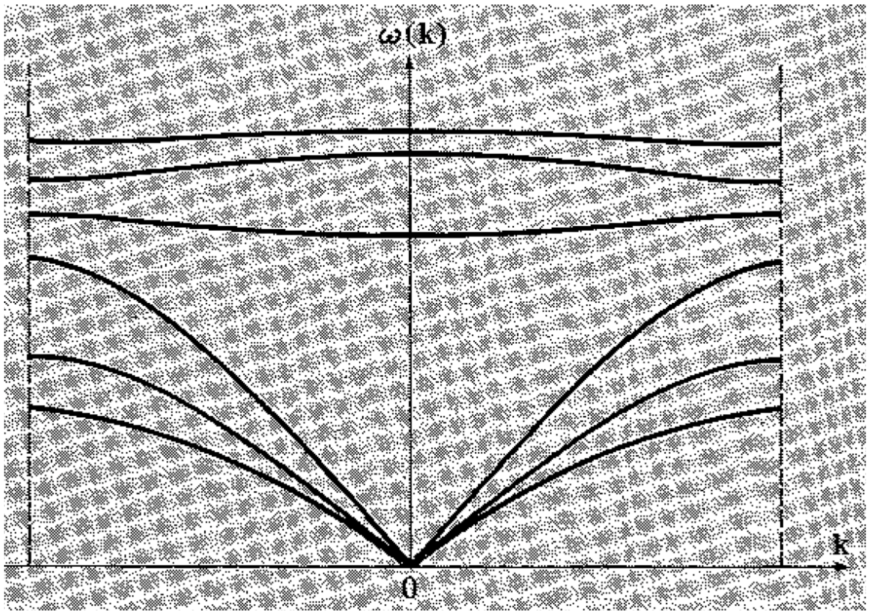
Phonon Contribution to Physical Properties

Recall: Crystal lattices vibrate



$$\varepsilon_{k,s} = (n_{k,s} + 1/2)\hbar\omega_s\left(k\right)$$

Phonon Density of States

1-D $$g(\omega)d\omega = \frac{L}{\pi}\frac{1}{|\nabla_k \omega|}$$

2-D $$g(\omega)d\omega = \frac{A}{(2\pi)^2}\int d^2k$$

3-D $$g(\omega)d\omega = \frac{V}{(2\pi)^3}\int_{shell} d^3k$$

Quantum theory: Lattice Specific Heat

$$\varepsilon_i = (n + 1/2)\hbar\omega$$

$$Z = \sum_{i=1}^{\infty} \exp[\frac{-\varepsilon_i}{k_B T}]$$

Partition Function

$$= \sum_{i=1}^{\infty} \mathbf{exp}[\frac{-(n+1/2)\hbar\omega}{k_B T}]$$

Do Series Expansion

$$Z = \frac{\exp(-\hbar\omega / k_B T)}{1 - \exp(-\hbar\omega / k_B T)}$$

$$\langle A \rangle = \frac{\sum_n A \exp(-\varepsilon_n / k_B T)}{\sum_n \exp(-\varepsilon_n / k_B T)}$$

Thermal Average

Lattice Specific Heat

from an evaluation of the thermal average occupancy of a mode

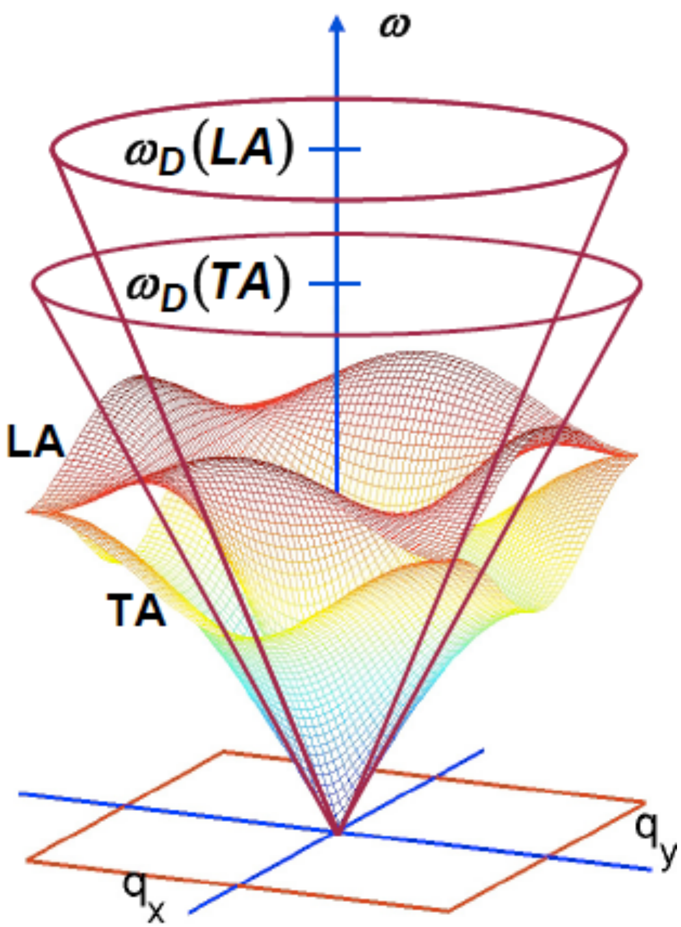
$$\langle n(s,k,T)\rangle = \frac{1}{\exp(\hbar\omega_k(s)/k_B T)-1}$$

$$C_v^p = \frac{\partial}{\partial T}\sum_s \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{\hbar\omega_s(\mathbf{k})}{\exp(\hbar\omega_s(\mathbf{k})/k_B T)-1}$$

s is the phonon branch

Debye Approximation

$$\omega_s(k) = c_s(\bar{k})k$$

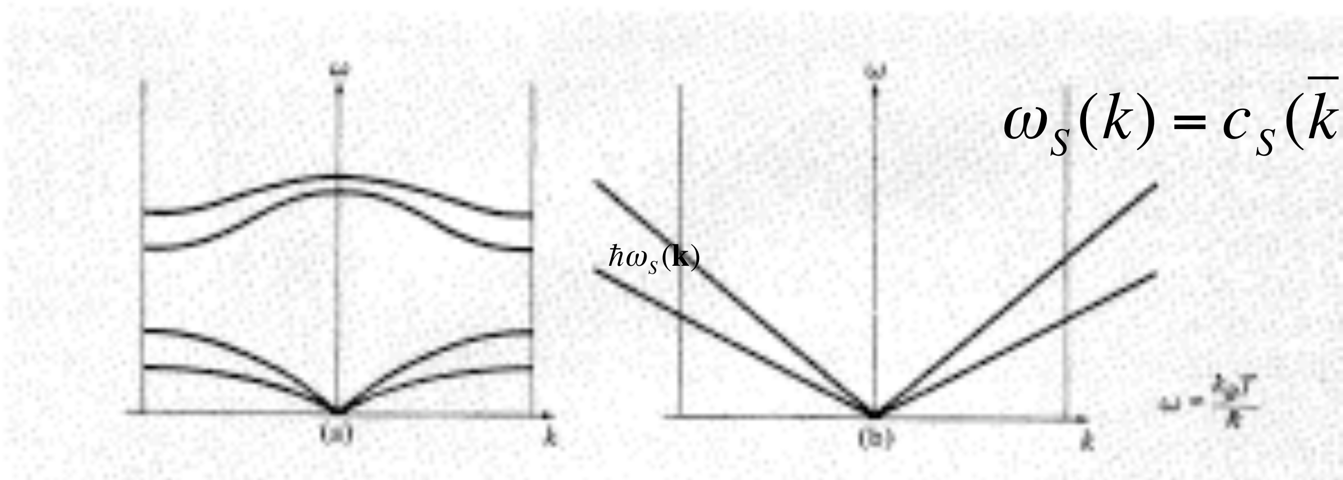


Peter Debye
(1884-1966)

Nobel Prize 1936

Debye Approximation

$$C_v^p = \frac{\partial}{\partial T} \sum_S \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\hbar \omega_S(\mathbf{k})}{\exp(\hbar \omega_S(\mathbf{k}) / k_B T) - 1}$$



$$\omega_S(k) = c_S(\bar{k}) k$$

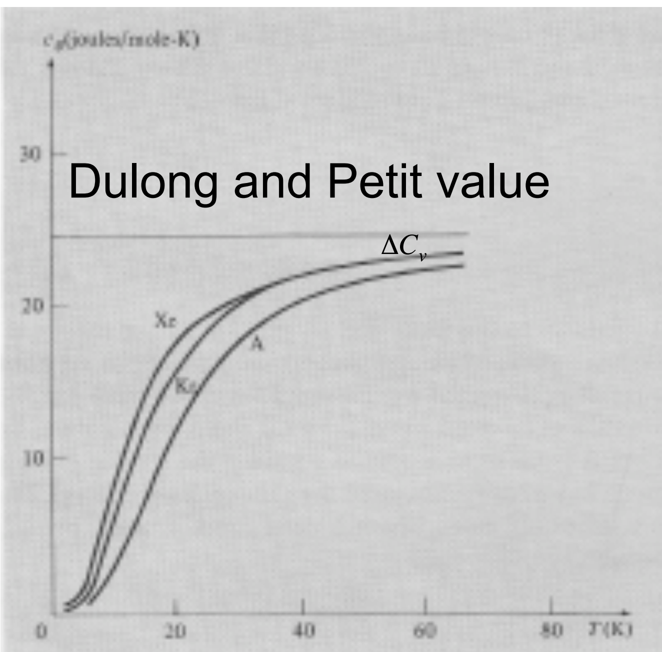
$$C_v^p = \frac{\partial}{\partial T} \sum_S \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\hbar c_S(\bar{\mathbf{k}}) \mathbf{k}}{\exp(\hbar c_S(\bar{\mathbf{k}}) / k_B T) - 1} = \frac{\partial}{\partial T} \frac{(k_B T)^4}{(\hbar \bar{c})^3} \frac{3}{2\pi^3} \int_0^\infty \frac{x^3 dx}{e^x - 1}$$

Debye approximation for specific heat at high T

$$x = \hbar\omega_s / k_B T << 1$$

$$C_v^p(high-T) \approx 3nk_B\left[1 - \frac{\hbar^2}{12(k_BT)^2}\frac{1}{3N}\sum\omega_s(k)^2\right]$$

$$\approx C_v^{Dulong-Petit} - \Delta C_v$$



quantum corrections

Debye approximation for specific heat: T intermediate

Assuming all branches $\omega = c_p k$, and all modes are within a sphere of radius k_D

$$\frac{(2\pi)^3}{V} N = \frac{4\pi k_D^3}{3} \qquad n = \frac{N}{V} = \frac{k_D^3}{6\pi^2}$$

Define **Debye frequency** $\omega_D = c_p k_D$

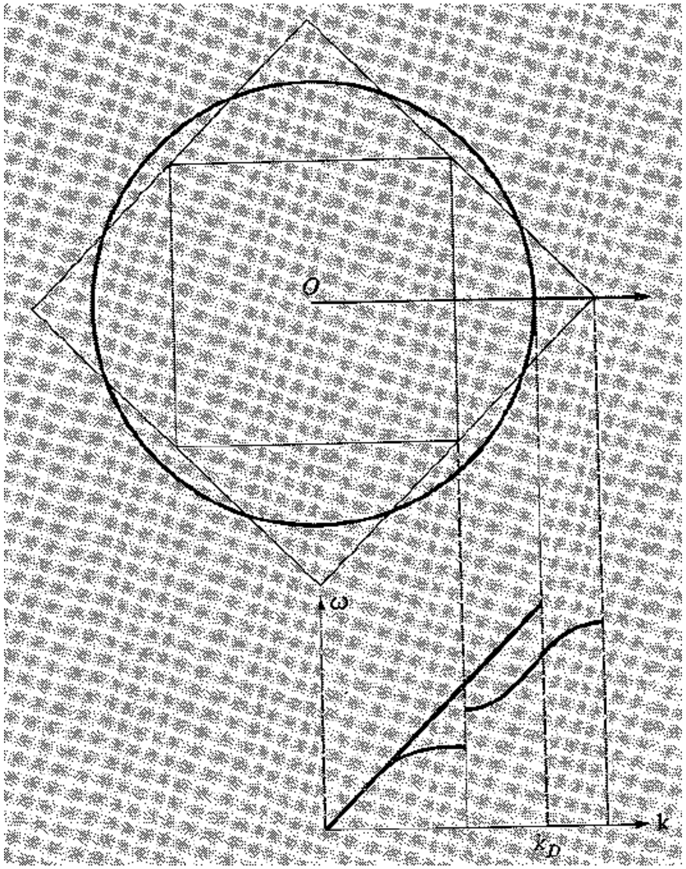
Define **Debye temperature** $\Theta_D = \frac{\hbar \omega_D}{k_B}$

$$\begin{cases} T > \Theta_D & \text{“soften”} \\ T < \Theta_D & \text{“harden”} \end{cases}$$

Debye approximation for specific heat: T intermediate

$$C_v^p = \frac{\partial}{\partial T}\frac{3\hbar c}{2\pi^2}\int_0^{k_D}\frac{k^3\,dk}{\exp(\hbar ck/k_B T)-1}$$

$$C_v^p = 9nk_B\left(\frac{T}{\Theta_D}\right)^3\int_0^{\Theta_D/T}\frac{x^4\,dx}{(e^x-1)^2}$$



Debye approximation for specific heat: T→0K

$$C_v^p = \frac{\partial}{\partial T}\sum_S \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{\hbar c_S(\bar{\mathbf{k}})\mathbf{k}}{\exp(\hbar c_S(\mathbf{k})/k_B T)-1}$$

$$C_v^p = \frac{\partial}{\partial T}\frac{(k_B T)^4}{(\hbar c)^3}\frac{3}{2\pi^3}\int_0^\infty \frac{x^3 dx}{e^x - 1}$$

$$\int_0^\infty \frac{x^3 dx}{e^x - 1} \overset{x>>1}{=} \sum_1^\infty \int_0^\infty x^3 e^{-nx} dx = 6\sum_1^\infty \frac{1}{n^4} = \frac{\pi^4}{15}$$

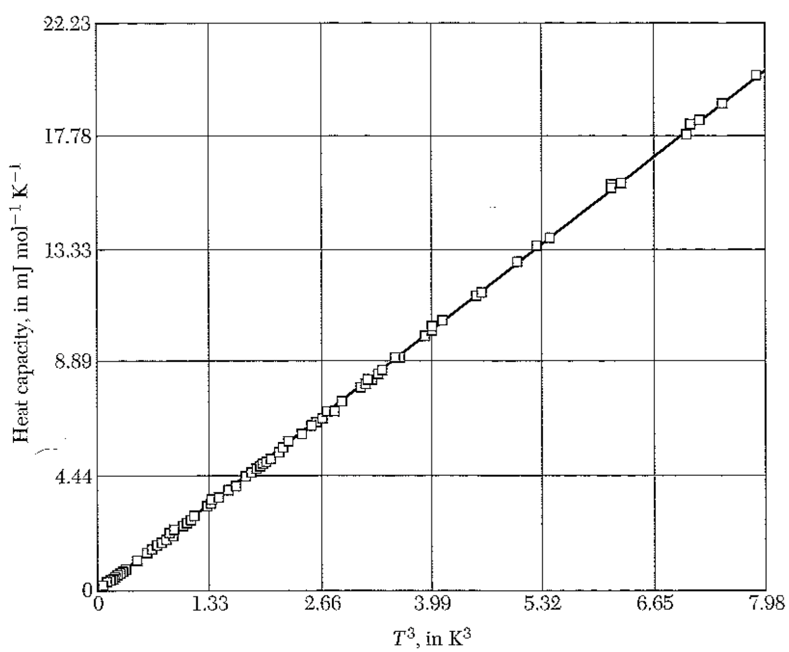
$$C_v^p \approx \frac{\partial}{\partial T}\frac{(k_B T)^4}{(\hbar c)^3}\frac{\pi^2}{10} = \frac{2\pi^2}{5}k_B\left(\frac{k_B T}{\hbar c}\right)^3$$

$$\lim(T \to 0)\frac{c_v^p}{T^3} = \frac{2\pi^2 k_B^4}{5(\hbar c)^3} = \frac{12\pi^4 k_B}{5(\Theta_D)^3}$$

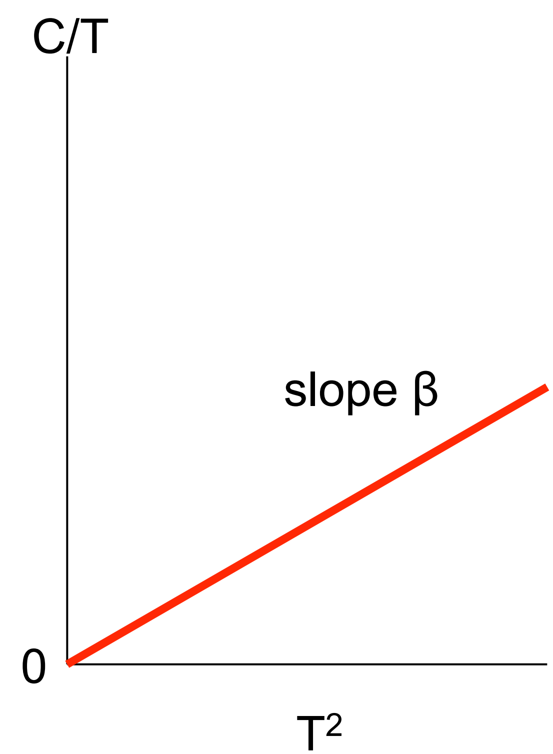
= Debye T^3 law

Experimental Confirmation

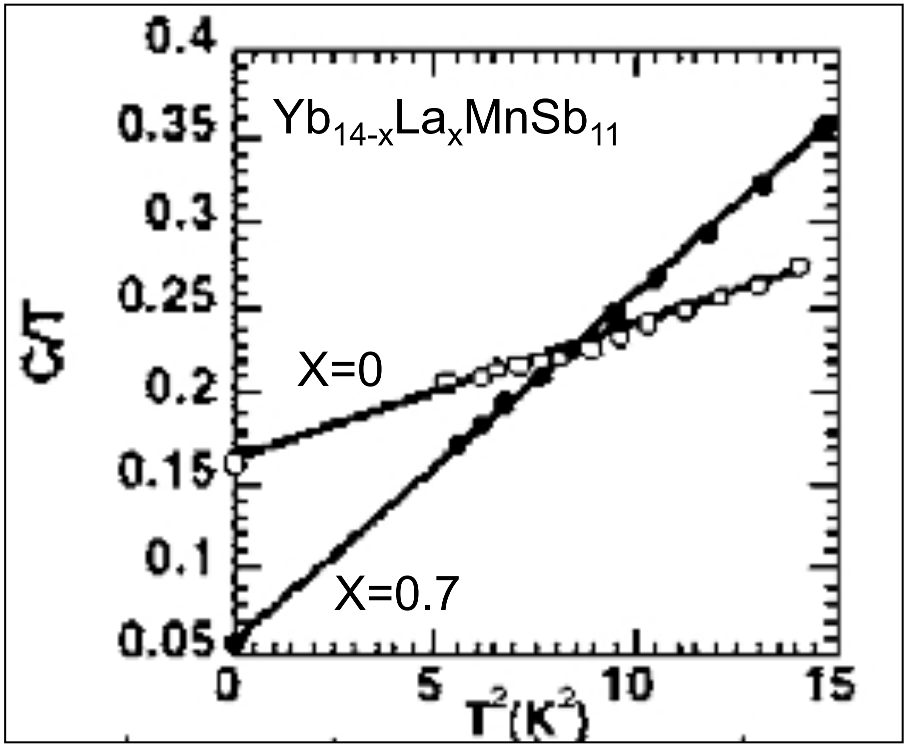
$$\lim(T \to 0)\frac{c_v^p}{T^3} = \frac{2\pi^2 k_B^4}{5(\hbar c)^3} = \frac{12\pi^4 k_B}{5(\Theta_D)^3} = \beta$$ = Debye T^3 law



or



Θ_D can be determined via β



$$C_{total} = C_{electron} + C_{phonon} = \gamma T + \beta T^3$$

Total Specific Heat at Low Temperatures for an non-magnetic system

When $C_D > C_e$?

$$\frac{C_v^{electron}}{C_v^{Debye-phonon}} = \frac{\frac{\pi^2}{2}\left(\frac{k_B T}{\varepsilon_F}\right) n k_B}{\frac{12\pi^4}{5} n k_B \left(\frac{T}{\Theta_D}\right)^3}$$

⇓

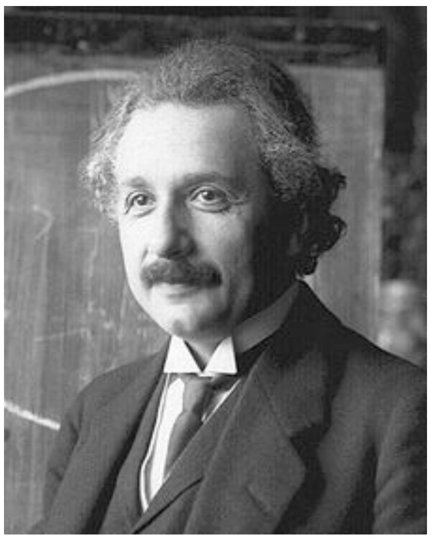
Crossover T

$$T_0 = 0.145\left(\frac{Z\Theta_D}{T_F}\right)^{1/2} \Theta_D$$

Einstein Model – deal with optical modes

treat ω_E^{OP} = constant

Debye Model $d\omega / dK = C$



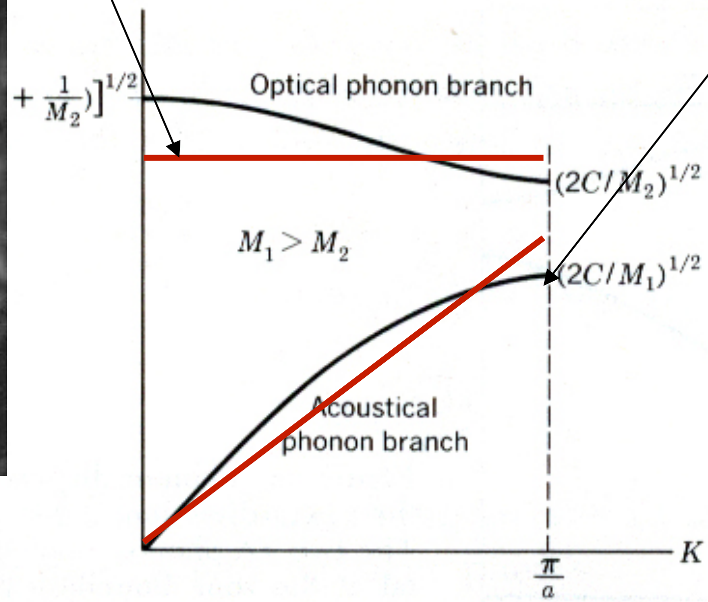


Figure 7 Optical and acoustical branches of the dispersion relation for a diatomic linear lattice, showing the limiting frequencies at $K = 0$ and $K = K_{max} = \pi/a$. The lattice constant is a.

Einstein Model

$$g_E(\omega) = N\delta(\omega - \omega_E)$$

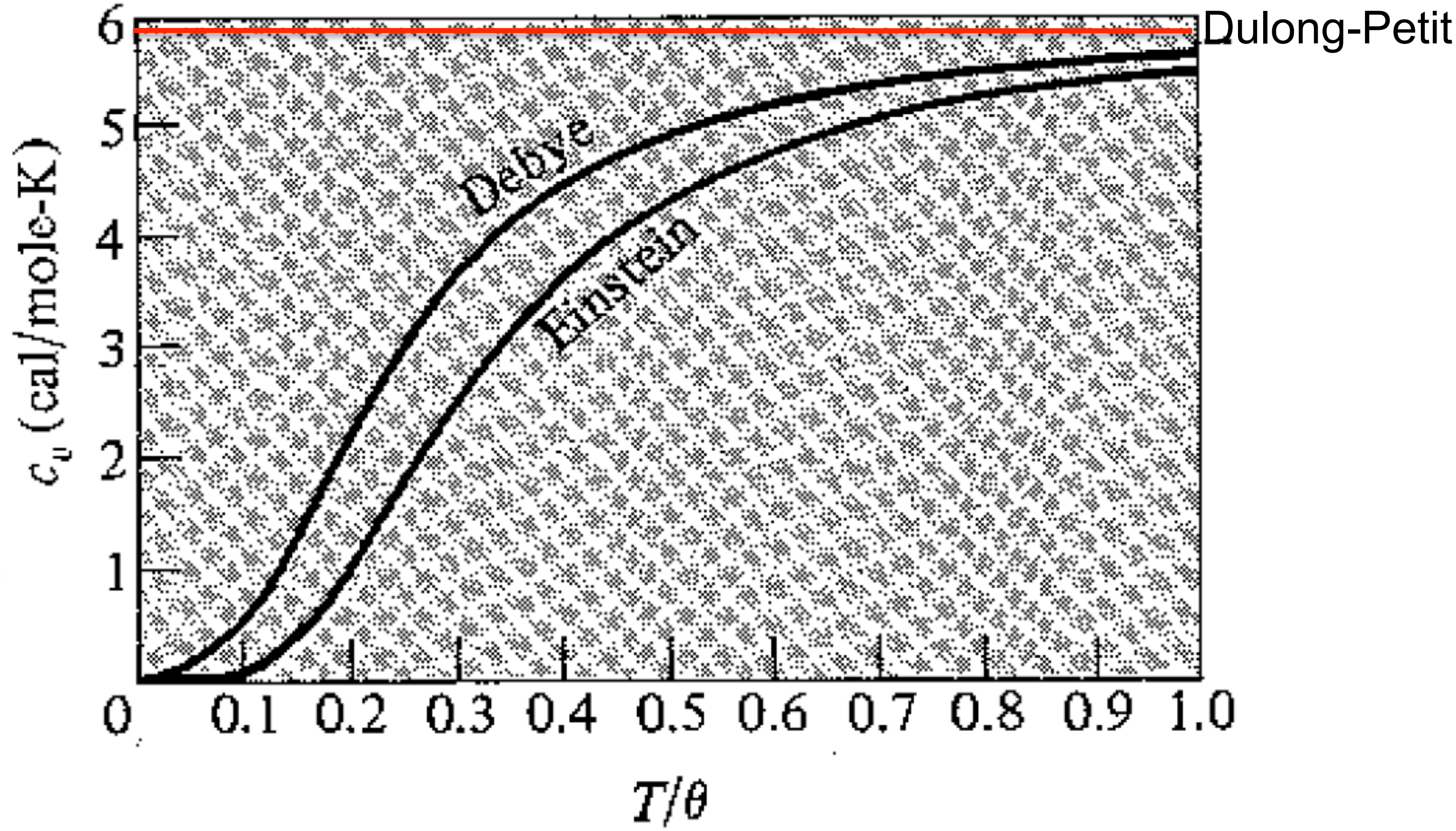
$$C_v^{optical} = pnk_B \frac{\left(\hbar\omega_E / k_B T\right)^2 e^{\left(\hbar\omega_E / k_B T\right)}}{\left[e^{\left(\hbar\omega_E / k_B T\right)} - 1\right]^2}$$

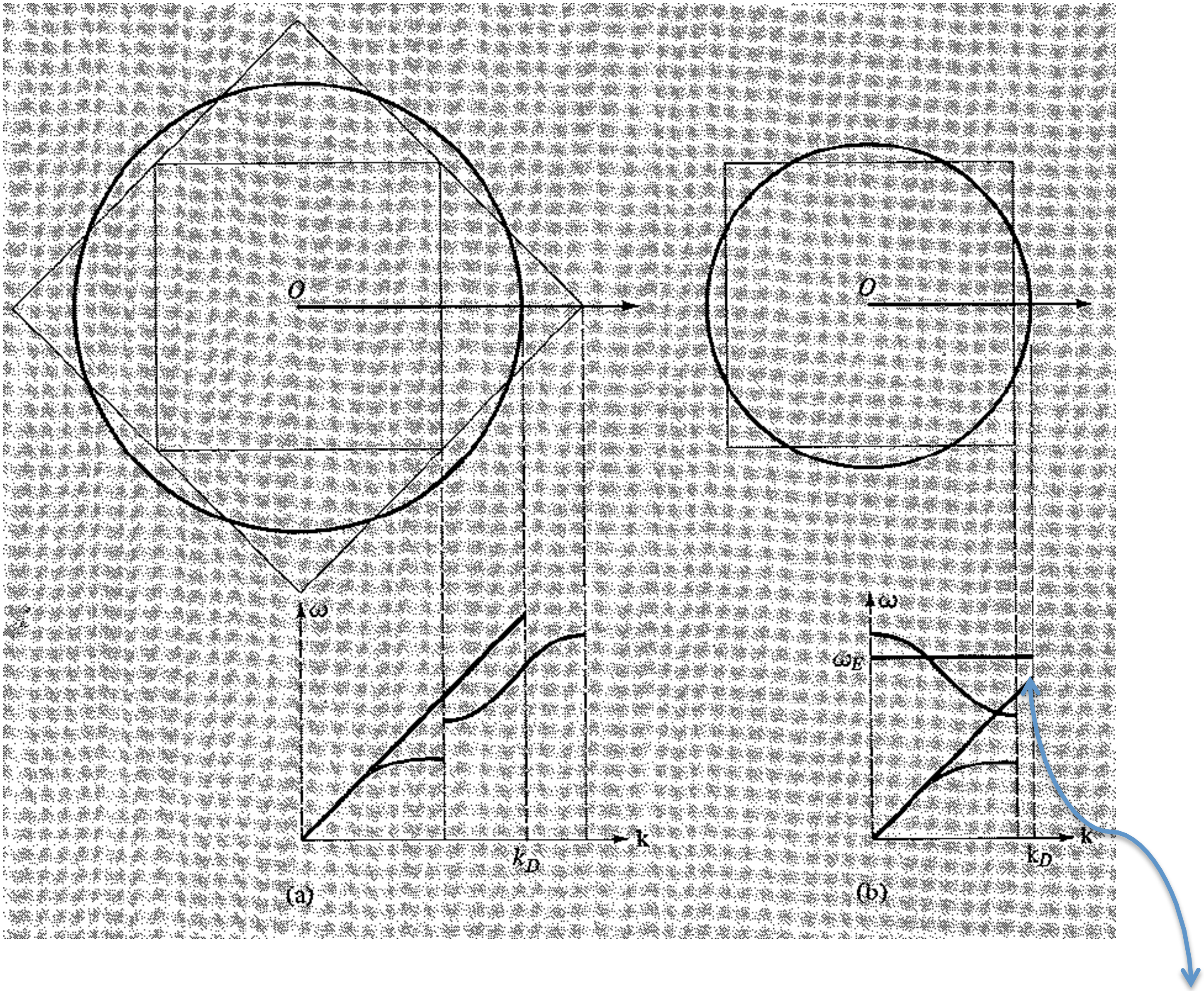
total number of such branches

$$C_v^{optical} = \begin{cases} \text{constant} & T >> \Theta_E \\ \text{exponential} & T << \Theta_E \end{cases}$$

Define **Einstein temperature** $\Theta_E = \dfrac{\hbar\omega_E}{k_B}$

Einstein and Debye Specific heats





Debye included optical phonon
Contribution via $k_{FBZ} < k < k_D$

Phonon Density of States: Einstein and Debye Approximation

$$g(\omega)=\sum_s \int_{surface-FBZ} \frac{dS}{(2\pi)^3}\frac{1}{\left|\nabla\omega_s(\mathbf{k})\right|}=\sum_s\int_k \frac{d\,\mathbf{k}}{(2\pi)^3}\delta\left(\omega-\omega_s(\mathbf{k})\right)$$

$$g_D(\omega)=3\int_{k<k_D}\frac{d\,\mathbf{k}}{(2\pi)^3}\delta\left(\omega-c_p k\right)=\frac{3}{(2\pi)^3}\int_0^{k_D}k^2\delta\left(\omega-c_p k\right)$$

$$=\begin{cases}\dfrac{3}{2\pi^2}\dfrac{\omega^2}{c_p^3} & \omega<\omega_D\\ 0 & \omega>\omega_D\end{cases}$$

$$g_E(\omega)=\int_{zone}\frac{d\,\mathbf{k}}{(2\pi)^3}\delta\left(\omega-\omega_E\right)=N\delta(\omega-\omega_E)$$

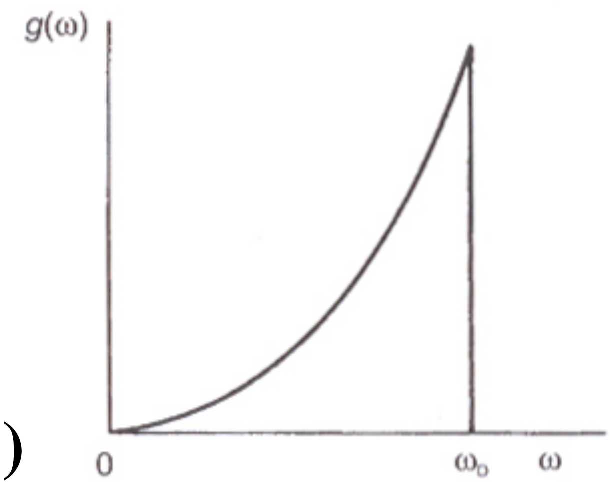
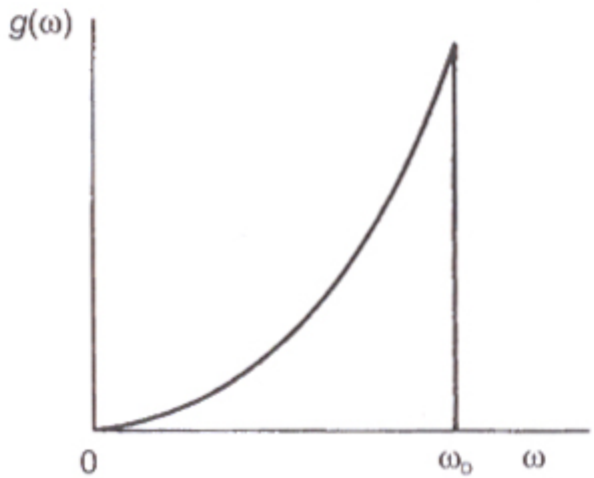


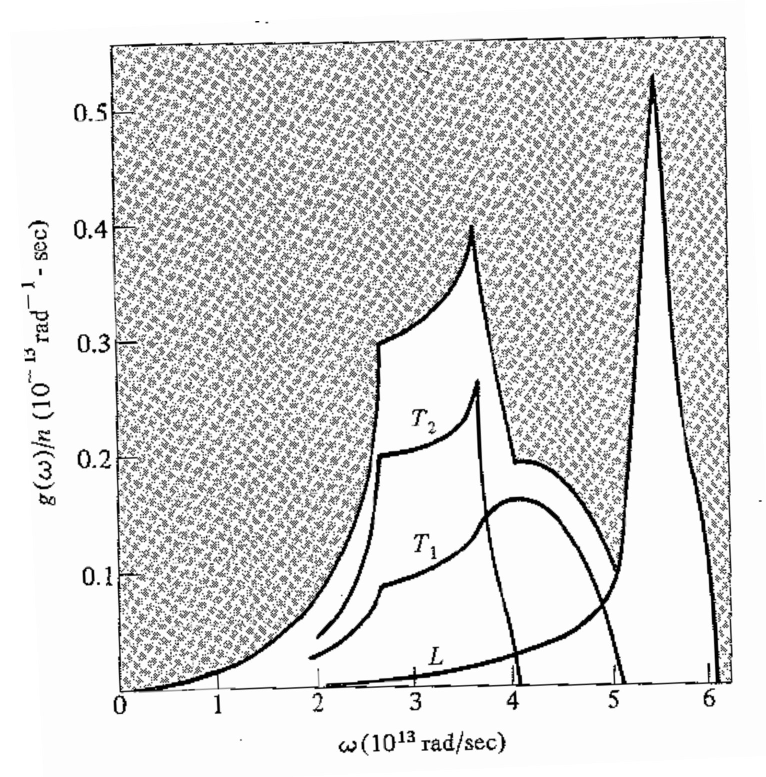
Fig. 4.5 The Debye density of vibrational states.

Phonon Density of States of Al

Phonon density of levels in Al as deduced from neutron scattering data. The three branches are shown as L, T_1, and T_2



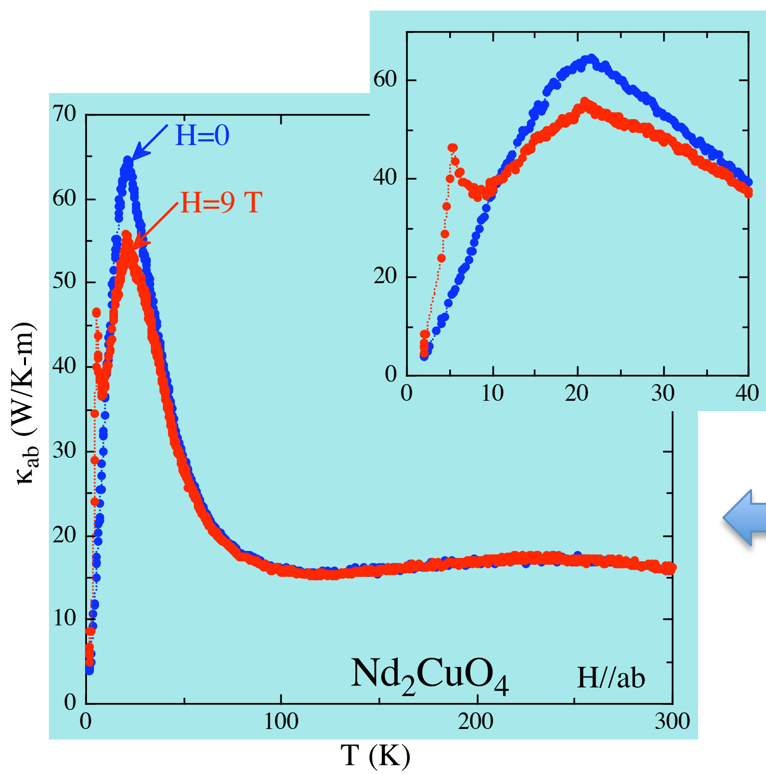
he Debye density of vibrational states.



Recall: Relationship between κ and C

Drude: $\kappa_e = 1/3\ C_e v_e l_e$

Sommerfeld: $\kappa_e/\sigma T = \text{constant}$



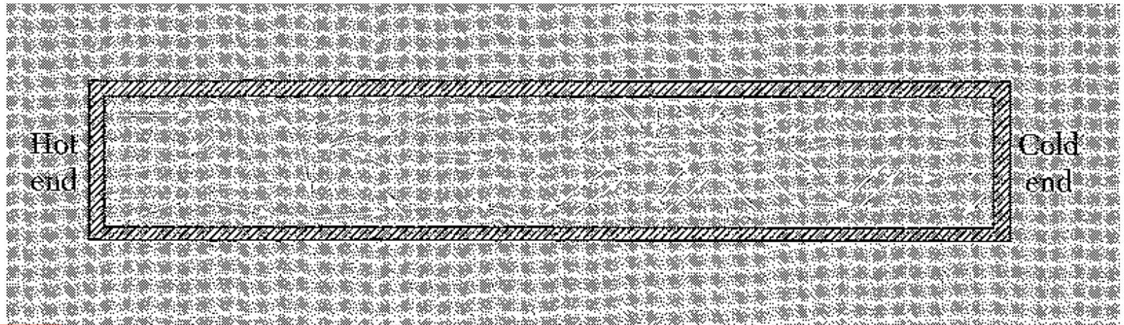
Nd_2CuO_4: an insulator

Where is finite κ coming from?

A Perfect Harmonic Crystal

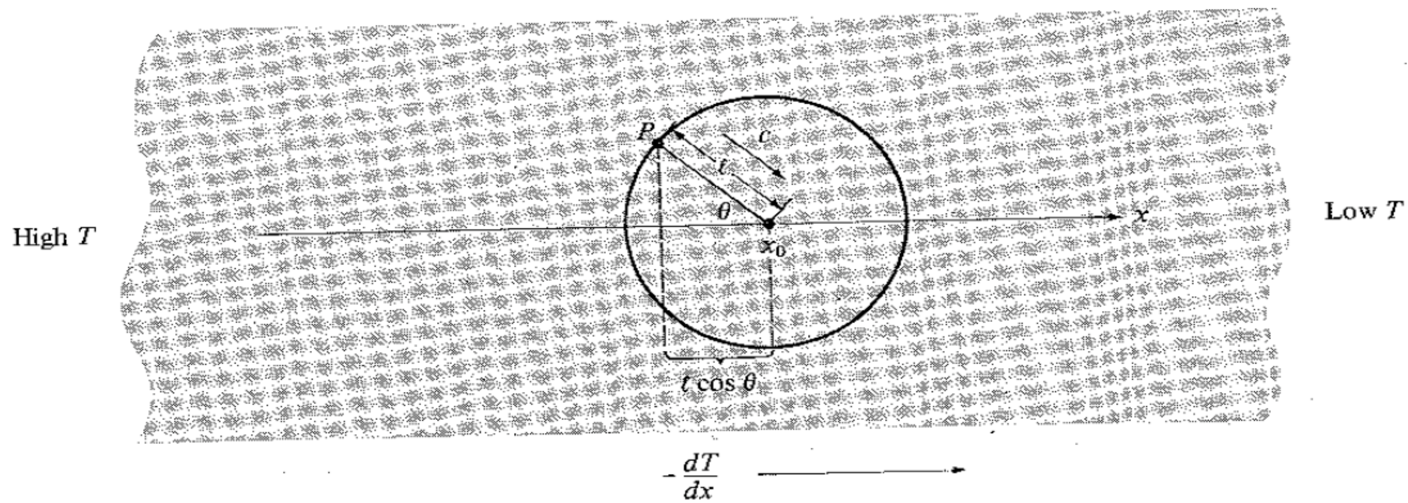
No collision between phonons

$$\kappa_{phonon}^{perfect} \rightarrow \infty$$



In reality:

- Crystal boundaries
- Lattice imperfections
- Anharmonic effects



$$J_{thermal}^{phonon} = \left\langle v_{phonon} u\left(x_0 - \ell_{phonon} \cos\theta\right)\right\rangle_\theta$$

$$J_{thermal}^{phonon} = \kappa_{phonon}\left(-\frac{\partial T}{\partial x}\right)$$

$$\kappa_{phonon} = \frac{1}{3} C_v^{phonon} v_{phonon} \ell_{phonon}$$

At high temperatures: $T >> \Theta_D$

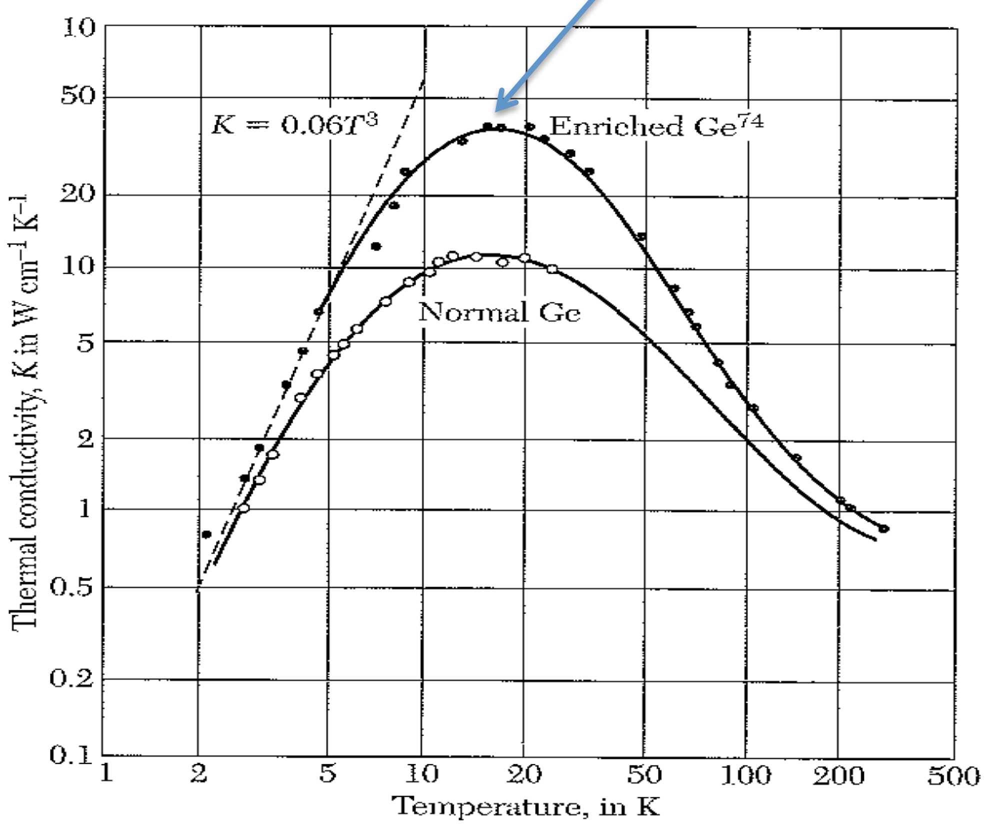
Number of excited phonons $n \propto T$

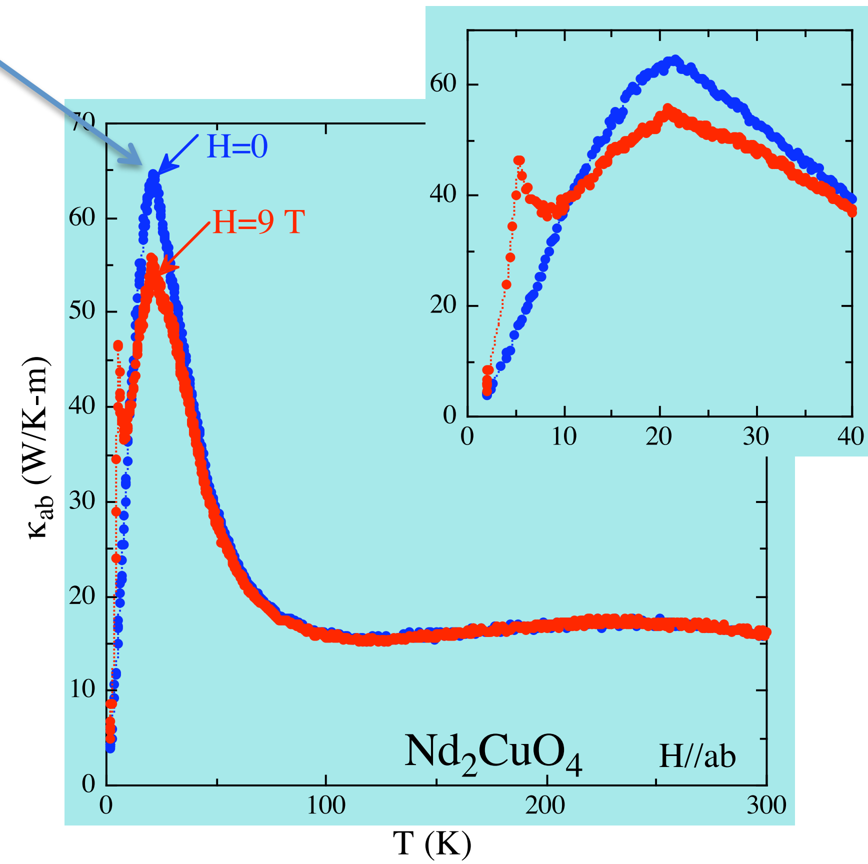
$$n_s(k) = \frac{1}{e^{\hbar\omega_s(k)/k_B T} - 1} \approx \frac{k_B T}{\hbar\omega_s(k)}$$

Phonon mean free path $l_{phonon} \propto \frac{1}{T}$

$$\kappa_{phonon} = \frac{1}{3} C_v^{phonon} v_{phonon} \ell_{phonon} \propto \frac{1}{T}$$

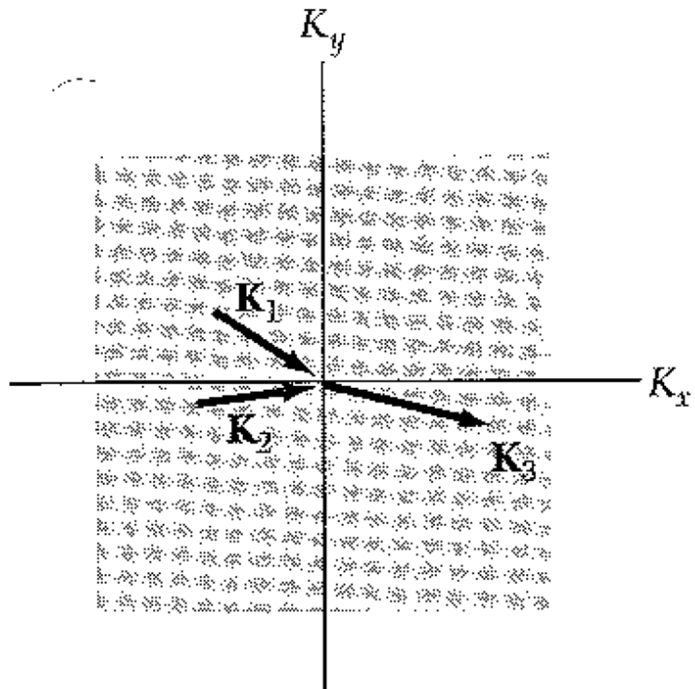
Why is there a peak (maximum) in $\kappa(T)$?





At low temperatures: $T << \Theta_D$

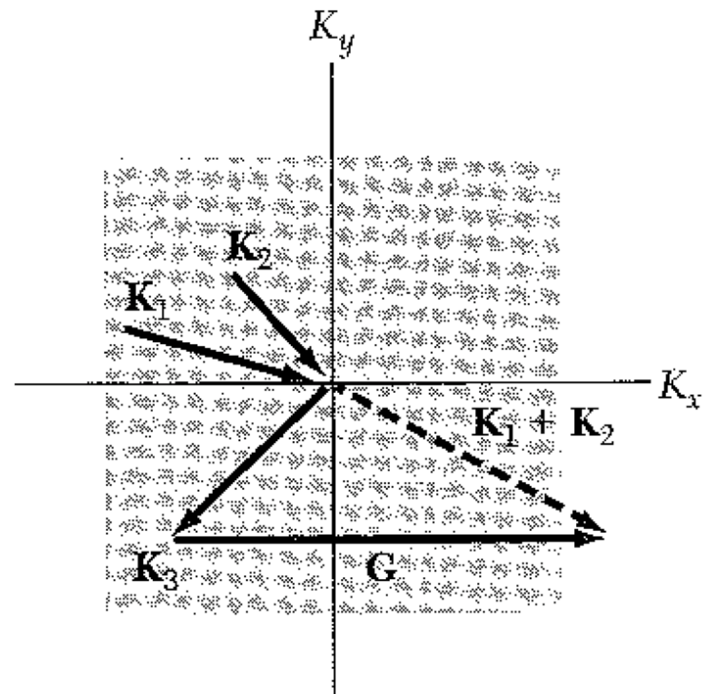
Normal Process



momentum is conserved

$$K_1 + K_2 = K_3$$

Umklapp Process



momentum is NOT conserved

$$K_1 + K_2 = K_3 + G$$

Thermal resistance = N-scattering + U-scattering

majority minority

Why ?

At low temperatures: $T << \Theta_D$

Normal Process

$$K_1 + K_2 = K_3$$

↓

small k (must be in FBZ)

↓

No impact to thermal transport

$$\omega(-k) = \omega(k)$$

Umklapp Process

$$K_1 + K_2 = K_3 + G$$

↓

large k ~ k_D

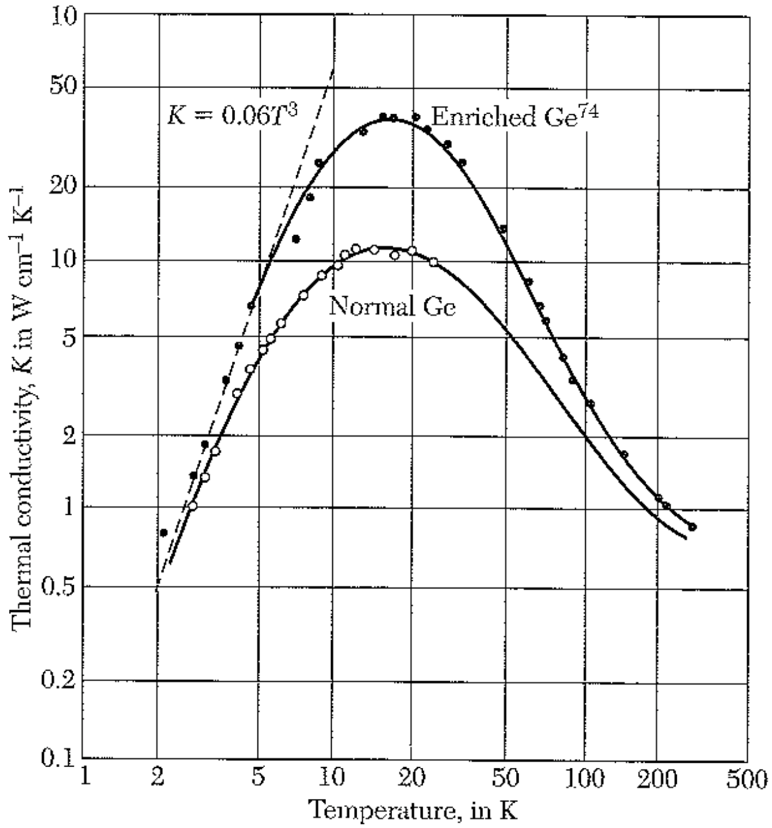
↓

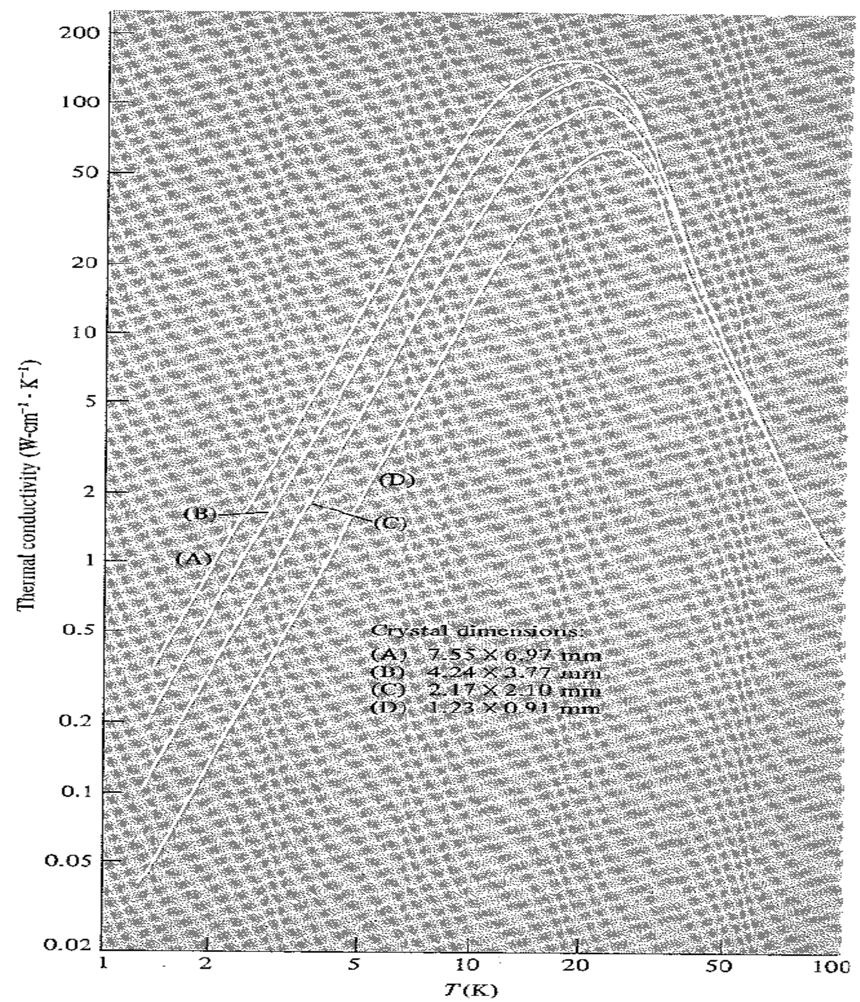
$$n_s(k) = \frac{1}{e^{\hbar\omega_s(k)/k_B T} - 1} \approx \frac{1}{e^{\Theta_D/T} - 1} \approx e^{-\Theta_D/T}$$

↓

$$\kappa_{phonon} = \frac{1}{3} C_v^{phonon} v_{phonon} \ell_{phonon} \propto C_v^{phonon} \propto T^3$$

At low temperatures: $T << \Theta_D$





Homework today (due on Oct. 7, 2010)

Problem 3 in page 468