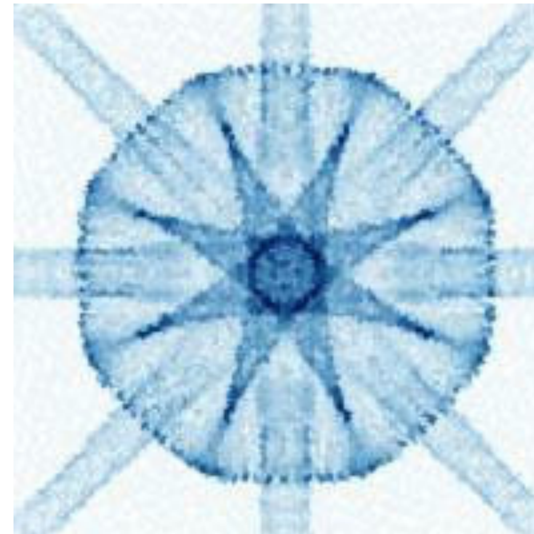
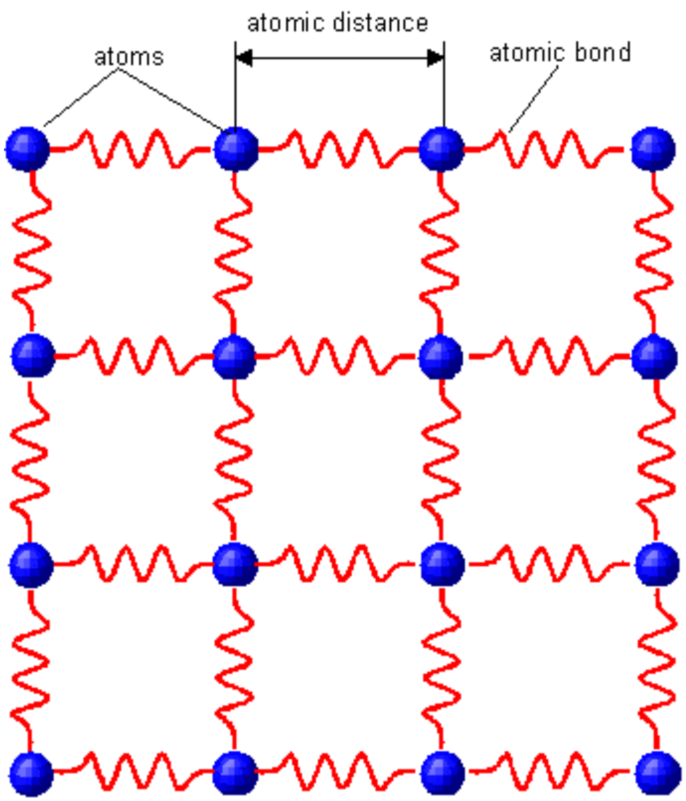
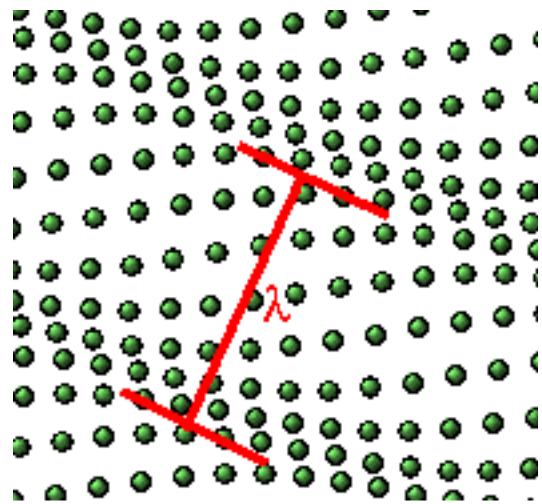
PH575 Spring 2019

Lecture #26 & 27

Phonons: Kittel Ch. 4 & 5







PH575 POP QUIZ

Is a phonons a:

A. Fermion?

B. Boson?

C. Lattice vibration?

D. Light/matter interaction?

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What does it mean for a phonons to be:

A. Longitudinal?
B. Transverse?
C. Acoustic?
D. Optic?

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The phonon dispersion relation is:

A. The same as the electron $E(k)$

B. Different from the electron $E(k)$

C. Undefined because there is no "k" for phonons

D. A linear $E(k)$

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Give an example of where phonons are relevant to:

A. Optical properties of solids
B. Electrical properties of solids
C. Thermal properties of solids
D. (Magnetic properties of solids?)

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What is an “umklapp” process?
How do phonons determine electrical resistivity?

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?

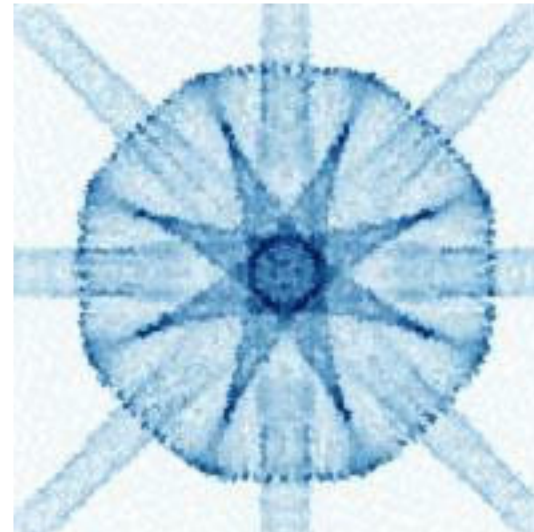
The overall nuclear motion can be organized into collective normal modes called phonons.

Phonons are partly responsible for heat transport.

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

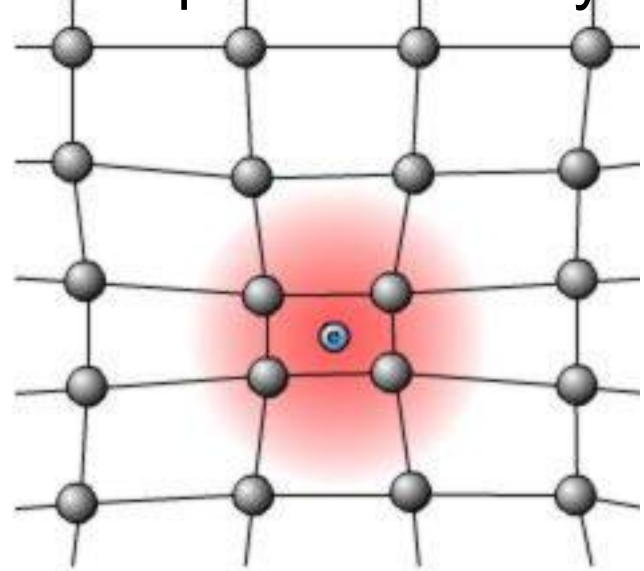
Phonons disrupt lattice periodicity and cause electrical resistivity.

And more ….



Phonon focussing

Superconductivity

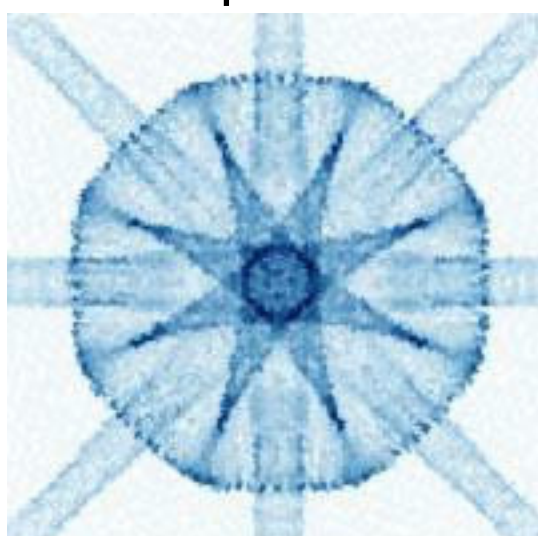


Phonon dispersion relation (monatomic)

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 -> 0 as k -> 0 and the speed of the low frequency propagation is the speed of sound.

Phonon imaging:



Java Applet that shows the different motions of a linear chain
http://fermi.la.asu.edu/ccli/applets/phonon/phonon.html

What is the difference between optic and acoustic?
Explore large and small *ka*.
Explore different mass ratios.

Dispersion relations and some more realistic phonon modes in real crystals: https://henriquemiranda.github.io/phononwebsite/phonon.html
(click on high symmetry points in dispersion relation)
Graphene: Explore differences between acoustic and optical
NaF: Explore differences between transverse and longitudinal

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

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

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

What is this?

What is this quantity?

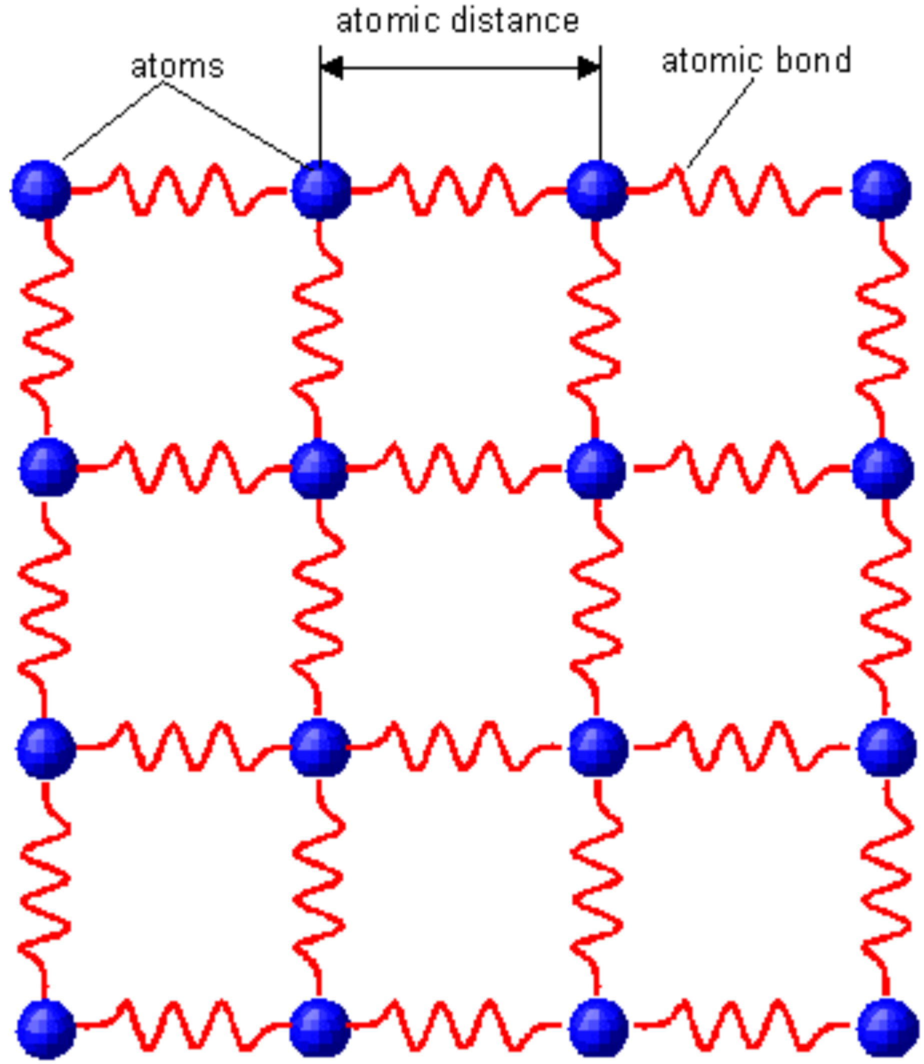
Phonon occupation number

- Each classical mode of frequency ω_k is assumed to be a quantum particle or phonon with energy $h\omega_k/2\pi$.
- Phonons are BOSONS – integer or zero spin.
- f_{BE} : Bose-Einstein function plays the same role as the Fermi function for electrons.

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

- No restriction on the number in the same quantum state (the PEP does not apply).
- In classical regime, E-μ>>kT, identical to Maxwell-Boltzmann distribution and occupation <<1
- In quantum regime, occupation can be >>1
- Phonons are massless, like photons

Phonon dispersion relation:

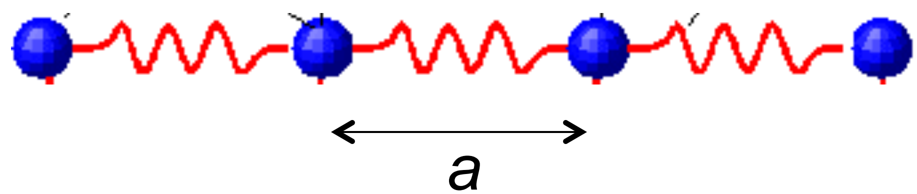


Use Newton's law to treat problem classically, but more refined quantum treatment yields similar results.

Positive ions coupled by springs. Individual spring force is characterized by vibration frequency, ω_0, stiffness κ, mass m.

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

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

$$m\frac{d^2x_p}{dt^2} = -m\omega_0^2\left(x_p - x_{p-1}\right) - m\omega_0^2\left(x_p - x_{p+1}\right)$$

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

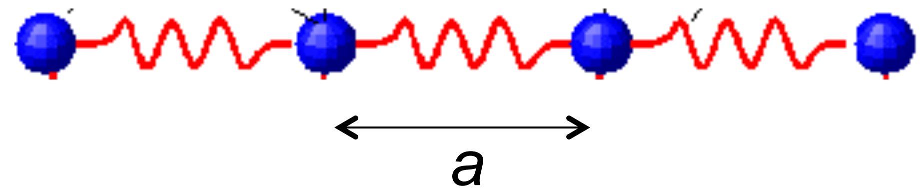
Normal modes: $x_p = A_k e^{ikpa} e^{i\omega_k t}$

Discuss normal modes.

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

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

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



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

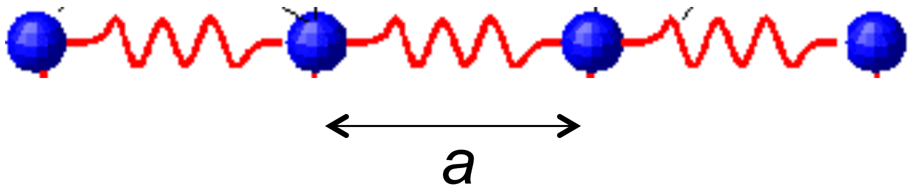
$$-m\omega_k^2 x_p = -m\omega_0^2\left(2x_p - x_{p-1} - x_{p+1}\right)$$

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

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

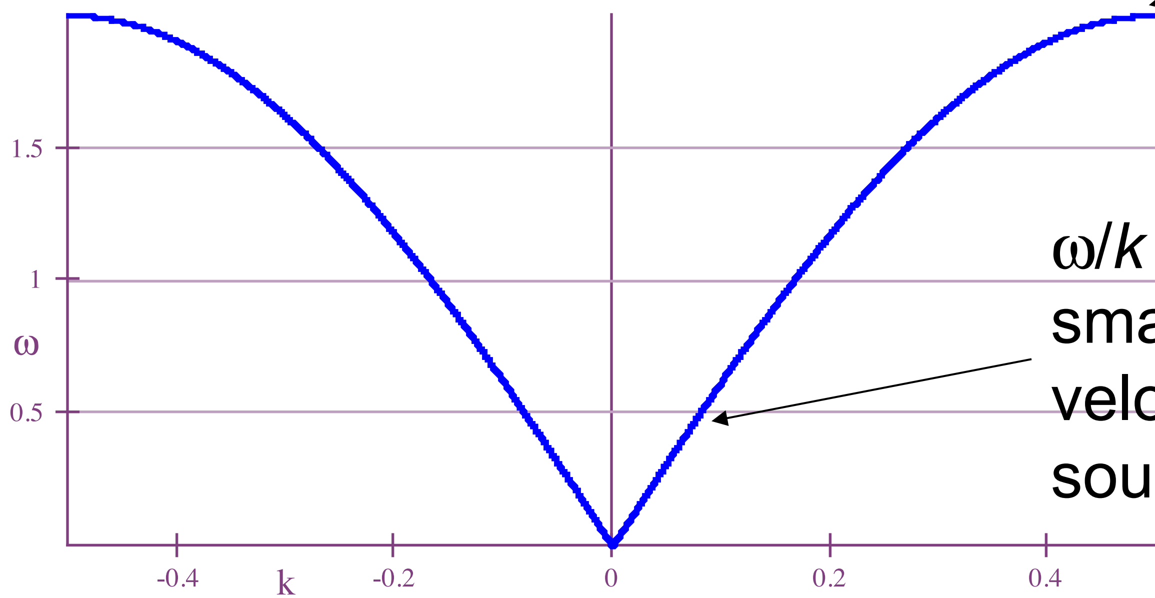
$$\omega_k = 2\omega_0 \sin\left(\frac{ka}{2}\right)$$ <-- Dispersion relation! $\omega(k)$

Phonon dispersion relation (1-D, periodic BCs)



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

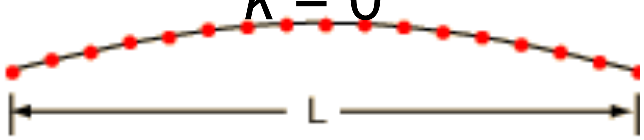
Group velocity is zero at BZB



ω/k is constant at small k. This velocity is the sound velocity!

$k = -\pi/a$

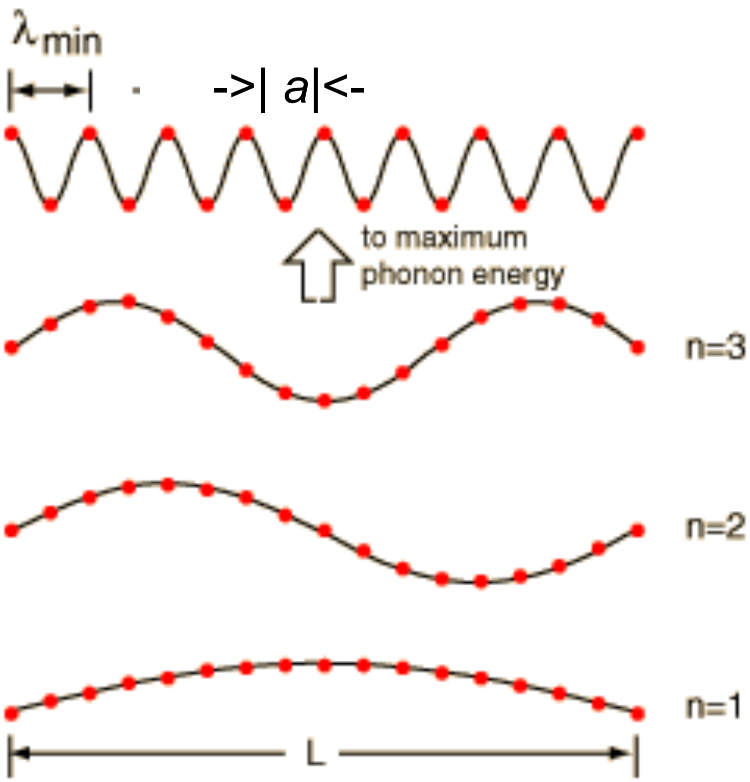
$k = 0$



$k = \pi/a$

<u>Phonons & phonon dispersion relation:</u>

Phonons are lattice vibrations (vibrations of heavy ions)
Simplest ("normal mode") cases are depicted below
Any motion is a superposition of the *normal modes*
Boundary conditions set the quantization conditions



1-D crystal, length *L*

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

$\lambda_n = \frac{2L}{n}$ $$k_{\mathrm{n}} = \frac{n\pi}{L}$$

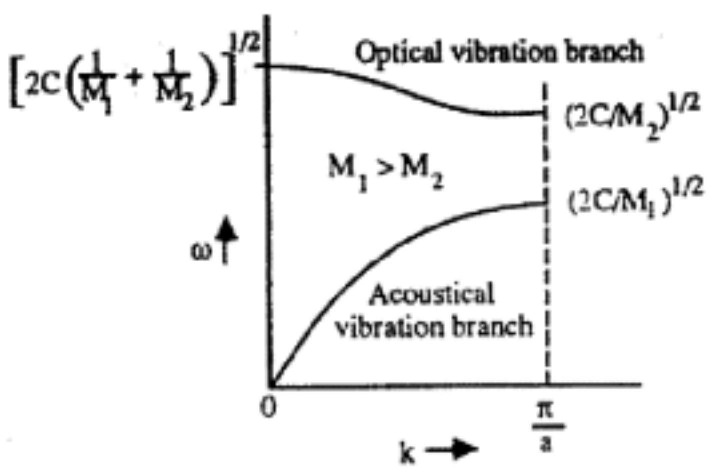
$\lambda_{max} = 2L$ $$k_{\min} = \frac{\pi}{L}$$

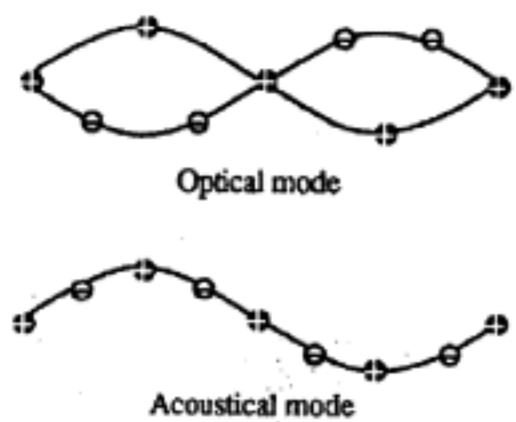
http://hyperphysics.phy-astr.gsu.edu/hbase/solids/imgsol/phonon.gif

Phonon dispersion relation (polyatomic)

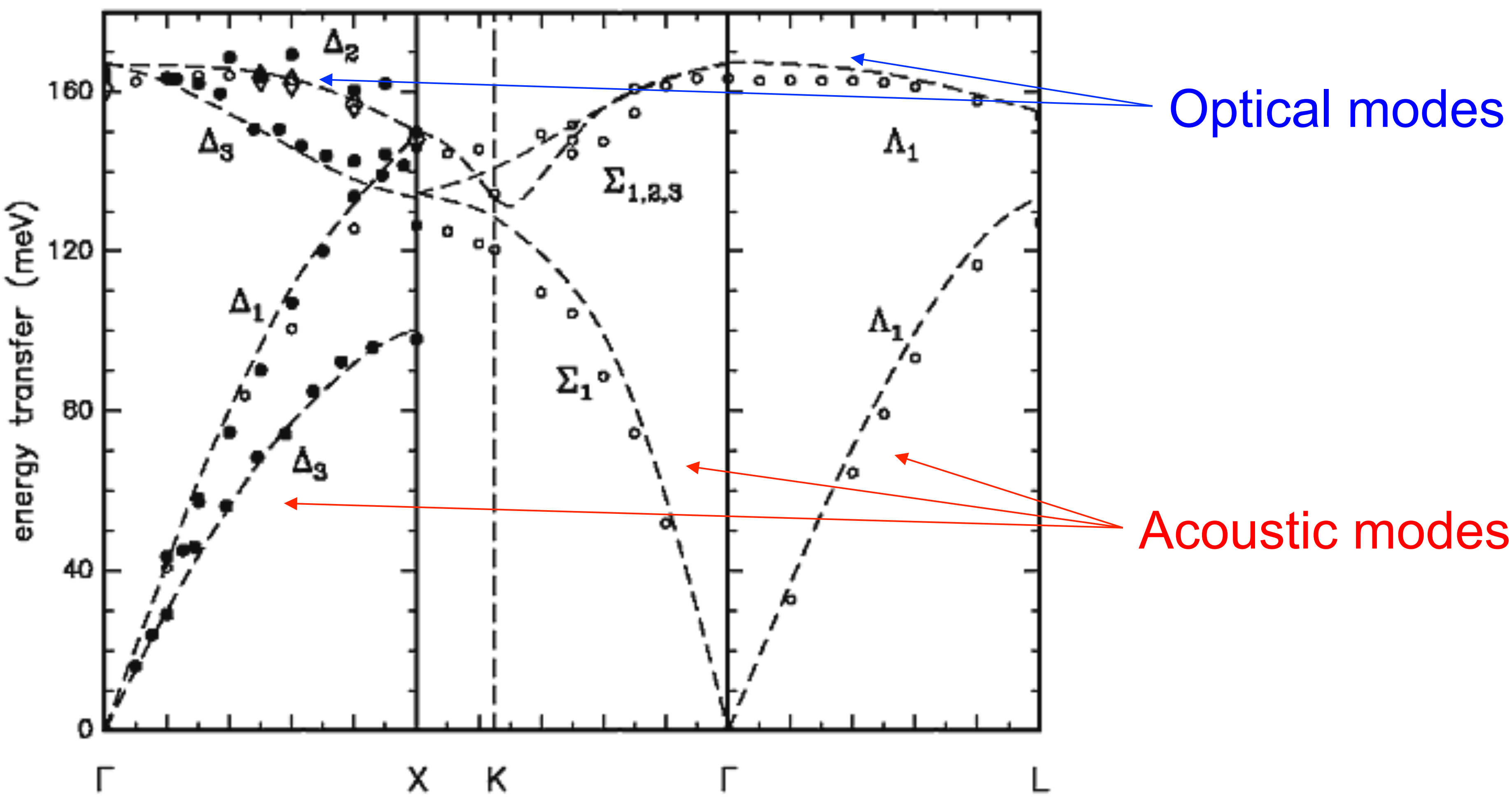
In a polyatomic lattice, the phonon modes are both "acoustic" and "optical". ω_k -> 0 as k -> 0 for acoustic modes as before, but for optical modes ω_k-> constant as k -> 0. There can be transverse and longitudinal modes of both types.

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.





http://edu.ioffe.ru/register/?doc=galperin/l2pdf2.tex



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

http://www.physik1.uni-rostock.de/user/radtke/Course_I/Chapter_IV/II_Chap4_2.html

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 t from the literature (Warren, Yarnell, Dolling and Cowley 1967).

Density of states:
We again recall the treatment for electrons.
Periodic boundary conditions: $k = 0, \pm 2\pi/L, \pm 4\pi/L, \ldots.$
In 1-D k space, there is 1 allowed mode per ($2\pi/L$) "k-volume".

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

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

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

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

Density of states:

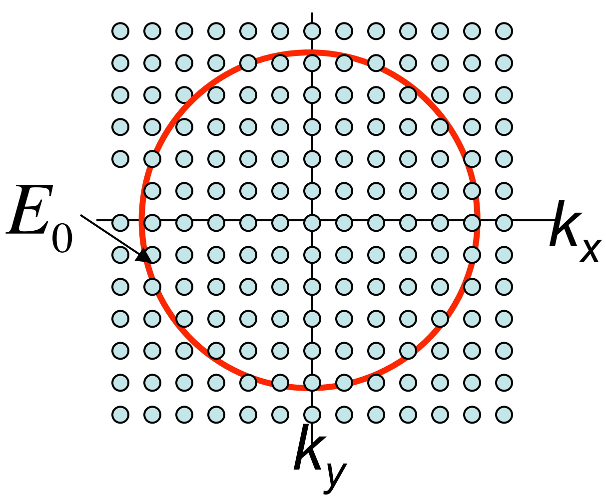
In 3-d k space, there is 1 allowed mode per $(2\pi/L)^3$ "k-volume".

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

$$S = \frac{\text{Vol k-space}}{\text{Vol k-space per mode}} = \frac{\frac{4}{3}\pi k^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{Vk^3}{6\pi^2}$$

for EACH longitudinal and transverse type and for each branch

The density of states is (for each polarization)

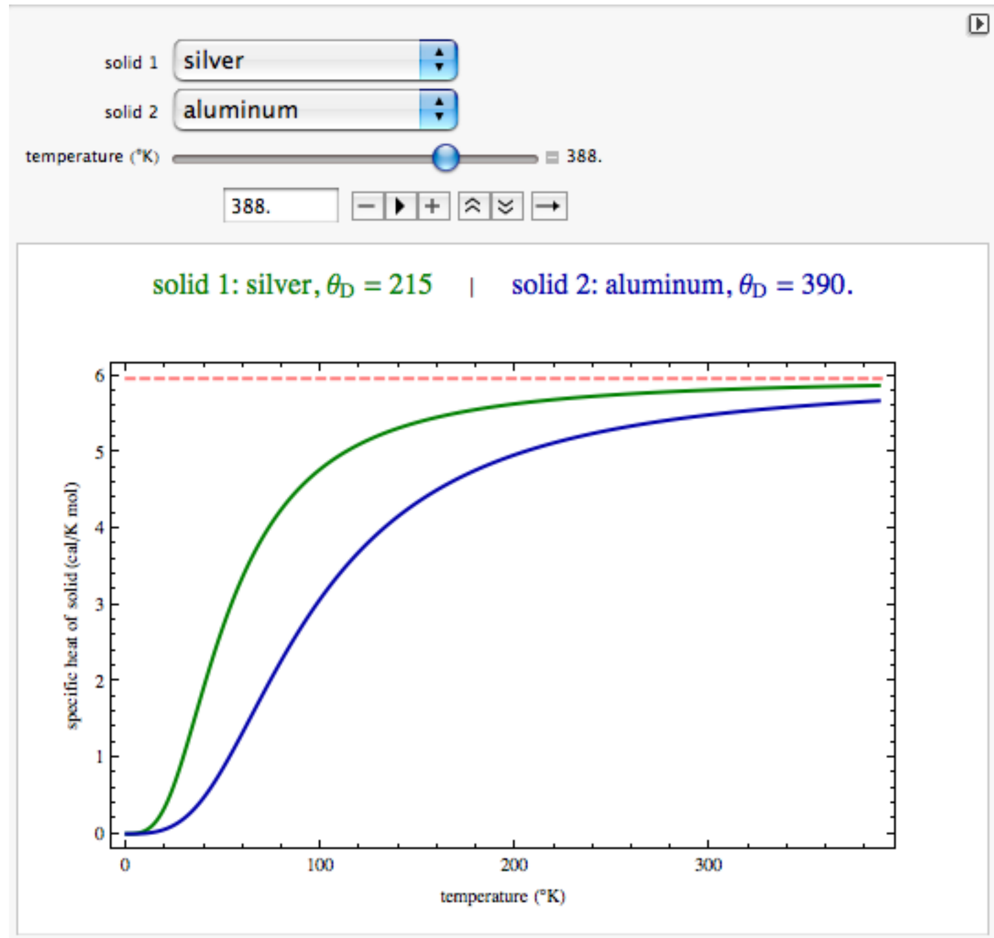


$$D(\omega) = \frac{dS}{d\omega} = \frac{dS}{dk}\frac{dk}{d\omega} = \frac{Vk^2}{2\pi^2}\frac{dk}{d\omega}$$

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

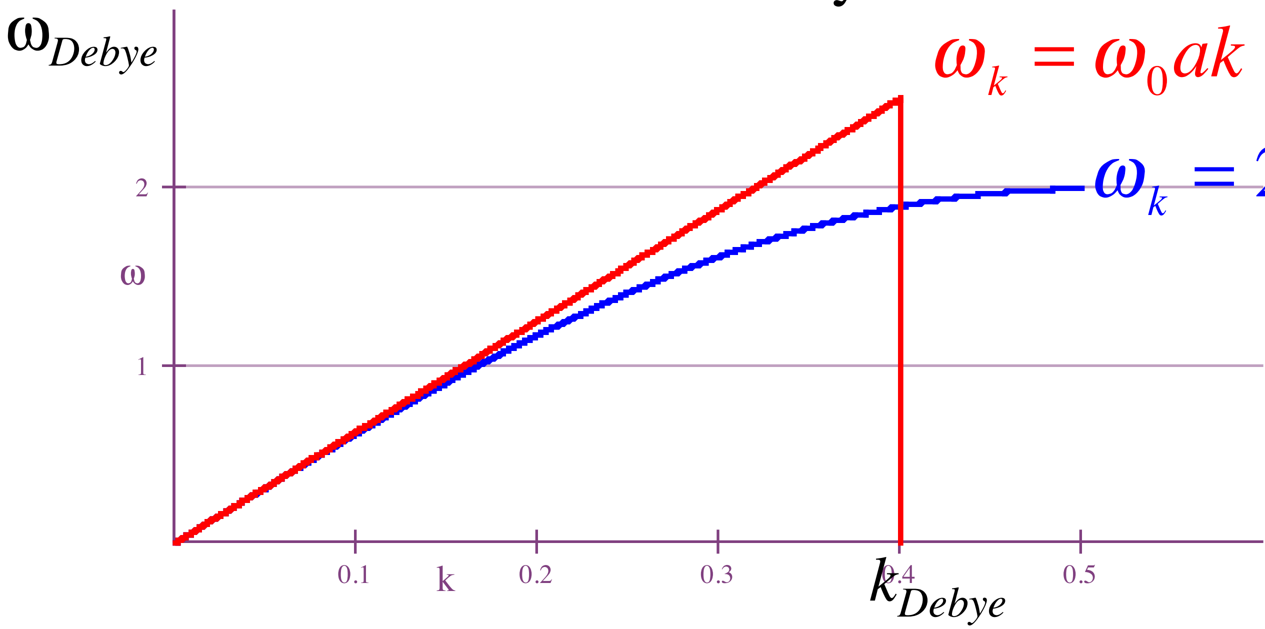
The Debye model assumes the linear relation holds for all k to a maximum k_D (Debye wave vector) or maximum ω_D (Debye frequency). Can also define T_D or θ_D (Debye temperature).

Peter Debye
(1884 –1966)
http://en.wikipedia.org/wiki/Peter_Debye



http://demonstrations.wolfram.com/HeatCapacityOfSolidsInTheDebyeApproximation/

Debye Model



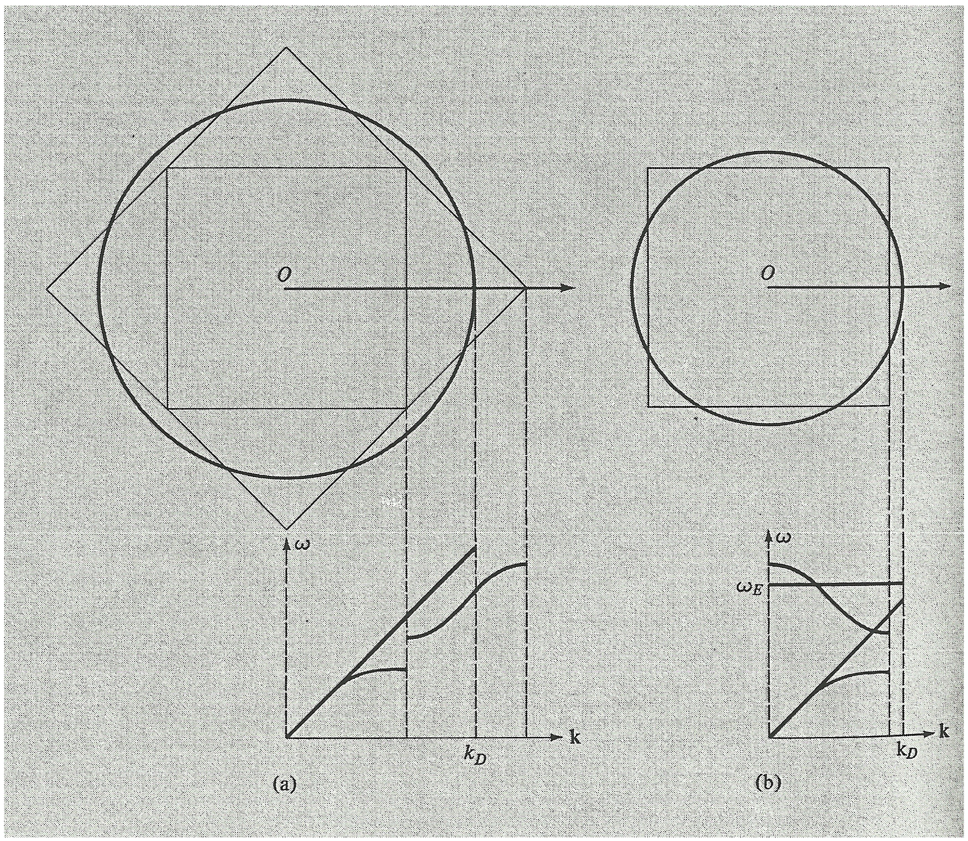
$$\omega_k = \omega_0 a k = v_s k$$

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

$$\omega_D = \left[\frac{6\pi^2 v_s^3 N}{V}\right]^{1/3} \qquad \theta_{Debye} \equiv \frac{\hbar\omega_D}{k_B}$$

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

The Debye model assumes the linear relation holds for all *k* to a maximum k_D (Debye wave vector) or maximum ω_D (Debye frequency).
(Einstein model uses flat dispersion for optical branch – hwk.)



Choose k_D to get correct number of modes (*N* modes per branch if *N* atoms)

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

$$\theta_D = \frac{\hbar\omega_D}{k_B} = \frac{h v_s}{2k_B}\sqrt{\frac{6N}{\pi V}}$$

Zero Temperature limit

$$E_{TOT} = E_{ZeroPt} + \frac{V}{2\pi^2 v_s^2} \int_0^\infty \left(\frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} \right) \omega^2 \, d\omega$$

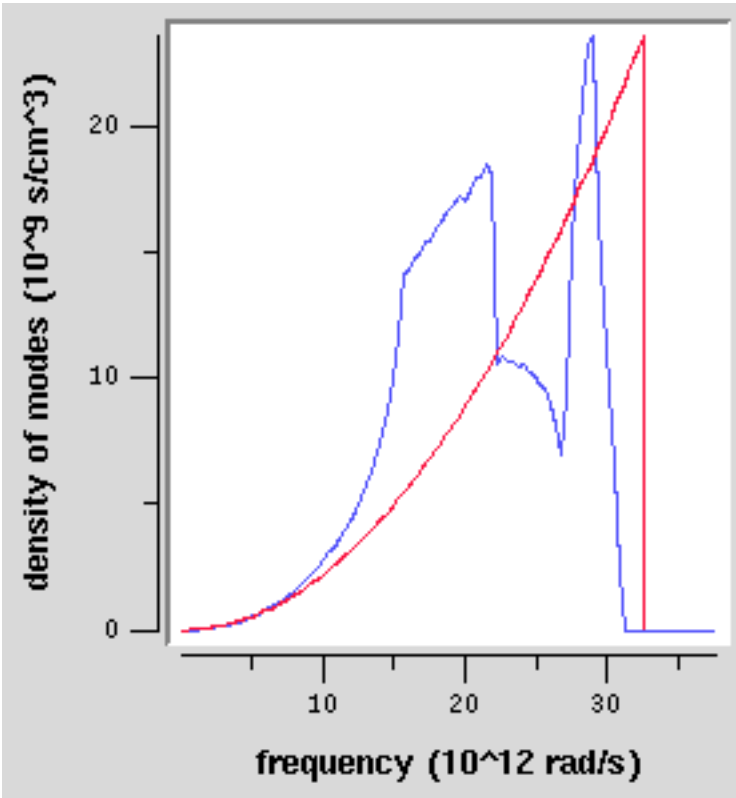
$$E_{TOT} = E_{ZeroPt} + \frac{V}{2\pi^2 v_s^3} \frac{\left(k_B T\right)^4}{\hbar^3} \int_0^\infty \left(\frac{x^3}{e^x - 1} \right) dx$$

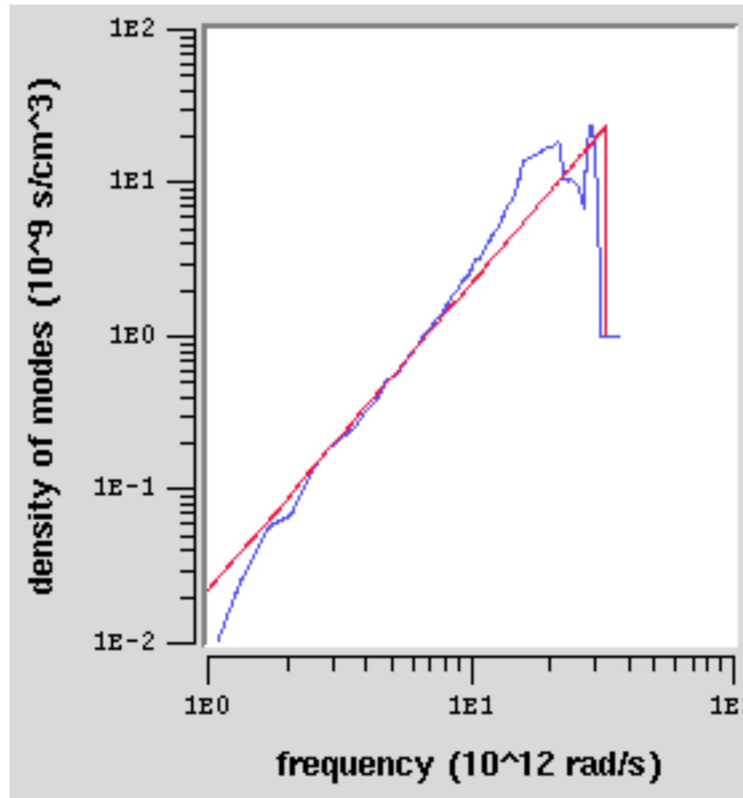
$$C = \frac{2V\pi^2}{15 v_s^3} \frac{\left(k_B T\right)^3}{\hbar^3}$$

Debye T^3 law at low temperatures

$$\frac{C}{N k_B} = \frac{12\pi^4}{5} \left(\frac{T}{\theta_D} \right)^3$$

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





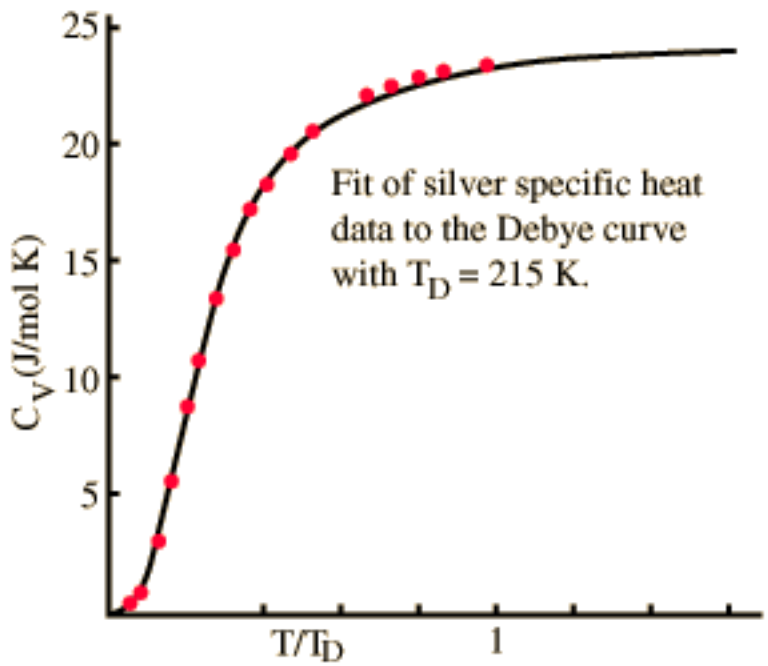
"debye" samples the reciprocal space randomly, calculates the 3 phonon frequencies associated with each sampled point, and develops a density of modes histogram. The density of modes (in blue) may be displayed either in a linear plot (left) or a log/log plot (right). A density of modes given by the Debye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

http://www.physics.cornell.edu/sss/debye/debye.html

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

Debye model of specific heat: similar to low T limit before (same dispersion), but Debye freq cutoff

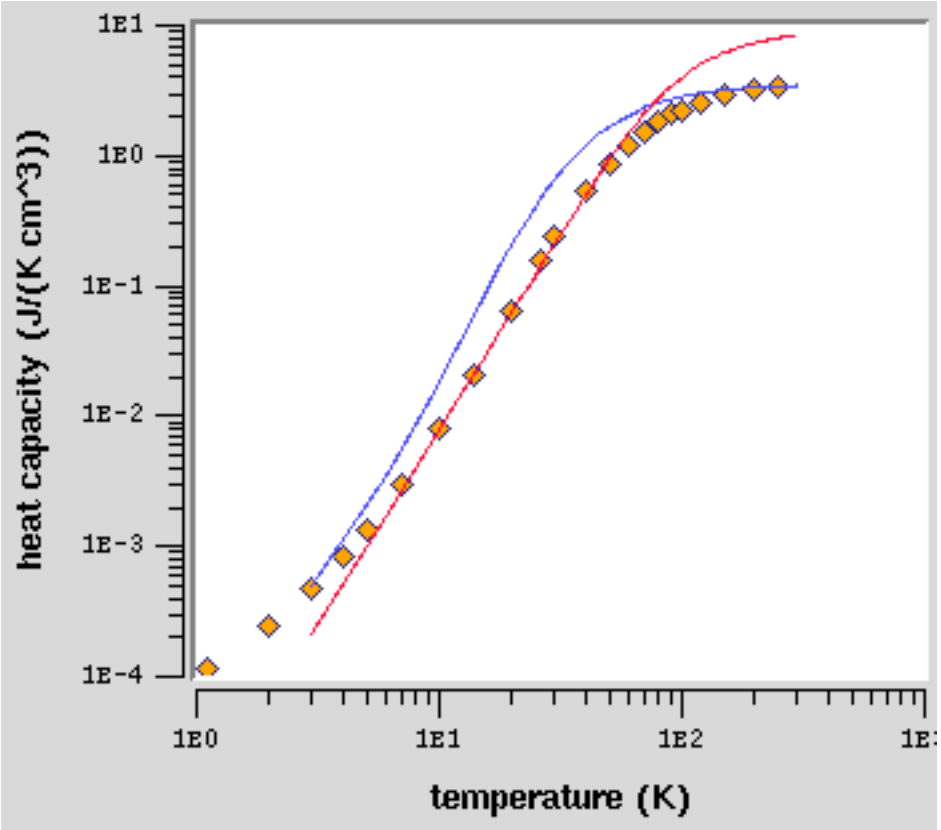
$$C = 9Nk_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{x_D} dx \frac{x^4 e^x}{\left(e^x - 1\right)^2}$$



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_{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.

http://hyperphysics.phy-astr.gsu.edu/hbase/solids/phonon.html http://www.physics.cornell.edu/sss/debye/debye.html

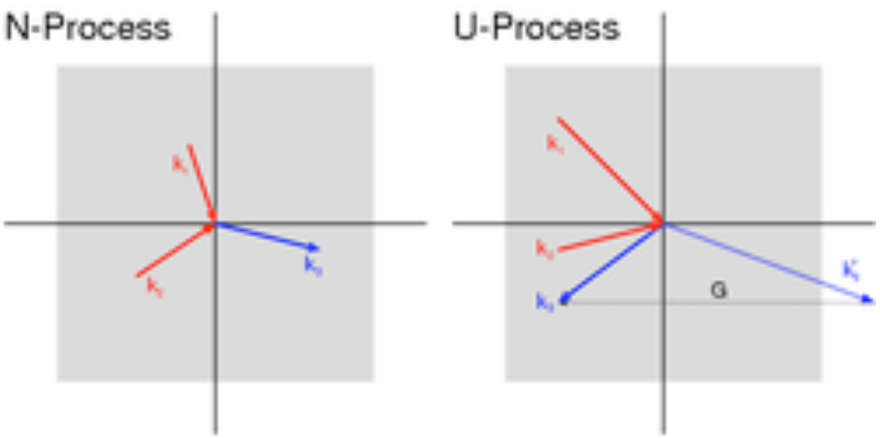


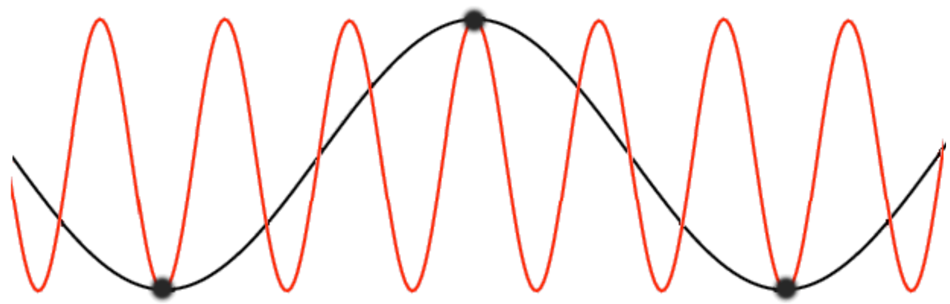
From the density of states, the specific heat is calculated, is displayed, and can be compared with experimental data and with a Debye model calculation. In the log/log plot, the wrong force constant was chosen for the numerical calculation (in blue). Should it be increased or decreased, and by what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

For the Debye model (in red), the wrong lattice constant was chosen! Should it be larger or smaller, and by what factor?

UMKLAPP and NORMAL PROCESSES:

"Normal" phonon collisions that conserve *k*-momentum (crystal momentum) do not limit thermal conductivity (N-processes), but "Umklapp processes" (U-processes) limit thermal conductivity. This is because the medium is discrete, and k-values outside the 1st BZB can be mapped back into the 1st BZB with a reciprocal lattice vector. Notice that two phonons with $k_x > 0$ collide to produce a phonon with $k_x < 0$!





http://en.wikipedia.org/wiki/Umklapp_scattering

THERMAL CONDUCTIVITY:

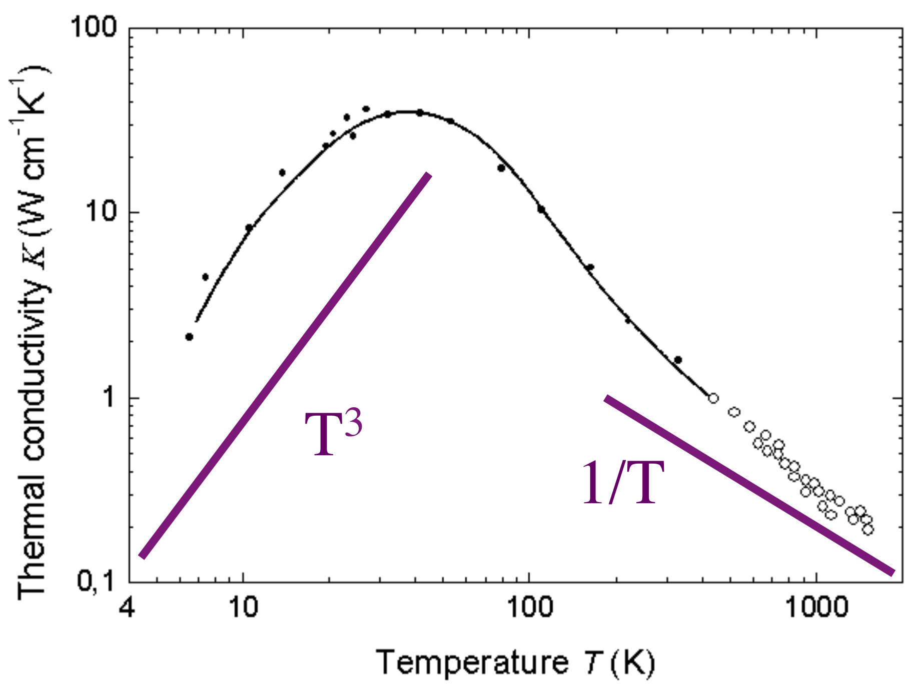
$$\kappa = \tfrac{1}{3} C v \ell_{mfp}$$

Low temp: $C \approx T^3$, $v \approx v_F$, mfp ≈ constant (not many phonons; impurity scattering dominates) => $\kappa \approx T^3$

High T: C ≈ constant, $v \approx v_F$; mfp ≈ $1/T$ (# phonons scattering ≈ T) => $\kappa \approx 1/T$

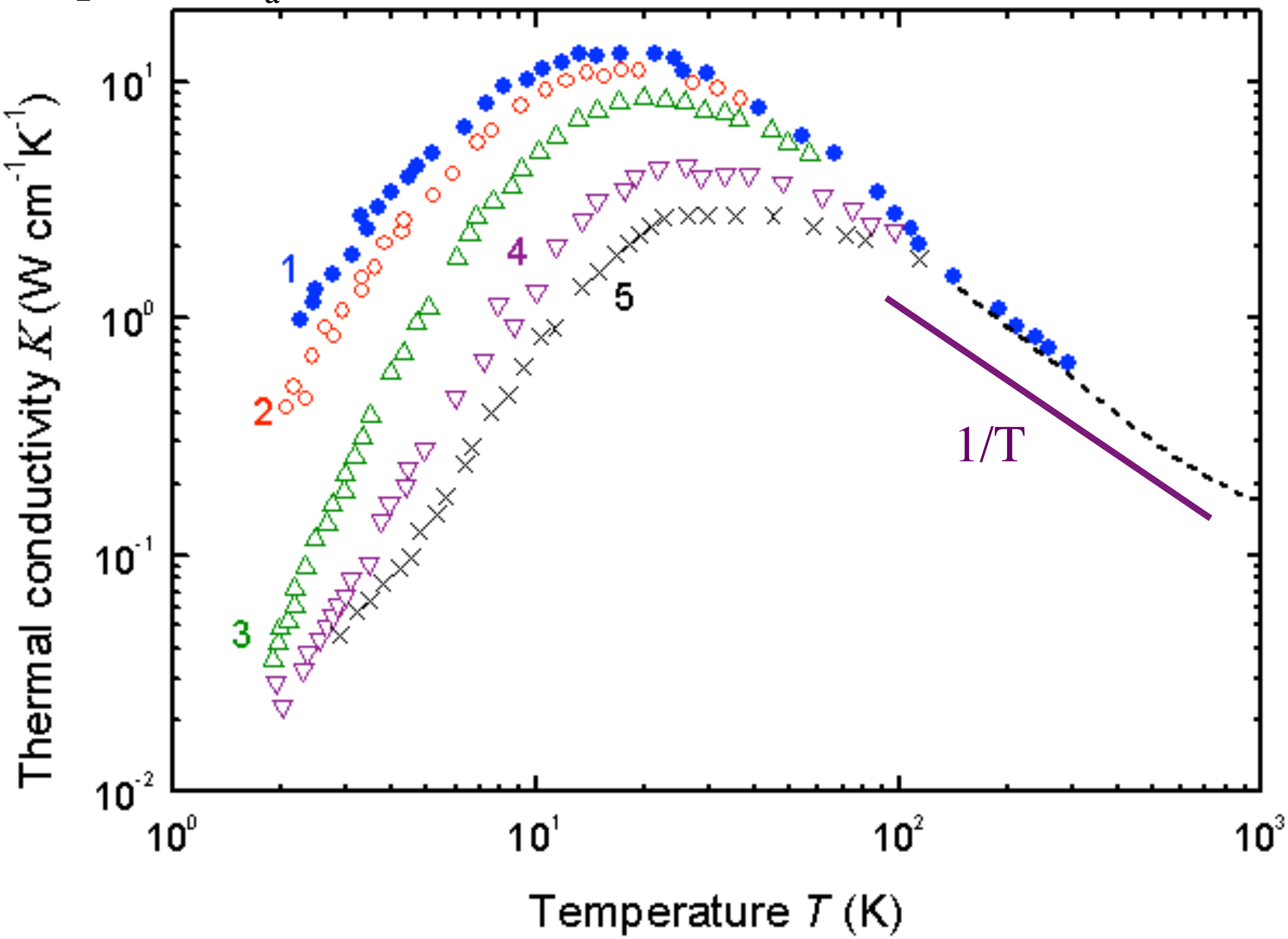
$$n(T) = \frac{1}{e^{\hbar\omega/k_B T} - 1} \xrightarrow[T \to \infty]{} \frac{1}{\hbar\omega / k_B T} = \frac{k_B T}{\hbar\omega}$$

$$\rho \sim n \sim T$$



http://www.ioffe.ru/SVA/NSM/Semicond/Si/Figs/151.gif

Temperature dependence of thermal conductivity at different doping level. *p*-Ge. N_a (cm^{-3}): **1**. 10^3; **2**. 10^{15}; **3**. $2.3 \cdot 10^{16}$; **4**. $2 \cdot 10^{18}$; **5**. 10^{19}.



http://www.ioffe.ru/SVA/NSM/Semicond/Ge/Figs/251.gif

ELECTRON-PHONON SCATTERING:
(Ashcroft ch. 26)

Resistivity of metals varies as T at high temperature.

At high $T >> \theta_D$, all phonon modes excited. # of phonons in normal mode is

$$n(q) = \frac{1}{e^{\hbar\omega/k_B T} - 1} \xrightarrow[T \to \infty]{} \frac{1}{\hbar\omega / k_B T} = \frac{k_B T}{\hbar\omega}$$

$$\rho \sim n \sim T$$

Resistivity of metals varies as T^5 at low temperature.

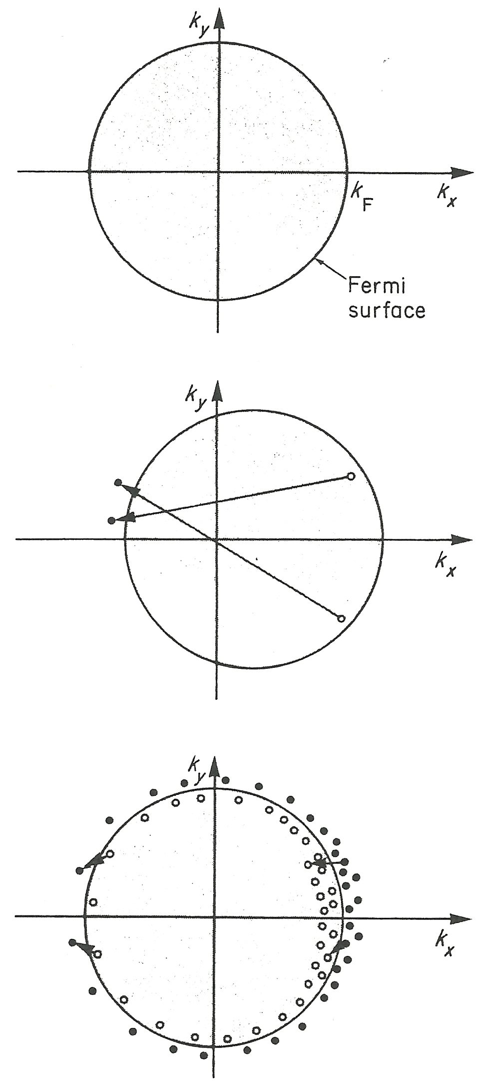
(1) Energy of phonons must be ≈ $k_B T$ (occupation near Fermi surface)
(2) Wave vector of phonon must be ≈ θ_{Debye}; + small energy ≈ $k_B T$
(3) El-Ph coupling constant scales as T
(4) Forward scattering predominates ≈ T^2

ELECTRON-PHONON SCATTERING IN METALS:
(Hook)

Wiedemann-Franz Law.

$$\frac{\kappa_{thermal}}{\sigma_{electrical} T} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 \sim const$$

$$\kappa_{thermal} = \frac{\pi^2}{3}\frac{nk_B^2\tau}{m^*}T; \quad \sigma_{electrical} = \frac{ne^2\tau}{m^*}$$



But scattering can be different!

(1) At lowest T, impurity scattering dominates: τ same for both – WF OK
(2) Low *T* – more phonon mechanisms for thermal relaxation: WF violated
(3) High *T* – same phonon mechanisms again – WF OK