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introduction of thermal transport

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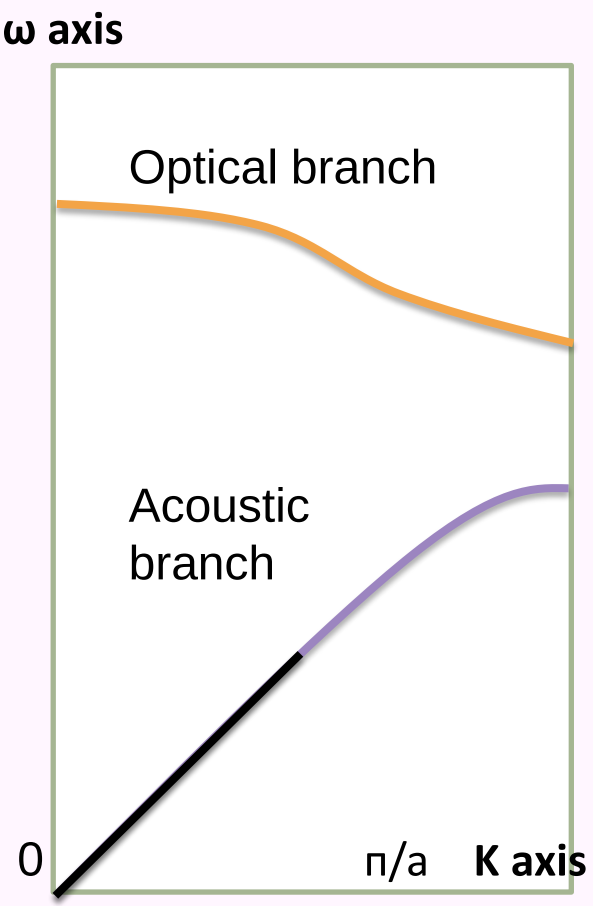
introduction of thermal transport
Phonon effect
Electron effect
Lattice vibration
phonon
Debye model of lattice vibration
K space, Reciprocal lattice
Scattering mechanism
Dispersion relation
Optical and Acoustic phonons
Bose-Einstein model
Dulong-petit model
Brillouin zone
Boundary scattering
Phonon-phonon scattering
Heat capacity
The contribution of electron of heat capacity
Normal Process
Debye temperature
Umklapp process

Outline

- Dispersion relation (review)
- Sepcific heat (review)
- Different temperature ranges
- Low temperature range
- Debye temperature

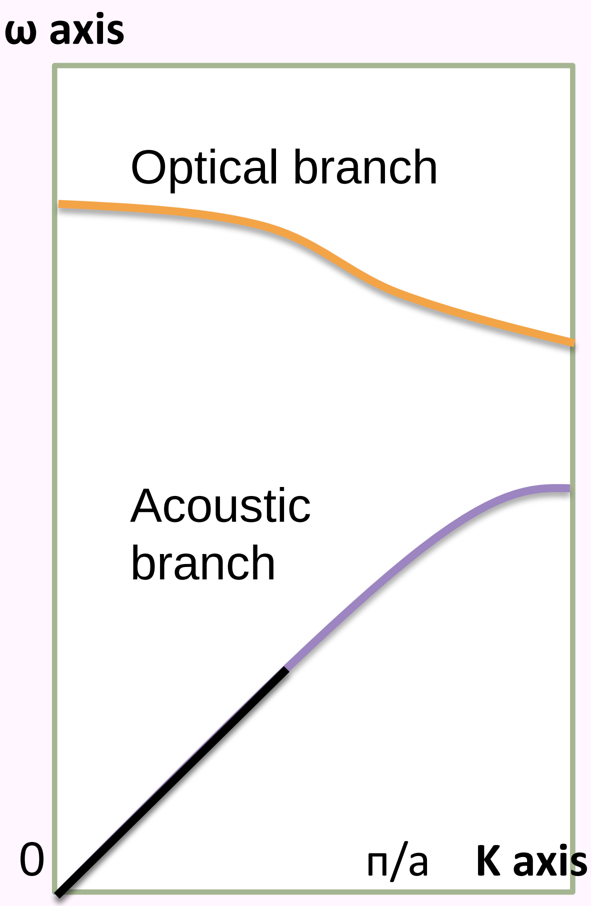
Disparsion relation

Electromagnetic wave
- ω/k=c
- c:light speed
- c is constant → linear dispersion relation



- At lower energy (lower k)
- Ka << π (near zero)
- The dispersion relation is regard as linear

Disparsion relation



$$\omega^2 = \frac{C(M+m)}{Mm} - \frac{C\sqrt{(M+m)^2 - 2Mm(1-\cos Ka)}}{Mm}$$

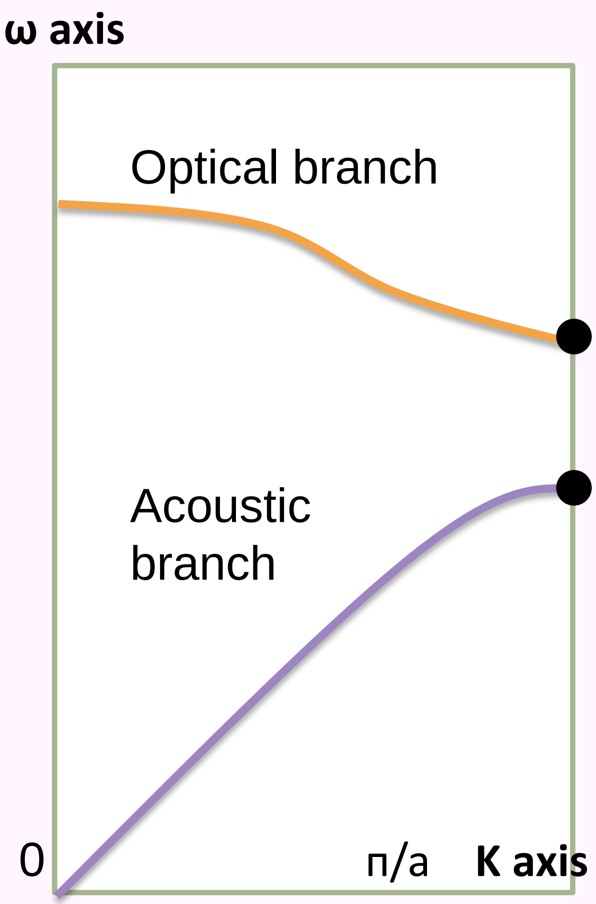
$$1 - \cos Ka = 1 - \left(1 - \frac{1}{2}K^2a^2\right) = \frac{1}{2}(Ka)^2$$

$$\frac{C\sqrt{(M+m)^2 - MmK^2a^2}}{Mm} = \frac{C(M+m)}{Mm} - \frac{CK^2a^2}{2(M+m)}$$

$$\omega \sim \sqrt{\frac{C}{2(M+m)}}Ka$$

We get linear part of dispersion relation.

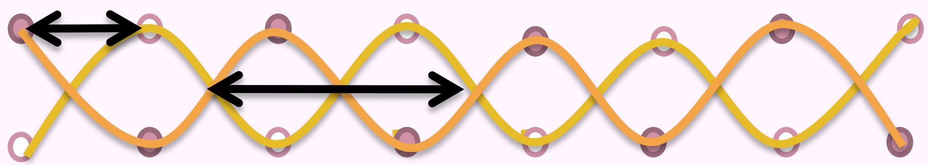
Disparsion relation



Standing wave

k= π/a   2a=λ

(k is fixed, ω is independent from k)



Group velocity $v_g = \frac{d\omega}{dk}$

$v_g = 0$ at k=π/a

Energy does not propagate in the medium (standing wave)

Disparsion relation

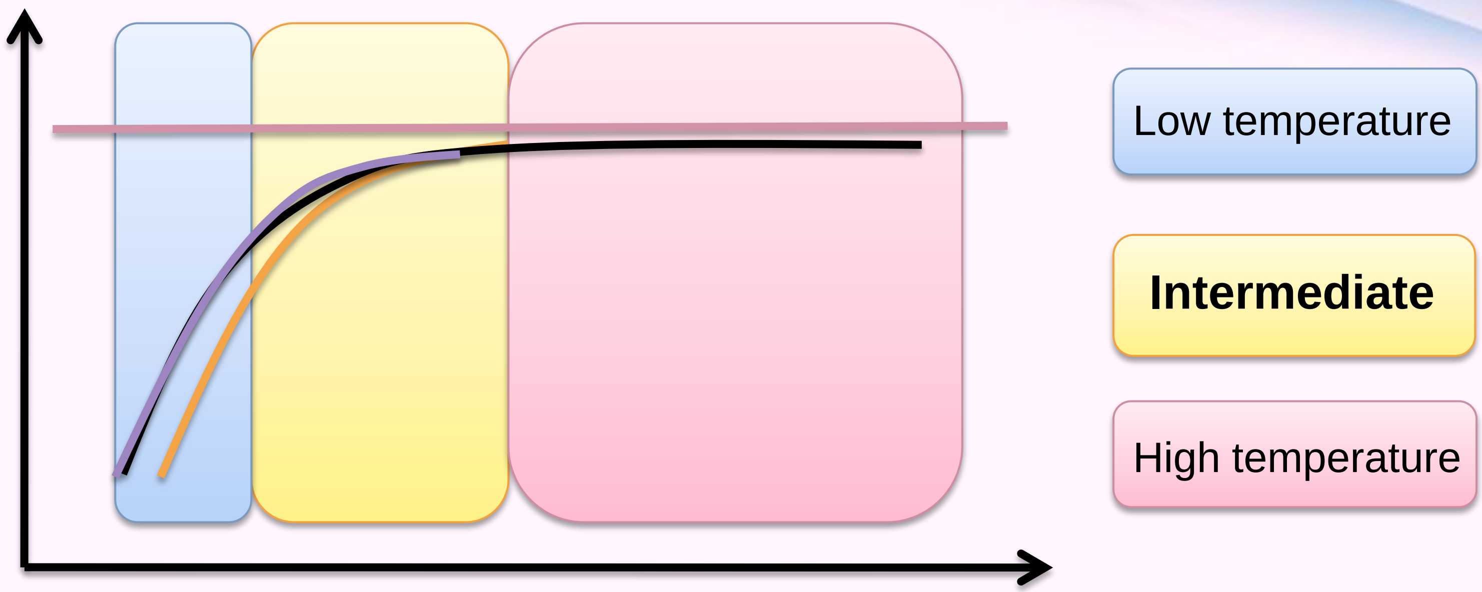
- Classical mechanism :

  Harmonic oscillator

  (conservative force and wave)

- We get dipersion relation by only classical assumption

Specific heat



There are three segments of the experiment curve of specific heat (Cv).

Specific heat

s: types of phonons
k: wave factor

Frequencies are functions of wave factor

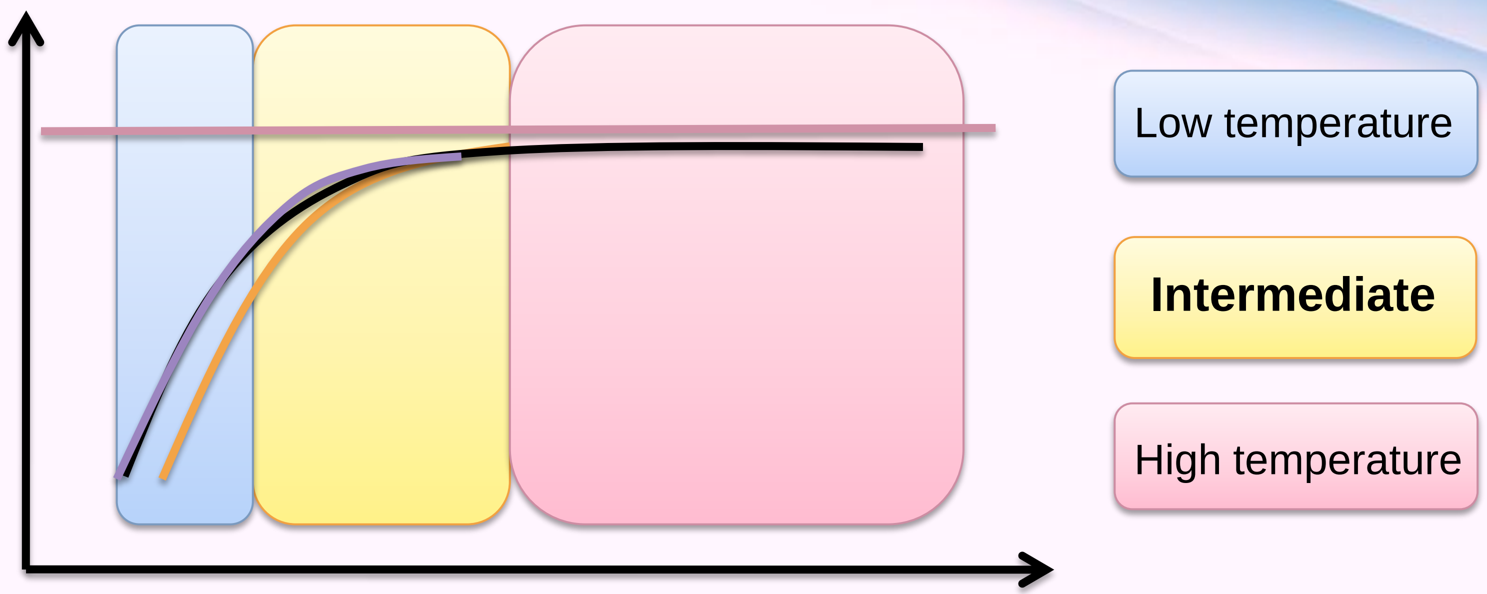
General form of specific heat

$$C_v = \frac{\partial}{\partial T}\frac{1}{V}\sum_s \int \frac{\hbar\omega_s(k)}{e^{\hbar\omega_s(k)/k_B T} - 1}\frac{4\pi k^2 L^3}{(2\pi)^3} dk$$

Quatum theory of Harmonic solid

- Bose-Einstein distribution function
- Stationary states of vibration

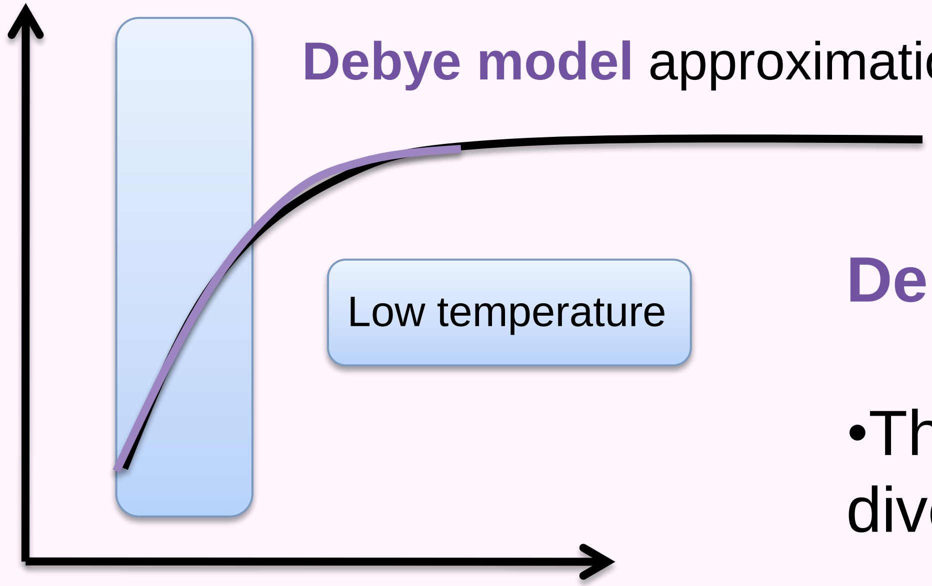
Specific heat

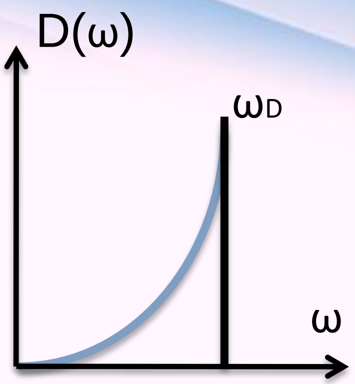


Different approximationa of temperature ranges:

- Low temperature: Debye model
- Intermediate temperature: Debye & Einstein
- High temperature: → Dulong-Petit

Specific heat
at Low temperature





Debye model

- The angular frequencies are diverse values.

- The maximum allowed value is cut-off frequency ω_D

Debye model

Specific heat

$$C_v = \frac{1}{V}\frac{\partial}{\partial T}\int_0^{\omega_D} D(\omega)\frac{\hbar\omega}{e^{\hbar\omega/k_B T}-1}d\omega$$

↓

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

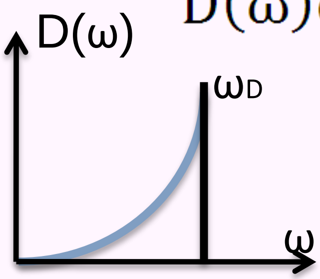
$$x = \frac{\hbar\omega}{k_B T}$$

- ✓Density of states
- ✓Energy per phonon
- ✓Bose-Einstein distribution
- ✓Cut-off frequency

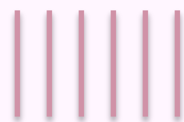
$$U = 9nk_B T\left(\frac{T}{\theta}\right)^3 \int_0^{x_D} \frac{x^3 dx}{e^x-1}$$

Debye model

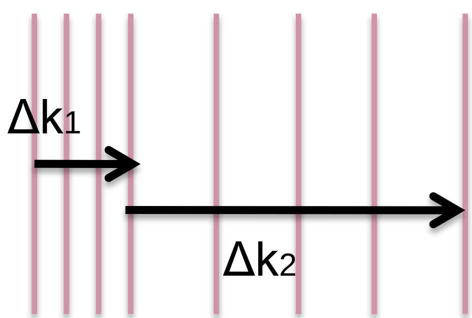
Density of states D(ω)



$$D(\omega)d\omega = \left(\frac{L}{2\pi}\right)^3 \int_0^{shell} d^3k$$



$$D(\omega) = \frac{V}{(2\pi)^3} \int^{shell} \frac{dS_\omega}{v_g}$$



The difference between constant ω surface is Δω

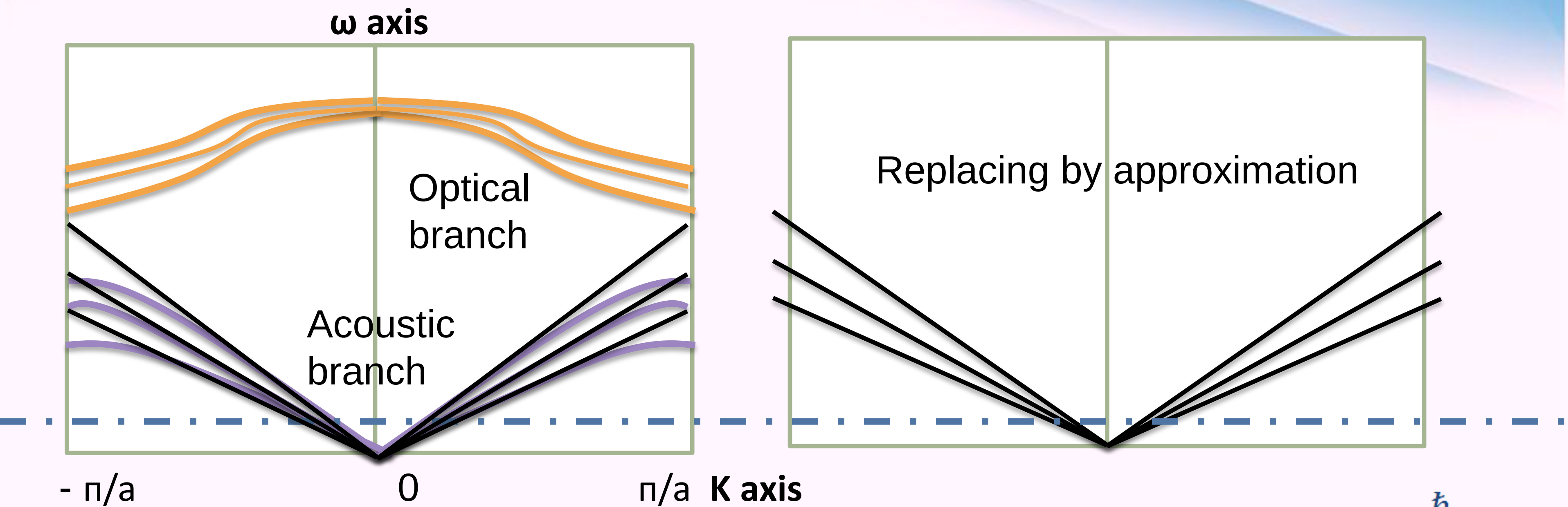
The spacing between constant frequency surface depends on (group velocity) dω/dk

For simple case that $v_p=v_g$
ω/k=constant=sound velocity

We can get approximation D(ω) of Debye model (low temperature)

$$D(\omega) = \frac{V\omega^2}{2\pi^2 v^3}$$

Specific heat at Low temperature



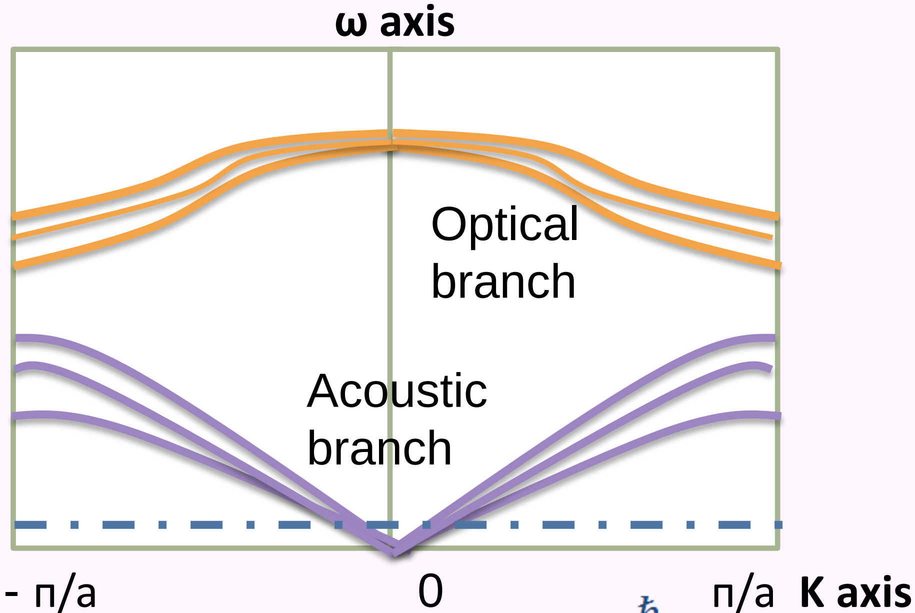
$$\omega = \frac{\hbar}{k_B T}$$

Dispersion relation

- Ignored optical branches
- Replace acoustic branch with liner branches

Specific heat at Low temperature

$$C_v = \frac{\partial}{\partial T}\frac{1}{V}\sum_s \int \frac{\hbar\omega_s(k)}{e^{\hbar\omega_s(k)/k_B T} - 1}\frac{4\pi k^2 L^3}{(2\pi)^3}dk$$



$$\omega = \frac{\hbar}{k_B T}$$

When T is small

High frequencies result in large $e^{\hbar\omega/k_B T}$

The contributions of high frequencies for **LOW** temperature are negligible.

Specific heat at Low temperature

$$C_V = \frac{\partial}{\partial T}\frac{1}{V}\sum_s \int \frac{\hbar\omega_s(k)}{e^{\hbar\omega_s(k)/k_B T}-1}\frac{4\pi k^2 L^3}{(2\pi)^3}dk$$

$$\omega_s(k) = c_s(k)k$$

$$C_V = \frac{\partial}{\partial T}\sum_s \int_0^\infty \frac{\hbar c_s(k)k^3}{e^{\hbar c_s(k)k/k_B T}-1}\frac{dk}{2\pi^2}$$

$$\frac{1}{c_{ave}^3} = \frac{1}{3}\sum_s \int \frac{d\Omega}{4\pi} \times \frac{1}{c_s(k)^3}$$

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

$$\sum s = 3$$

$$x = \frac{\hbar\omega}{k_B T}$$

$$C_V = \frac{\partial}{\partial T}\frac{(k_B T)^4}{(\hbar c_{ave})^3}\frac{\pi^2}{10} = \frac{2\pi^2}{5}\frac{k_B^4 (T)^3}{(\hbar c_{ave})^3}$$

$$\int_0^\infty \frac{x^3}{e^x-1}dx = \frac{\pi^4}{15}$$

Specific heat at Low temperature

At very **low temperature**

Specific heat

$$C_V \cong \frac{2\pi^2}{5}\frac{k_B^4 (T)^3}{(\hbar c_{ave})^3}$$

Which is **Debye** T^3 **law**

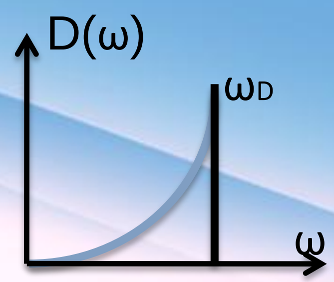
Condition assumption:

- Only Acoustic modes are thermally excited
- For actual crystals Temperature may necessary to be below T=θ/50

θ :Debye temperature

$$C_V \cong \frac{12\pi^4}{5} N k_B \left(\frac{T}{\theta}\right)^3$$

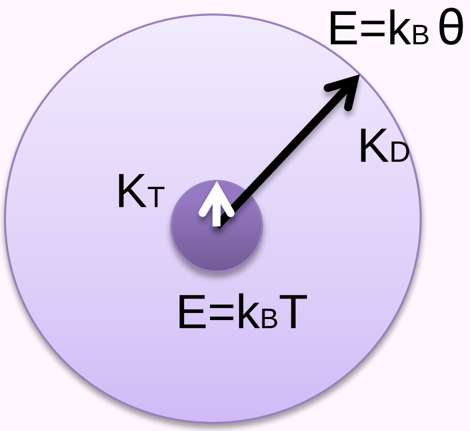
Debye temperature



Determine a cut-off frequency of specimen

$$N = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi k^3}{3} = \frac{V}{6\pi^2}(\omega v)^3$$

$$\omega_D^3 = 6\pi^2 v^3 N/V \qquad K_D = \left(\frac{6\pi^2 N}{V}\right)^{\frac{1}{3}}$$



$$C_v = \frac{1}{V}\frac{\partial}{\partial T}\int_0^{\omega_D} D(\omega)\frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}\,d\omega$$

Define Debye temperature θ in terms of cut-off frequency

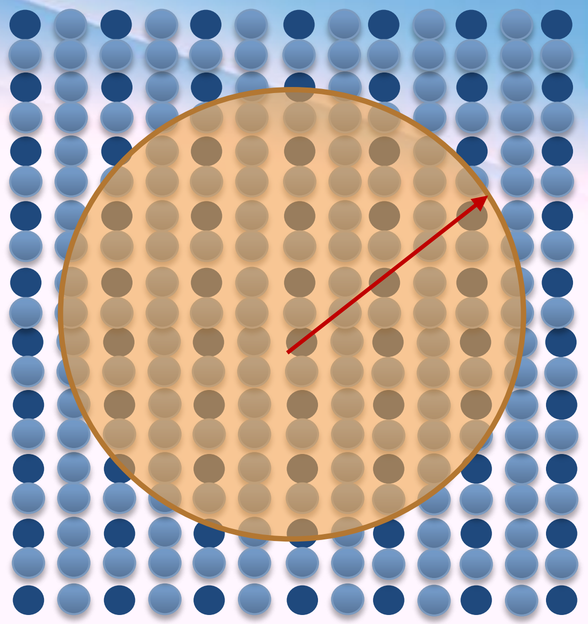
$$x_D = \frac{\hbar\omega_D}{k_B T} \equiv \frac{\theta}{T} \qquad \theta = \frac{\hbar v}{k_B}\left(\frac{6\pi^2 N}{V}\right)^{\frac{1}{3}}$$

Debye temperature

$$\theta = \frac{\hbar v}{k_B}\left(\frac{6\pi^2 N}{L^3}\right)^{\frac{1}{3}}$$

L: length of specimen

N: number of ions in specimen (total vibration modes)



Compare boundary conditions:

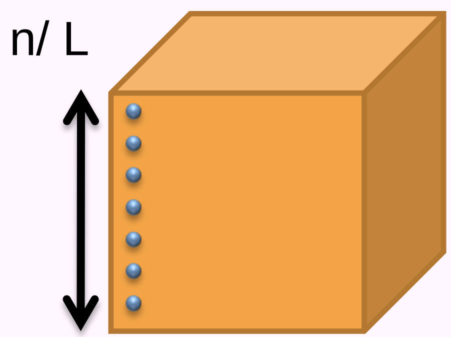
Brillion Zone (atom spacing) $K \leq \frac{\pi}{a}$

Cut off frequency (atom packing) $K \leq K_D = \left(\frac{6\pi^2 N}{V}\right)^{\frac{1}{3}}$

For ideal simple cubic specimen

$$\frac{\sqrt[3]{N}}{L} = \frac{n}{L} = \frac{1}{a} \qquad K_D = \frac{(6\pi^2)^{\frac{1}{3}}}{a}$$

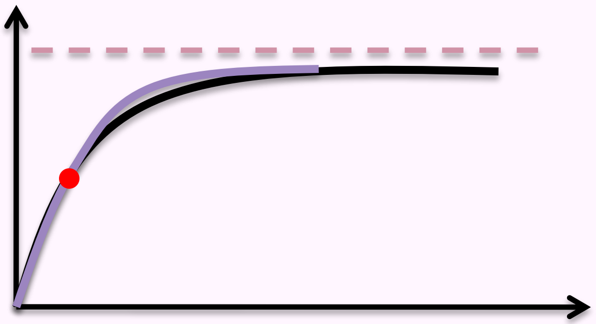
KD are different with different kinds of lattice packing



Debye temperature

What are the factors that determine Debye temperature?

Theoretical : $\theta = \frac{\hbar v}{k_B}(\frac{6\pi^2 N}{V})^{\frac{1}{3}}$



v(ρ,K,G): sound velocity in the specimen
N/V: atom concentration (packing density)

Experimental:

The Debye temperature were determined by fitting the observed specific heats Cv formula at the point of ½ Dulong-Petit value ($3Nk_B/2$)

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

Debye temperature

$$\theta \propto v \times (\frac{N}{V})^{\frac{1}{3}}$$

Element	Li	Na	K	Rb	Cs
Crystal structure	Bcc	Bcc	Bcc	Bcc	Bcc
Concentration 10^22 /cm^3	4.7	2.652	1.402	1.148	0.905
Sound speed m/s	6000	3200	2000	1300	~
Debye temperature	344	158	91	56	38
	334	151.6	76.6	46.6	
Element	Be	Mg	Ca	Sr	Ba
Crystal structure	Hcp	Hcp	Fcc	Fcc	Bcc
Concentration 10^22 /cm^3	12.1	4.3	2.3	1.78	1.6
Sound speed m/s	12870	4640	3810	~	1620
Debye temperature	1440	400	230	147	110
	1011.3	258.3	172.1		64.9

Future work

- Intermediate region
- High temperature region

- Electron Effect

Thanks for your attention