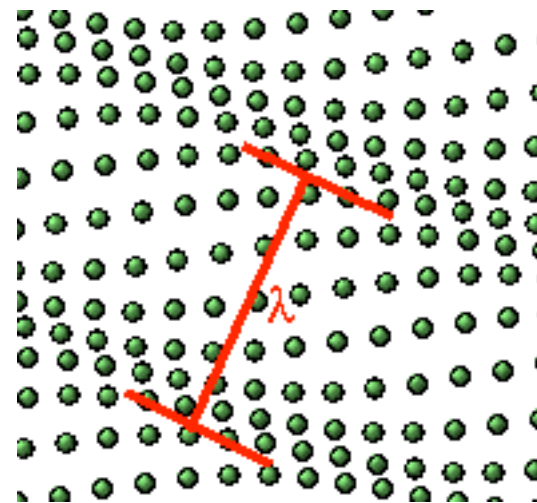
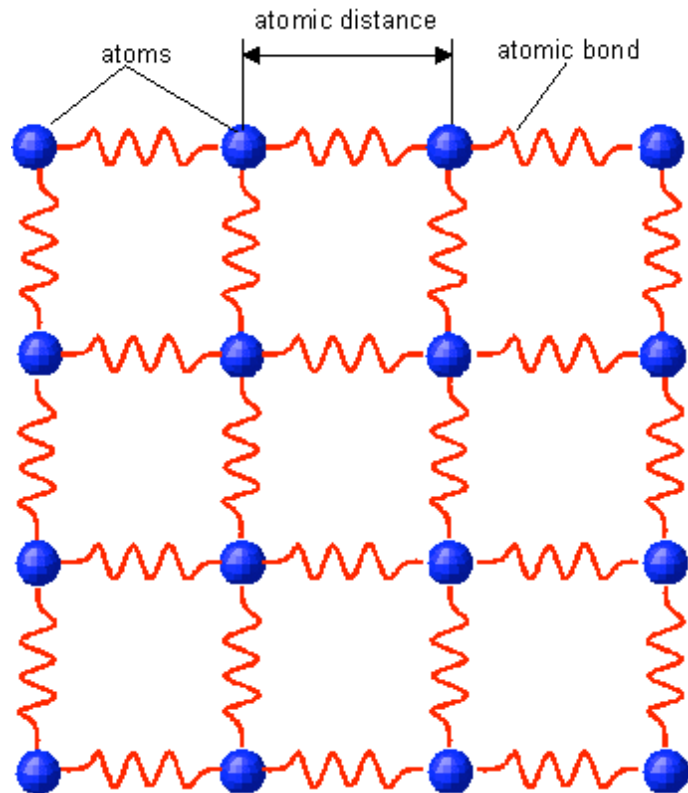
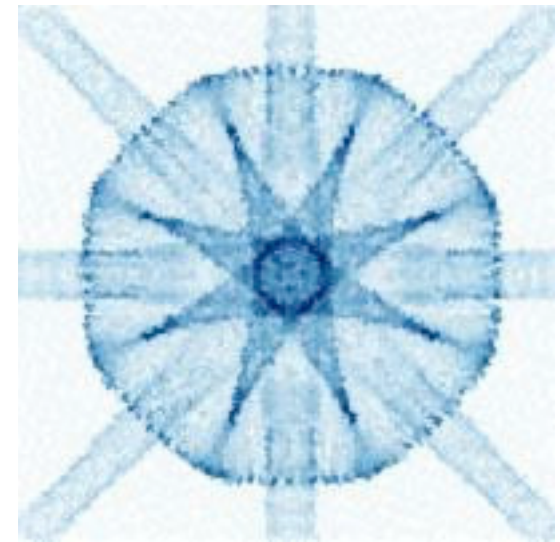


PH575 Spring 2009

Lecture #26 & 27

Phonons: Kittel Ch. 4 & 5



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POP QUIZ

Phonons are:

A. Fermions

B. Bosons

C. Lattice vibrations

D. Light/matter interactions

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POP QUIZ

Phonon dispersion relation:

- A. Same as electron  $E(k)$
- B. Different from electron  $E(k)$
- C.  $k$  undefined for phonons
- D. Linear  $E(k)$

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POP QUIZ

Phonons relevant to:

- A. Optical properties of solids
- B. Electrical properties of solids
- C. Thermal properties of solids
- D. Magnetic properties of solids

Until now, we have considered that nuclei in the solid are fixed in space - a good assumption at  $T = 0$ , but not otherwise. What extra energy does this motion add and what are the consequences?

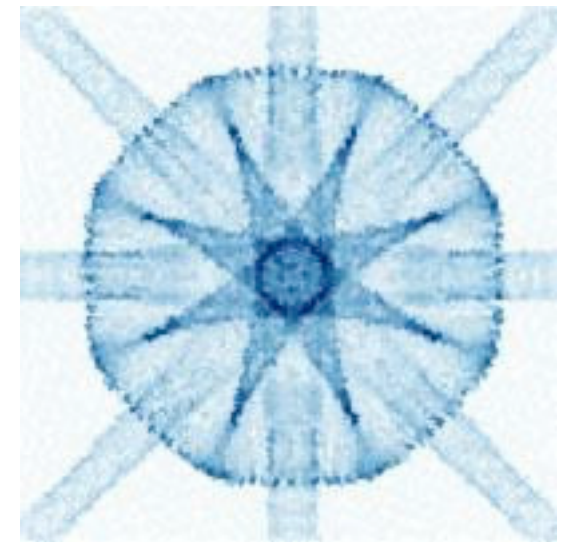
The overall nuclear motion can be organized into collective normal modes called phonons.

Phonons are partly responsible for **heat transport**.

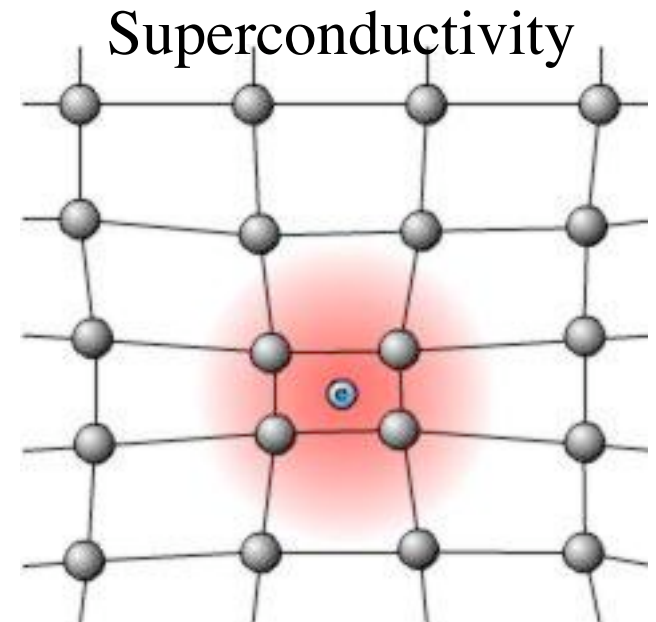
Phonons provide the interaction that yields a net attractive interaction between electrons to give **superconductivity**.

Phonons disrupt lattice periodicity and cause electrical resistivity.

And more .....



Phonon focussing



Superconductivity

Focus on one example: energy transport - calculate specific heat due to phonons. Start with total energy.

$$U(T) = \int_0^{\infty} D(E)_{\text{phonons}} E f(E, T)_{\text{phonons}} dE$$

What is this quantity?  
What do we need to know to  
find it?

What is this quantity?

What is this?

Occupation function:

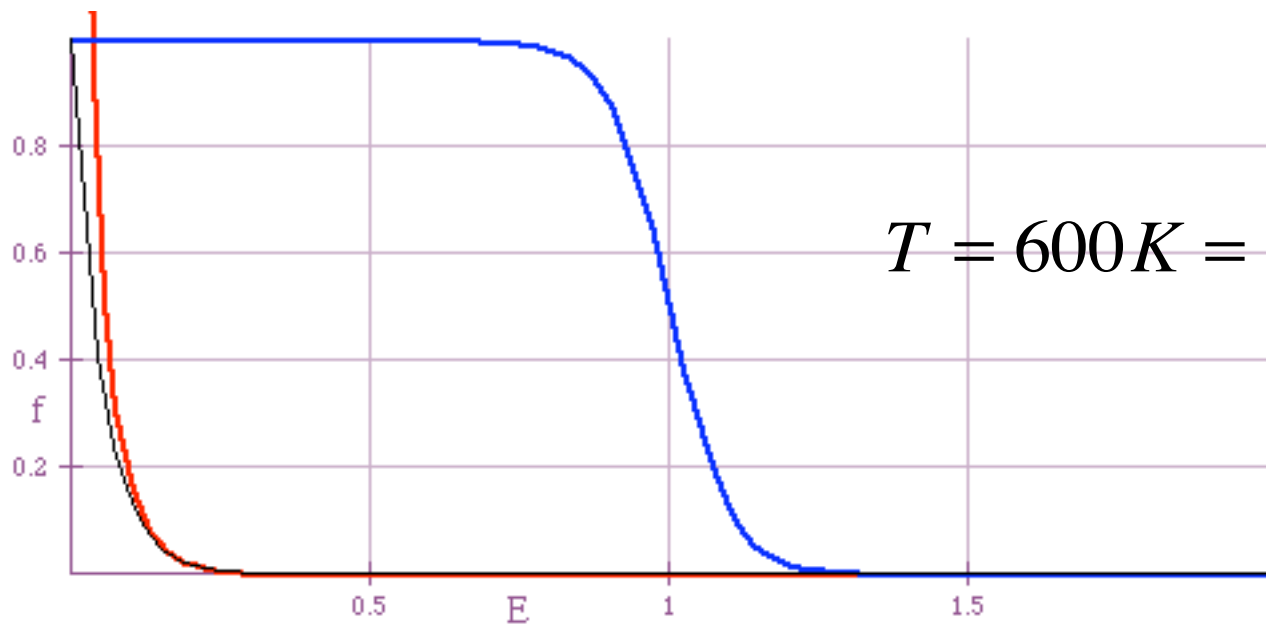
Each classical mode of frequency  $\omega_k$  is assumed to be a quantum particle or phonon with energy  $\hbar\omega_k/2\pi$ .

Phonons are BOSONS. Bosons have integer (or zero) spin. Like photons, phonons are massless. There is no restriction on the number in the same quantum state (the PEP does not apply).

Bosons occupy states with probability

$$f_{BE}(\omega) = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

$f_{BE}$  is called the Bose-Einstein function and it plays the same role as the Fermi function for electrons. Note that the “-1” in the denominator, and note also that there is nothing analogous to the Fermi energy for bosons.



$$T = 600\text{ K} = 327^\circ\text{C} = 0.05\text{ eV}$$

$$f_{BE}(\omega) = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

$$f_{FD}(\omega) = \frac{1}{e^{(\hbar\omega - 1\text{ eV})/k_B T} + 1}$$

$$f_{MB}(\omega) = e^{-\hbar\omega/k_B T}$$

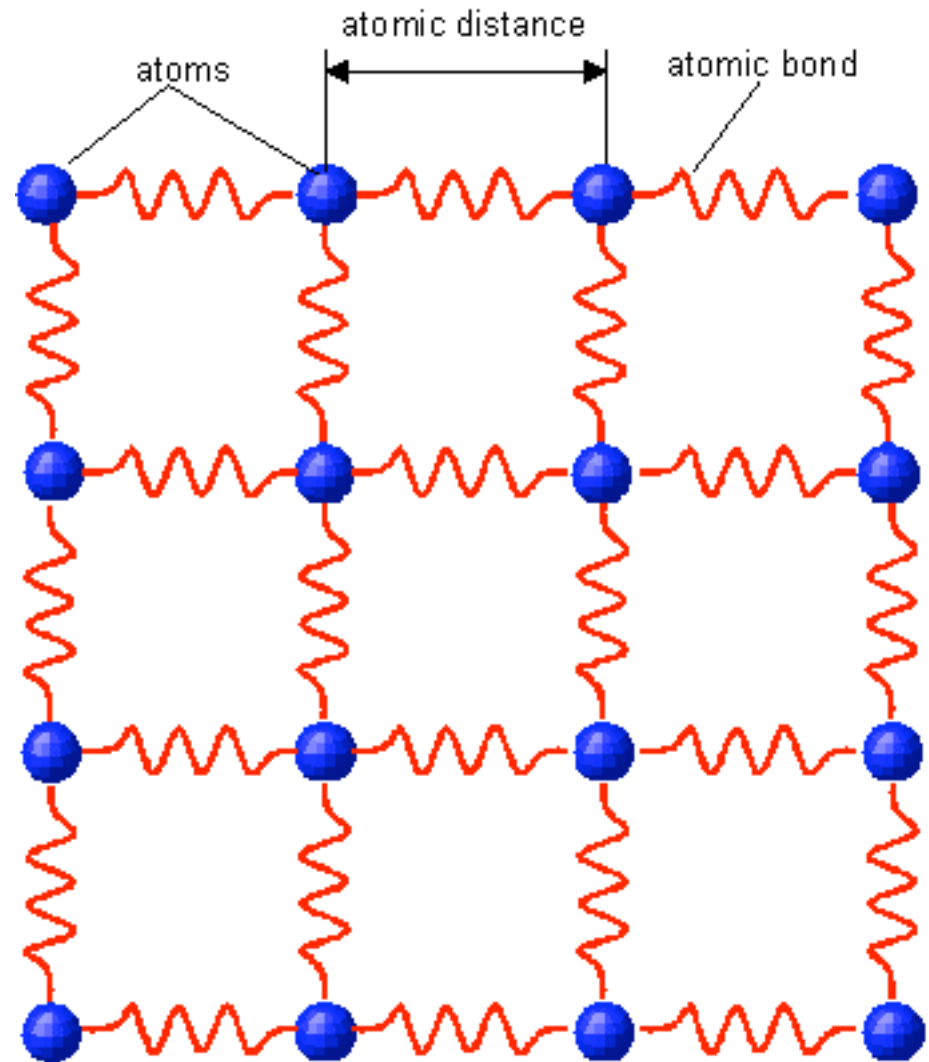
$f_{BE}$  is called the Bose-Einstein function and it plays the same role as the Fermi function for electrons. Note that the “-1” in the denominator, and note also that there is nothing analogous to the Fermi energy for bosons.



Phonon dispersion relation:

Use Newton's law to treat problem classically, but more refined quantum treatment yields similar results.

Positive ions coupled by springs. Individual spring force is characterized by vibration frequency,  $\omega_0$ , stiffness  $\kappa$ , mass  $m$ .

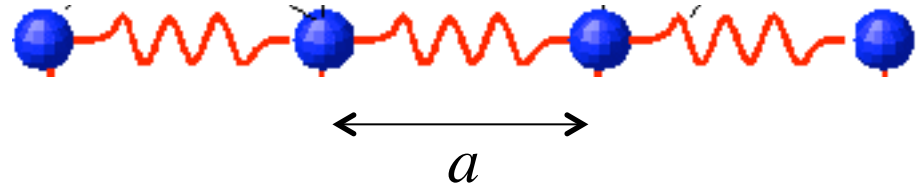


$$F = -\kappa(x - x_0) = -m\omega_0^2(x - x_0)$$

Phonon dispersion relation: 1-dimension for illustration.

Ions' equilibrium positions are  $pa$  where integer  $p$  labels ion, but each ion executes (mostly small) motion from equilibrium.

Displacement is denoted as  $x_p$ . In true 1-D, this motion would have to be along the spring direction (longitudinal).

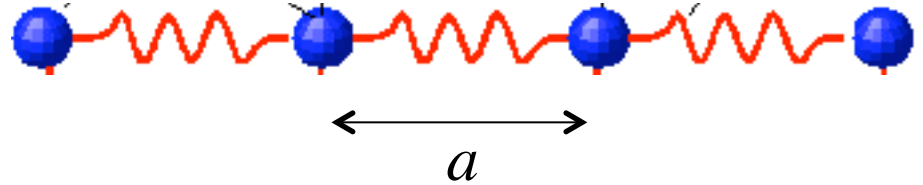


mass \* acceleration = force

$$\begin{aligned} m \frac{d^2 x_p}{dt^2} &= -m\omega_0^2 (x_p - x_{p-1}) - m\omega_0^2 (x_p - x_{p+1}) \\ &= -m\omega_0^2 (2x_p - x_{p-1} - x_{p+1}) \end{aligned}$$

Normal modes:  $x_p = A_k e^{ikpa} e^{i\omega_k t}$

Assumption! Discuss.  
Just like electron case.



$$x_p = A_k e^{ikpa} e^{i\omega_k t}$$

$$x_{p+1} = A_k e^{ik(p+1)a} e^{i\omega_k t}$$

$$x_{p-1} = A_k e^{ik(p-1)a} e^{i\omega_k t}$$

$$\frac{d^2 x_p}{dt^2} = -\omega_k^2 x_p \quad \text{Put this into} \quad m \frac{d^2 x_p}{dt^2} = -m\omega_0^2 (2x_p - x_{p-1} - x_{p+1})$$

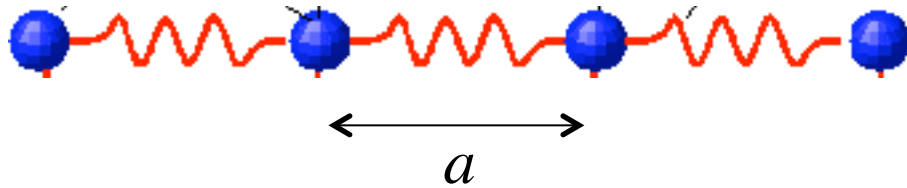
$$-m\omega_k^2 x_p = -m\omega_0^2 (2x_p - x_{p-1} - x_{p+1})$$

Now plug in expressions for  $x_p$ ,  $x_{p-1}$ ,  $x_{p+1}$ , lots of happy cancellations.

$$\omega_k^2 = \omega_0^2 (2 - e^{-ika} - e^{+ika}) = \omega_0^2 (2 - 2\cos(ka)) = 4\omega_0^2 \sin^2\left(\frac{ka}{2}\right)$$

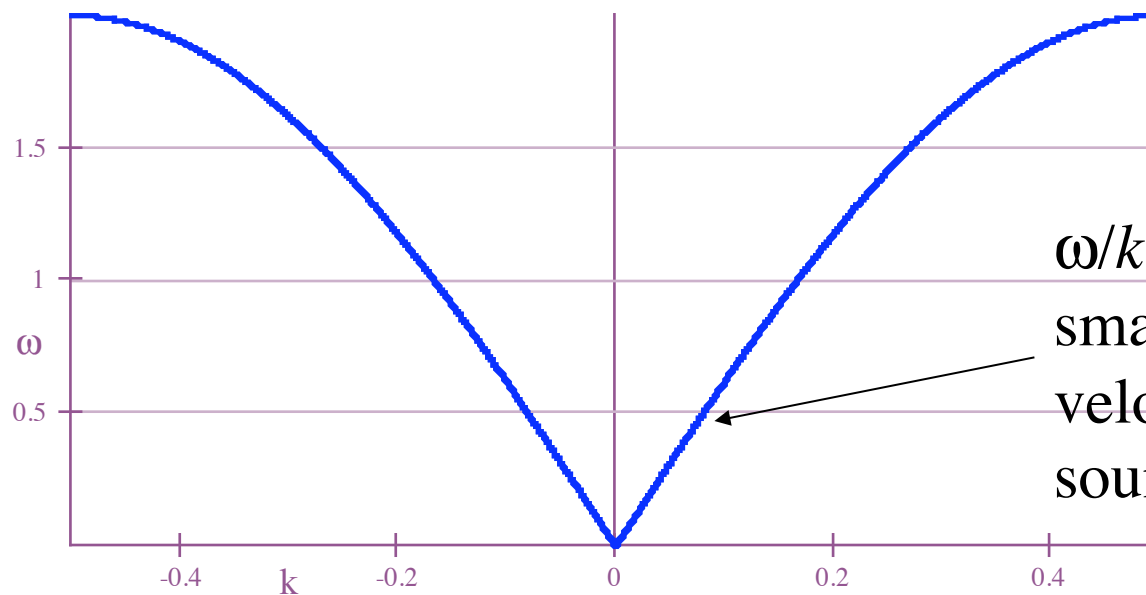
$$\omega_k = 2\omega_0 \sin\left(\frac{ka}{2}\right) \quad \leftarrow \text{Dispersion relation! } \omega(k)$$

# Phonon dispersion relation (1-D, periodic BCs)



$$\omega_k = 2\omega_0 \sin\left(\frac{ka}{2}\right)$$

Group velocity is zero at BZB



$\omega/k$  is constant at small  $k$ . This velocity is the sound velocity!

$k = -\pi/a$

$k = 0$

$k = \pi/a$



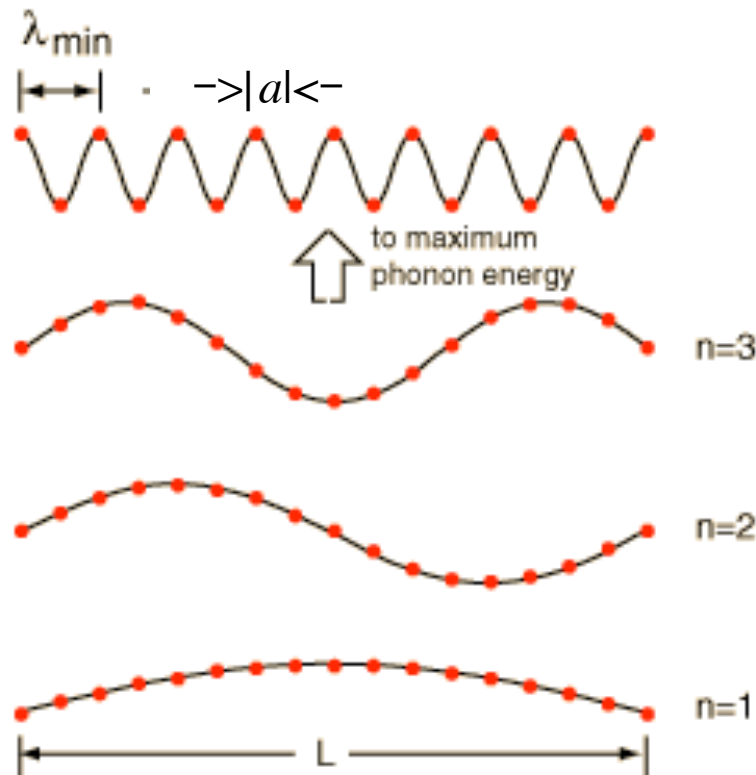
## Phonons & phonon dispersion relation:

Phonons are lattice vibrations (vibrations of heavy ions)

Simplest (“normal mode”) cases are depicted below

Any motion can be written as a superposition of the *normal modes*

The application of boundary conditions sets the quantization conditions



1-D crystal, length  $L$

$$\lambda_{\min} = 2a \quad k_{\max} = \frac{\pi}{a} = \frac{N\pi}{L}$$

$$\lambda_n = \frac{2L}{n} \quad k_n = \frac{n\pi}{L}$$

$$\lambda_{\max} = 2L \quad k_{\min} = \frac{\pi}{L}$$

Here's a good Java Applet that shows the different motions of a linear chain: <http://fermi.la.asu.edu/ccli/applets/phonon/phonon.html>

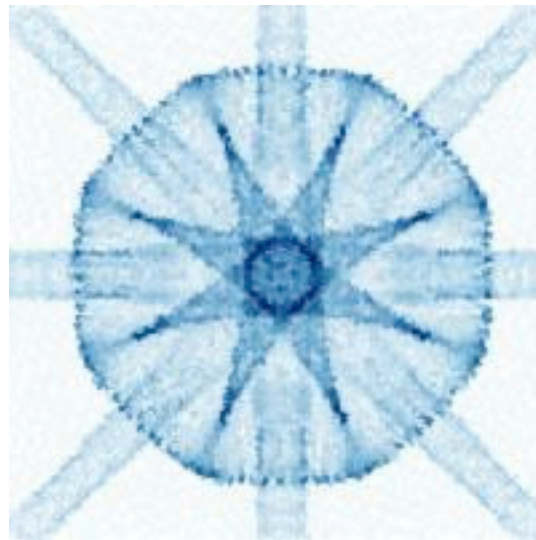
Dispersion relations and some more realistic phonon modes (including surface phonons) in real crystals: <http://www.phonon.fc.pl/index.php>

## Phonon dispersion relation (monatomic)

In 3 dimensions, there are 3 branches of the dispersion relation, 2 transverse and 1 longitudinal. Different crystal structures have different propagation speeds along different directions.

In a monatomic lattice, the phonon modes are called “acoustic” modes. The frequency  $\rightarrow 0$  as  $k \rightarrow 0$  and the speed of the low frequency propagation is the speed of sound.

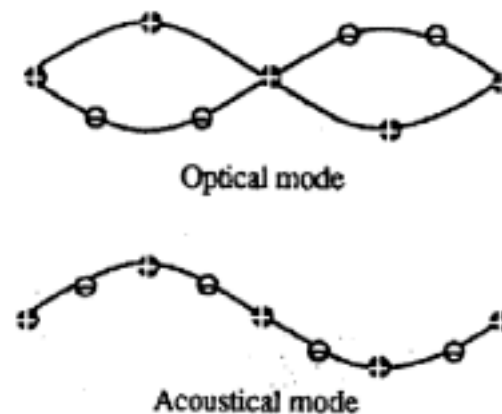
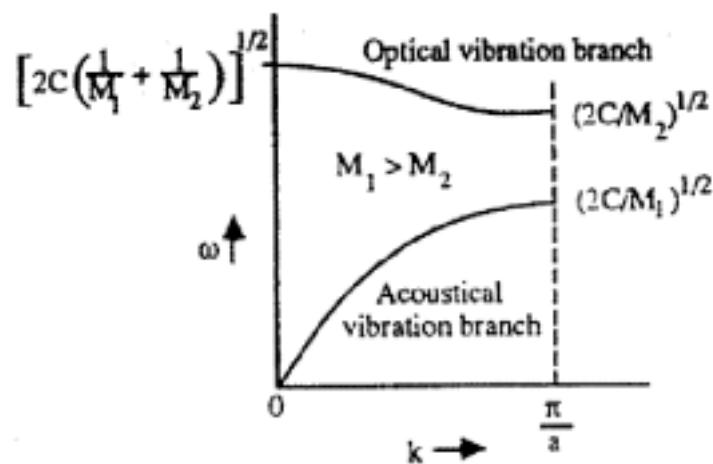
Phonon imaging:



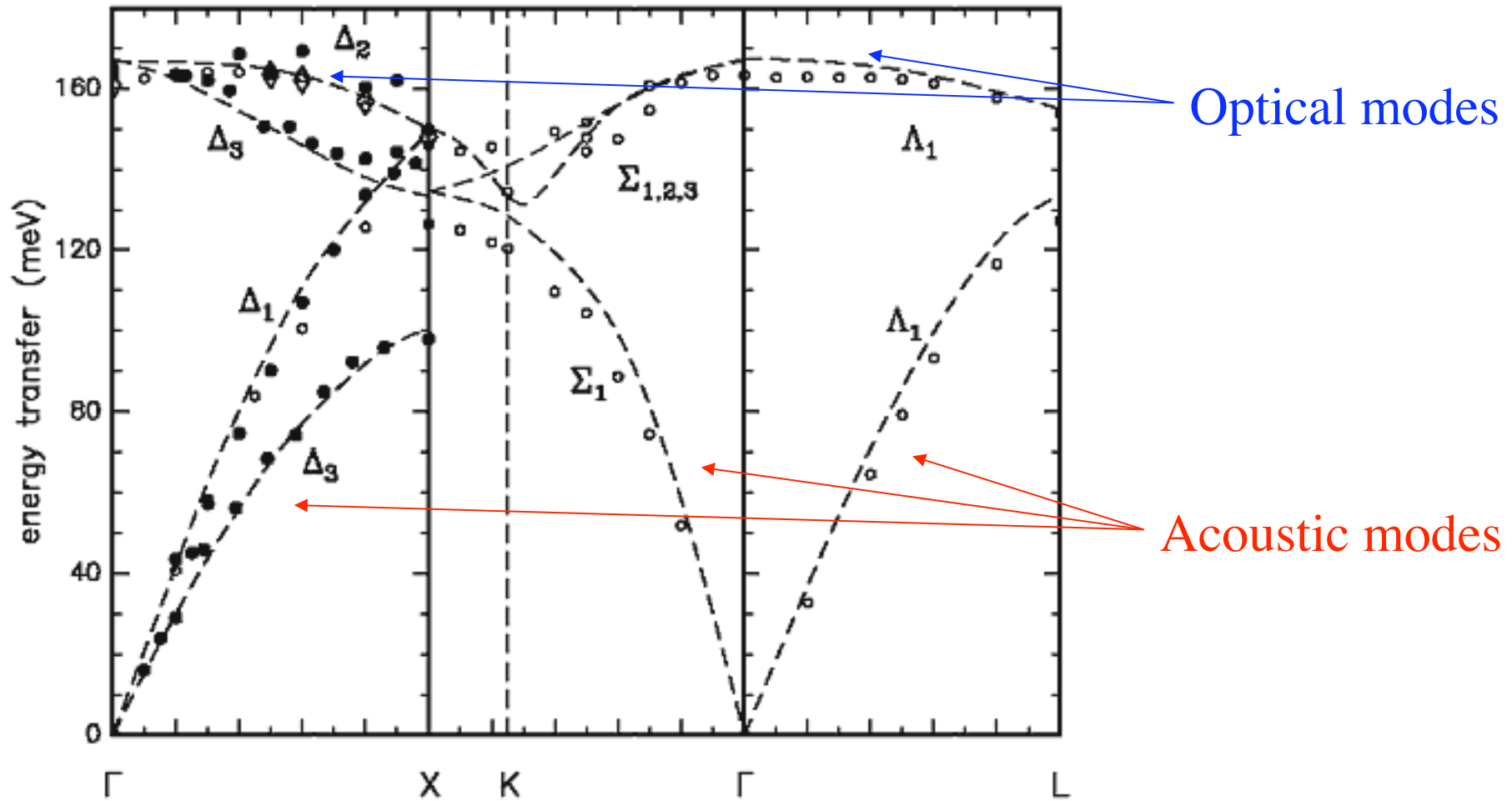
## Phonon dispersion relation (polyatomic)

In a polyatomic lattice, the phonon modes are both “acoustic” and “optical”.  $\omega_k \rightarrow 0$  as  $k \rightarrow 0$  for acoustic modes as before, but for optical modes  $\omega_k \rightarrow \text{constant}$  as  $k \rightarrow 0$ . There can be transverse and longitudinal modes of both types.

The origin of this effect is EXACTLY the same as we discussed for electron dispersion when we had 2 different types of atom, or 2 different coupling constants.







The phonon dispersion relation can be measured experimentally by inelastic X-ray or neutron scattering

Figure 6. Phonon dispersion curves for the longitudinal and the transverse modes in diamond as obtained with X-ray scattering by Burkel (1991), by Röll and Burkel (1993) and Schwoerer-Böhning et al (1998). The results are shown together with a shell-model from the literature (Warren, Yarnell, Dolling and Cowley 1967).

Density of states:

We again recall the treatment for electrons.

Periodic boundary conditions:  $k = 0, \pm 2\pi/L, \pm 4\pi/L, \dots$

In 1-D  $k$  space, there is 1 allowed mode per  $(2\pi/L)$  “ $k$ -volume”.

$$D(\omega) = D(k) \frac{dk}{d\omega} = \frac{L}{2\pi} \frac{dk}{d\omega}$$

$$\omega(k) = 2\omega_0 \sin\left(\frac{ka}{2}\right)$$

$$\frac{d\omega}{dk} = \omega_0 a \cos\left(\frac{ka}{2}\right) \xrightarrow{k \rightarrow 0} \omega_0 a$$

$$D(\omega) = \frac{L}{2\pi} \frac{1}{\omega_0 a \cos(ka/2)}$$

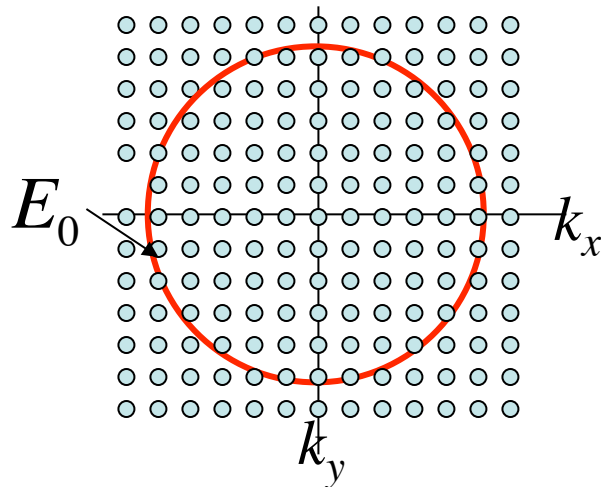
Density of states:

In 3-d  $k$  space, there is 1 allowed mode per  $(2\pi/L)^3$  “ $k$ -volume”.

Total number of modes  $S$  in a sphere of radius  $k$  is

$S = (4\pi k^3/3) / (2\pi/L)^3$  for EACH of longitudinal and transverse type and for each branch

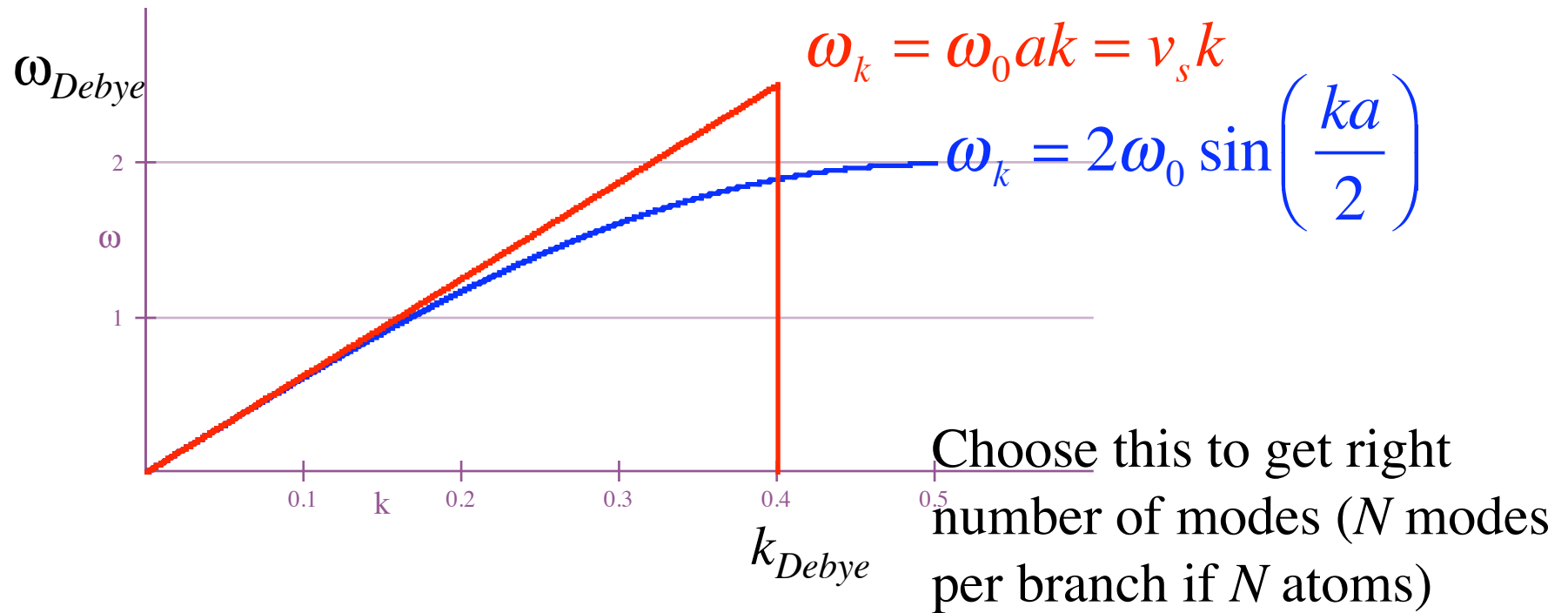
The density of states is (for each polarization)



$$D(\omega) = \frac{dS}{d\omega} = \frac{Vk^2}{2\pi^2} \frac{dk}{d\omega}$$

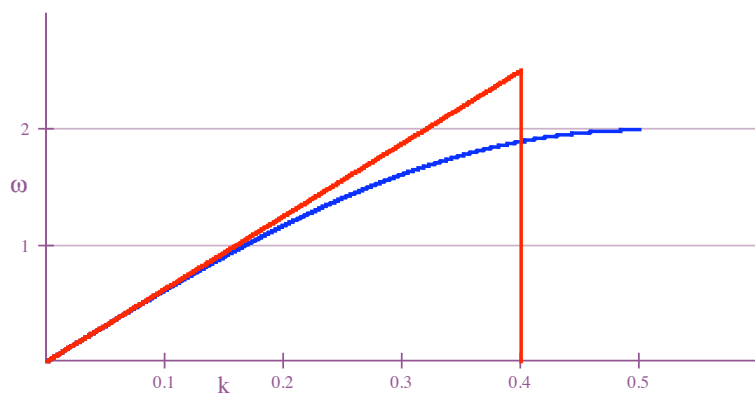
$$\omega(k) = 2\omega_0 \sin\left(\frac{ka}{2}\right)$$

The Debye model assumes the linear relation holds for all  $k$  to a maximum  $k_D$  or maximum  $\omega_D$  called the “Debye wavevector or Debye frequency”



$$D(\omega) = \frac{V k^2}{2\pi^2} \frac{dk}{d\omega} \quad \frac{d\omega}{dk} = v_s \quad D(\omega) = \frac{V k^2}{2\pi^2 v_s} = \frac{V \omega^2}{2\pi^2 v_s^3}$$

Let's calculate the Debye frequency, Debye temperature etc.



$$\omega_k = \omega_0 a k = v_s k \quad \frac{d\omega}{dk} = v_s$$

Number of modes (per branch) is  $N$  if there are  $N$  cells

$$N = \int_0^{\omega_D} D(\omega) d\omega$$

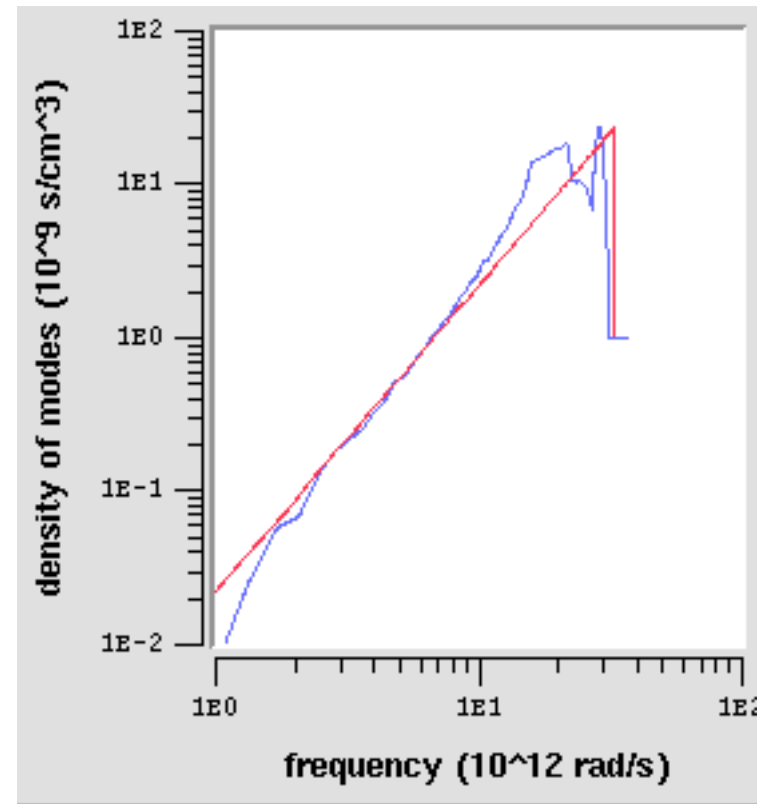
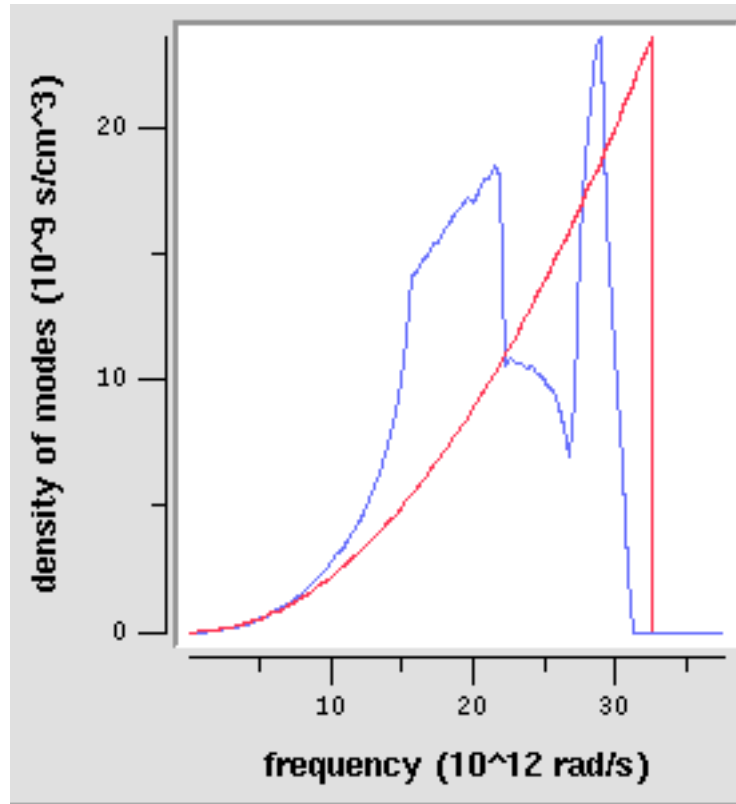
Quick class calc ... show

$$\omega_D = \left[ \frac{6\pi^2 v_s^3 N}{V} \right]^{1/3}$$

Define Debye temperature

$$\theta_{Debye} \equiv \frac{\hbar \omega_D}{k_B}$$

**Debye model** is useful, but only an approximation - nowadays, **computers** can crank out numerics very easily.



"debye" samples the reciprocal space randomly, calculates the 3 phonon frequencies associated with each sampled point, and develops a density of modes histogram. The density of modes (in blue) may be displayed either in a linear plot (left) or a log/log plot (right). A density of modes given by the Debye model (in red) is shown for comparison.

Debye model of specific heat:

$$C = \frac{dU}{dT}$$

$$C = 9Nk_B \left( \frac{T}{\theta_D} \right)^3 \int_0^{x_D} dx \frac{x^4 e^x}{(e^x - 1)^2}$$

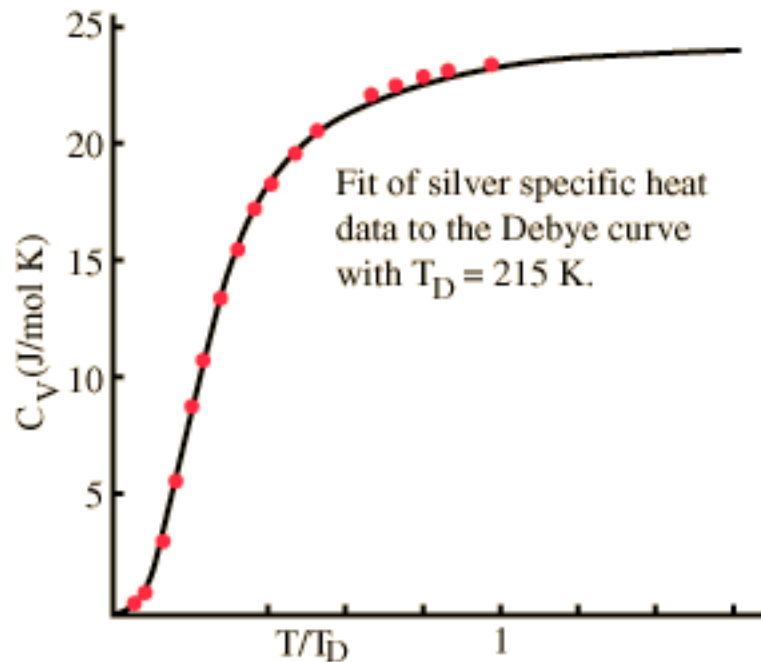
$C$  prop. to  $T^3$  at low temp ( $\ll \theta_D$ ),

$C$  constant at high temp ( $> \theta_D$ )

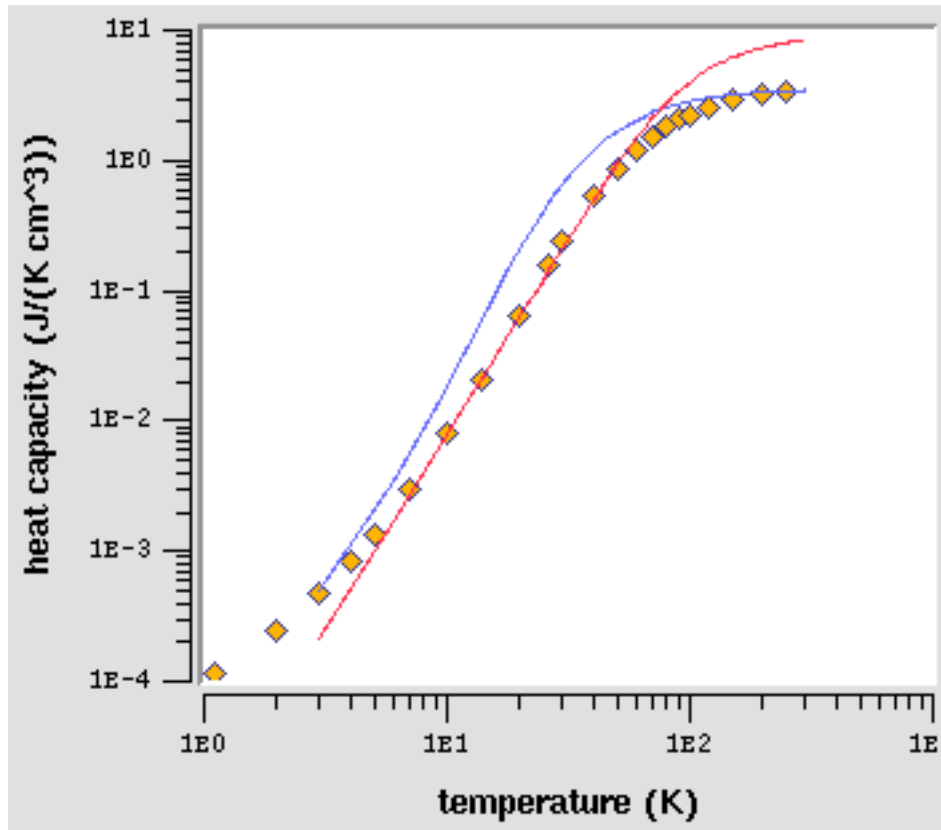
Na: 158 K, Si: 645 K,

$C_{\text{dia}}$ : 2230 K

Debye temp measures sound speed or bond stiffness.



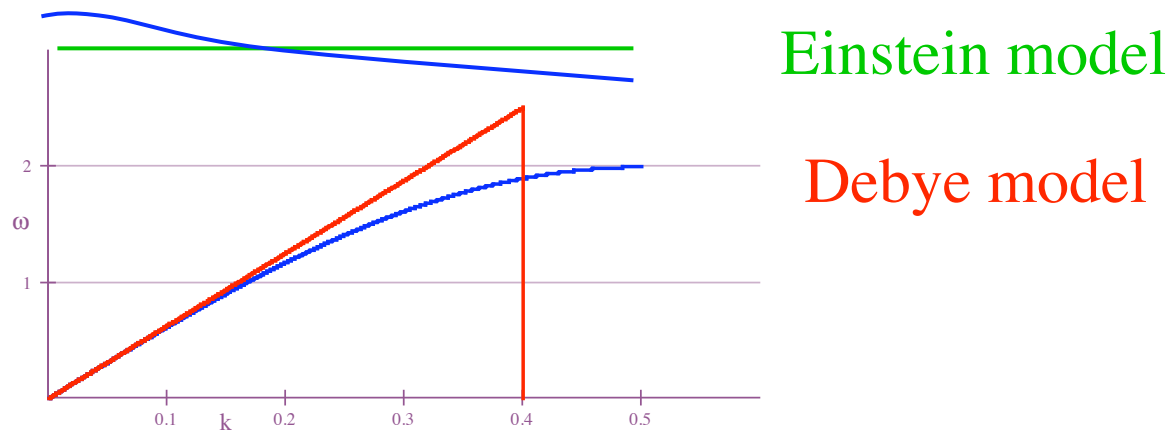
The data for silver shown is from Meyers. It shows that the specific heat fits the Debye model at both low and high temperatures.



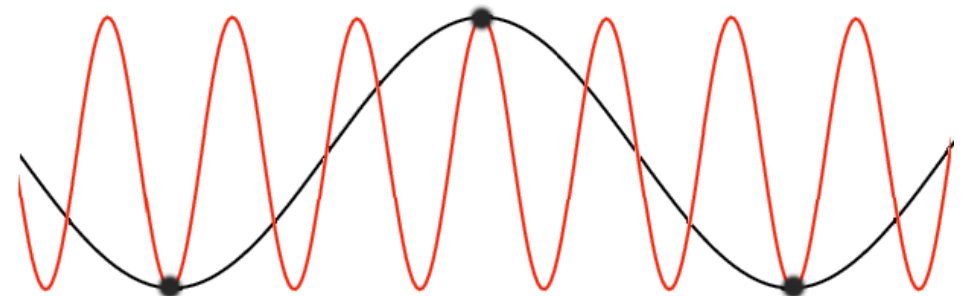
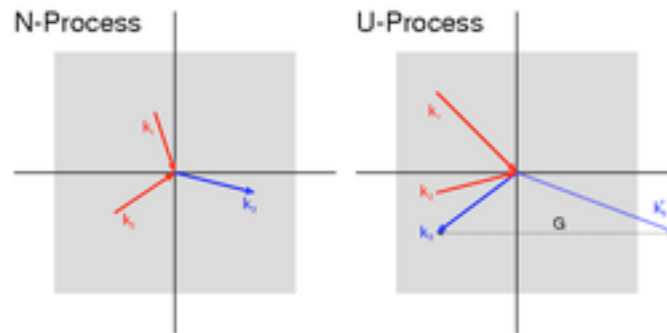
From the density of states, the specific heat is calculated, is displayed, and can be compared with experimental data and with a Debye model calculation. In the log/log plot, the wrong force constant was chosen for the numerical calculation (in blue). Should it be increased or decreased, and by what factor? For the Debye model (in red), the wrong lattice constant was chosen! Should it be larger or smaller, and by what factor?



Another important model of the phonon density of states is the Einstein model. This model works well for optical modes. Einstein model says all phonons have the same frequency!



“Normal” phonon collisions that conserve  $k$ -momentum (crystal momentum) do not allow relaxation (N-processes), but “Umklapp processes” (U-processes) do allow relaxation and limit thermal conductivity. This is because the medium is discrete, and  $k$ -values outside the 1<sup>st</sup> BZB can be mapped back into the 1<sup>st</sup> BZB with a reciprocal lattice vector.



[http://vatlieu.us/definition/methods.html?view=mediawiki&article=Umklapp\\_scattering](http://vatlieu.us/definition/methods.html?view=mediawiki&article=Umklapp_scattering)