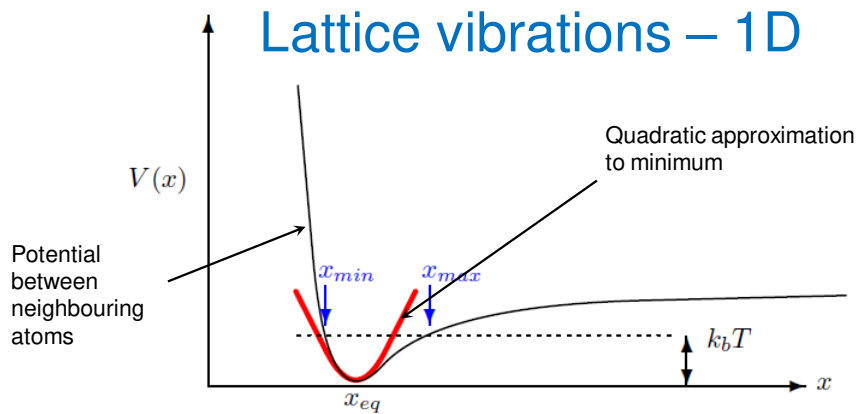
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## Lattice vibrations – 1D



Consider one dimensional system of atoms in a line.  
Recall: the potential between two neighbouring atoms has the form above.

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In region of minimum, Taylor expansion:

No linear term since  $x_{eq}$  is the minimum

$$V(x) \approx V(x_{eq}) + \frac{\kappa}{2}(x - x_{eq})^2 + \frac{\kappa_3}{3!}(x - x_{eq})^3 + \dots$$

$\kappa$  spring constant

If deviations from position  $x_{eq}$  are small, higher terms are much smaller than leading quadratic term, and can neglect. General principle that any smooth potential close to minimum is quadratic

At finite temperature  $T$  the atoms can oscillate between  $x_{max}$  and  $x_{min}$ . Since potential is asymmetric away from minimum, this leads to an average position greater than  $x_{eq}$

- **Thermal Expansion** (though not all systems behave like this)

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## Lattice vibrations – 1D

*First consider sound waves*

Compressibility/elasticity

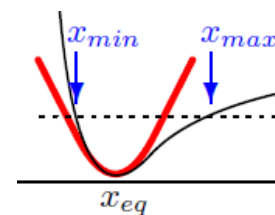
Hooke's Law – quadratic potential about minimum

$$-\kappa(\delta x_{eq}) = F$$

Applying a force to compress system

- reduces distance between atoms

Compressibility:  $\beta = -\frac{1}{V} \frac{\partial V}{\partial P}$  (assuming  $T = S = 0$ )



In one dimension, with  $L$  the length:

$$\beta = -\frac{1}{L} \frac{\partial L}{\partial F} = \frac{1}{\kappa x_{eq}} = \frac{1}{\kappa a} \quad (1)$$

(taking  $x_{eq} = a$ )

$T$  temperature

$P$  pressure

$S$  entropy

$V$  volume

$\kappa$  spring constant

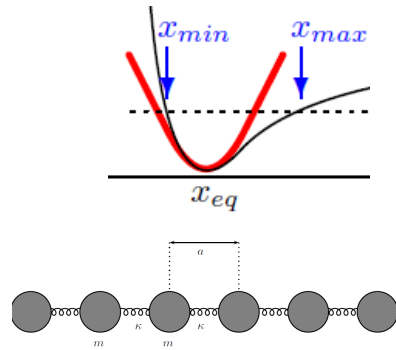
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# Lattice vibrations – 1D

In an isotropic compressible fluid  
sound waves with velocity:

$$v = \sqrt{\frac{B}{\rho}} = \sqrt{\frac{1}{\rho\beta}} \quad (2)$$



For the 1-D solid take the density  $\rho$  as  $m/a$  where  $m$  is the mass of atom  
Substitute (1) into (2) then

$$v = \sqrt{\frac{\kappa a^2}{m}} \quad \text{bulk modulus} \quad B = 1/\beta$$

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## Summary

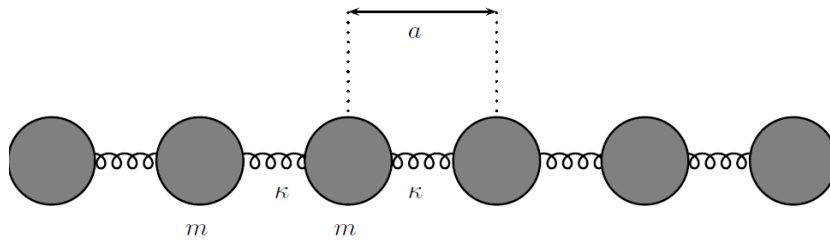
- Forces between atoms determine ground-state structure.
- These same forces, perturbing around the ground state, determine elasticity, sound velocity, and thermal expansion.
- Thermal expansion comes from the non-quadratic part of the interatomic potential.

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# Lattice vibrations -1 D chain

Oxford Basics, Ch.9  
Ashcroft &  
Mermin Ch.22

One dimensional monatomic harmonic chain



$m$ , mass  
 $a$ , lattice spacing  
 $\kappa$ , spring constant

Let the position of the  $n^{th}$  atom be  $x_n$   
And the equilibrium position be  $x_n^{eq} = na$

Allowing motion of atoms:  $\delta x_n = x_n - x_n^{eq}$   
Only in one dimension (longitudinal motion, not transverse)  
Can write total potential energy as:

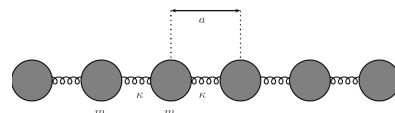
*Assume at low enough  $T$ , the potential is quadratic*

$$\begin{aligned} V_{tot} &= \sum_i V(x_i - x_{i+1}) \\ &= V_{eq} + \sum_i \frac{\kappa}{2} (\delta x_i - \delta x_{i+1})^2 \end{aligned}$$

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# Lattice vibrations -1 D chain

The force on the  $n^{th}$  atom:



$$F_n = -\frac{\partial V_{tot}}{\partial x_n} = \kappa(\delta x_{n+1} - \delta x_n) + \kappa(\delta x_{n-1} - \delta x_n)$$

$$m(\ddot{\delta x}_n) = F_n = \kappa(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n) \quad (1)$$

*Want to find the "normal modes" – all atoms oscillate with a common frequency*

Ansatz (guess) solution:  $\delta x_n = Ae^{i\omega t - ikx_n^{eq}} = Ae^{i\omega t - ikna}$

Substitute solution into (1)

$$-m\omega^2 Ae^{i\omega t - ikna} = \kappa Ae^{i\omega t} \left[ e^{-ika(n+1)} + e^{-ika(n-1)} - 2e^{-ikan} \right]$$

*Cancelling terms*

$$m\omega^2 = 2\kappa[1 - \cos(ka)] = 4\kappa \sin^2(ka/2)$$

*get frequency of normal modes*

$$\omega = 2\sqrt{\frac{\kappa}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

$k$ , wavevector, either  
+ or - (right or left travelling)  
 $\omega$  frequency ( $> 0$ )

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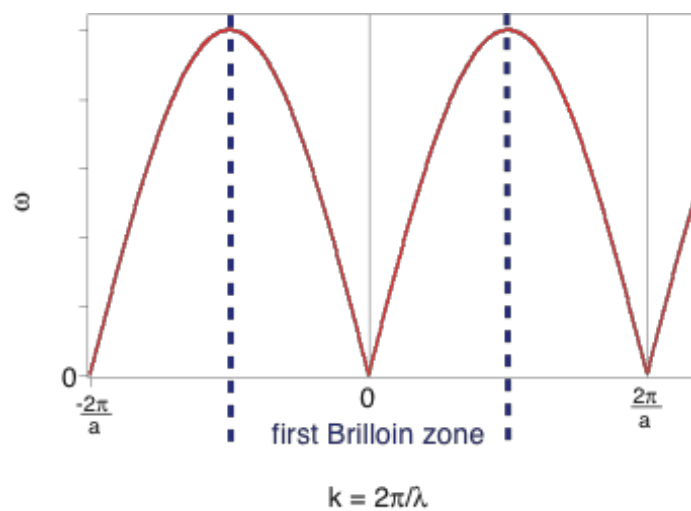
# Working

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## Dispersion of 1D chain

$$\omega = 2\sqrt{\frac{\kappa}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

$\omega(k)$  is called the *dispersion relation*. Periodic in  $k \rightarrow k + 2\pi/a$

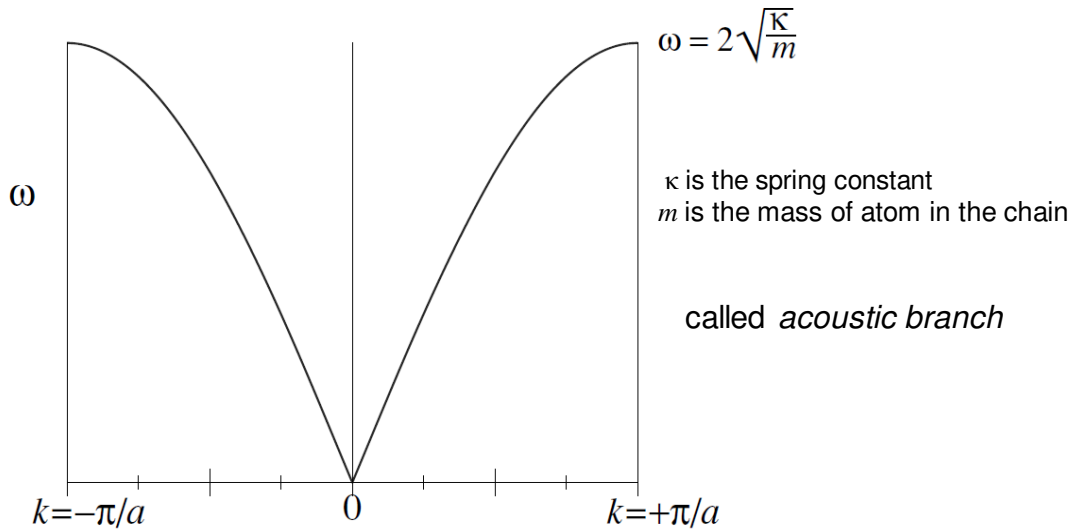
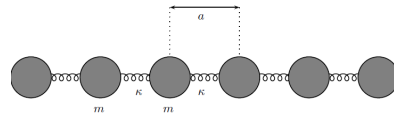


We only need to consider the dispersion relation in the first Brillouin zone.

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## Dispersion of 1D chain

$$\omega = 2\sqrt{\frac{\kappa}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

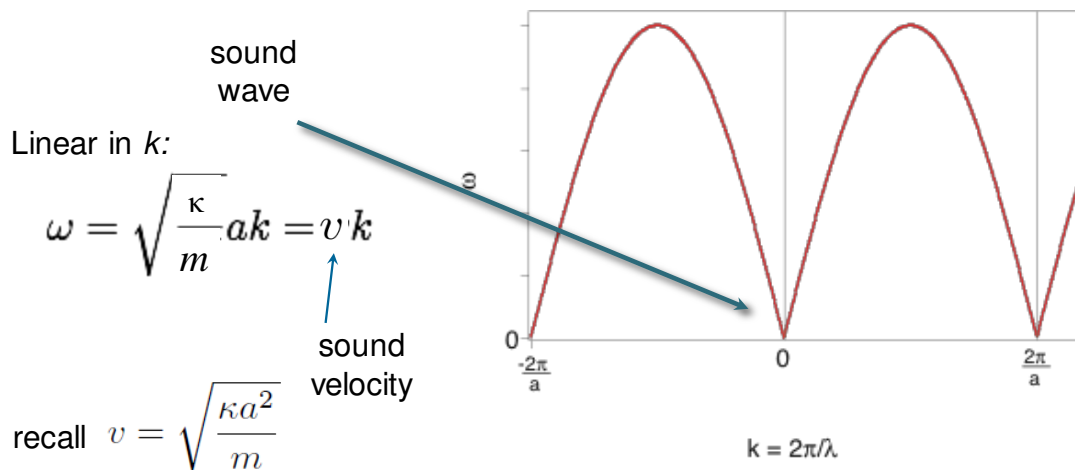


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## Dispersion of 1D chain

Dispersion relation  $\omega = 2\sqrt{\frac{\kappa}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$

For small  $k$  the sin is equal to its argument



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## Dispersion of 1D chain

We expect periodicity since:  $\delta x_n = Ae^{i\omega t - ikna}$

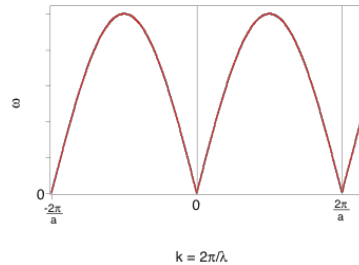
$$k \rightarrow k + 2\pi/a$$

$$\delta x_n = Ae^{i\omega t - i(k+2\pi/a)na} = Ae^{i\omega t - ikna} e^{-i2\pi n} = Ae^{i\omega t - ikna}$$

since  $e^{-i2\pi n} = 1$

In general for integer  $p$ ,  $k + 2\pi p/a$

$$e^{-i2\pi np} = 1$$



The set of points in  $k$ -space which are equivalent to  $k=0$  is the *reciprocal lattice* (we know this!)

$$\begin{aligned} x_n &= \dots -2a, & -a, & 0, & a, & 2a, & \dots \\ G_n &= \dots -2\left(\frac{2\pi}{a}\right), & -\frac{2\pi}{a}, & 0, & \frac{2\pi}{a}, & 2\left(\frac{2\pi}{a}\right), & \dots \end{aligned}$$

$$G_m \text{ belongs to the reciprocal lattice if } e^{iG_m x_n} = 1$$

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## Dispersion of 1D chain

At shorter wavelength (larger  $k$ ) we define:

*group velocity*

$$v_{group} = d\omega/dk$$

Speed at which a wave packet moves  
-gradient of dispersion curve

*phase velocity*

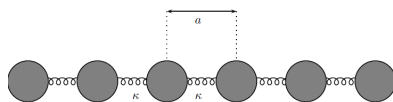
$$v_{phase} = \omega/k$$

-can see goes to zero at the zone boundary

Speed at which maxima and minima move

For small  $k$ , in the linear region, these are equal

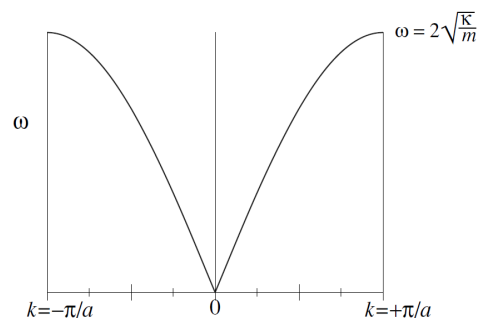
<https://www.youtube.com/watch?v=tIM9vq-bepA>



$$v_{phase} = \frac{\text{distance wave travels}}{\text{time period}} = \lambda/\tau = \omega/k$$

$$k = 2\pi/\lambda$$

$$\omega = 2\pi f \quad \tau = 1/f$$



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# Normal modes of monoatomic chain

<http://lampx.tugraz.at/~hadley/ss1/phonons/1d/1dphonons.php>

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End

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