Subgroup meeting-08/24

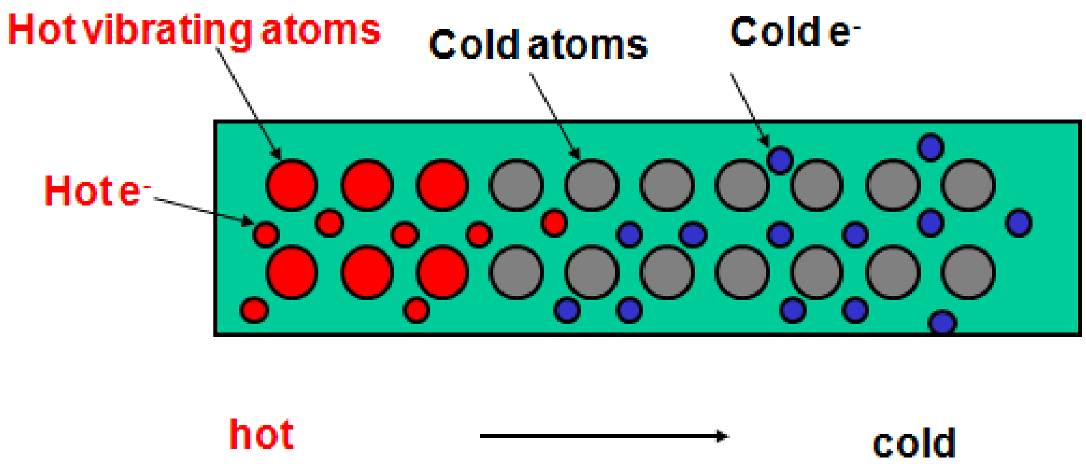
Introduction of thermal transport

Members: 盧孟珮
楊祥宏
王虹之

Outline

- Introduction
- Phonons
- Specific heat of solid
- Conclusion
- Q and A

Introduction



- **Electronic charge carriers** and **Phonons**.

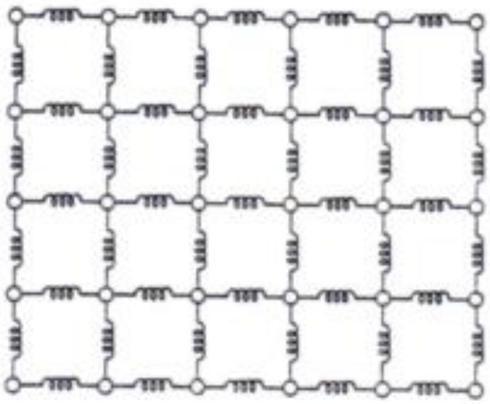
$$\kappa_{total} = \kappa_e + \kappa_L$$

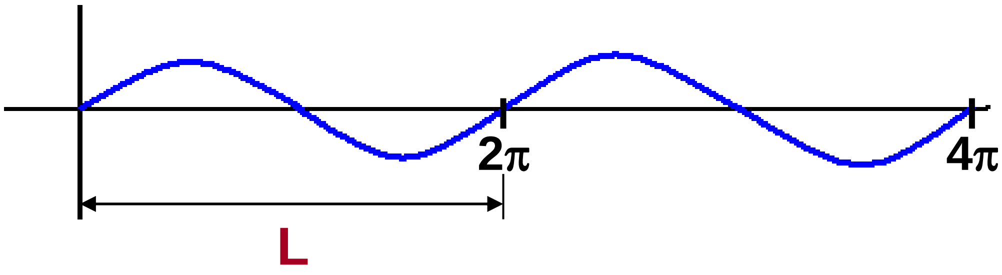
(κ is thermal conductivity)

Phonons

- **Quasiparticle**
  quantization of the modes of lattice vibrations of periodic ,elastic crystal structure of solid.

- **Lattice waves(lattice vibration)**





Moreover..

Specific heat of solids

- $c = Q/m\Delta T$

- *For fixed volume:* $C_v = \left(\frac{\partial E}{\partial T}\right)_V$

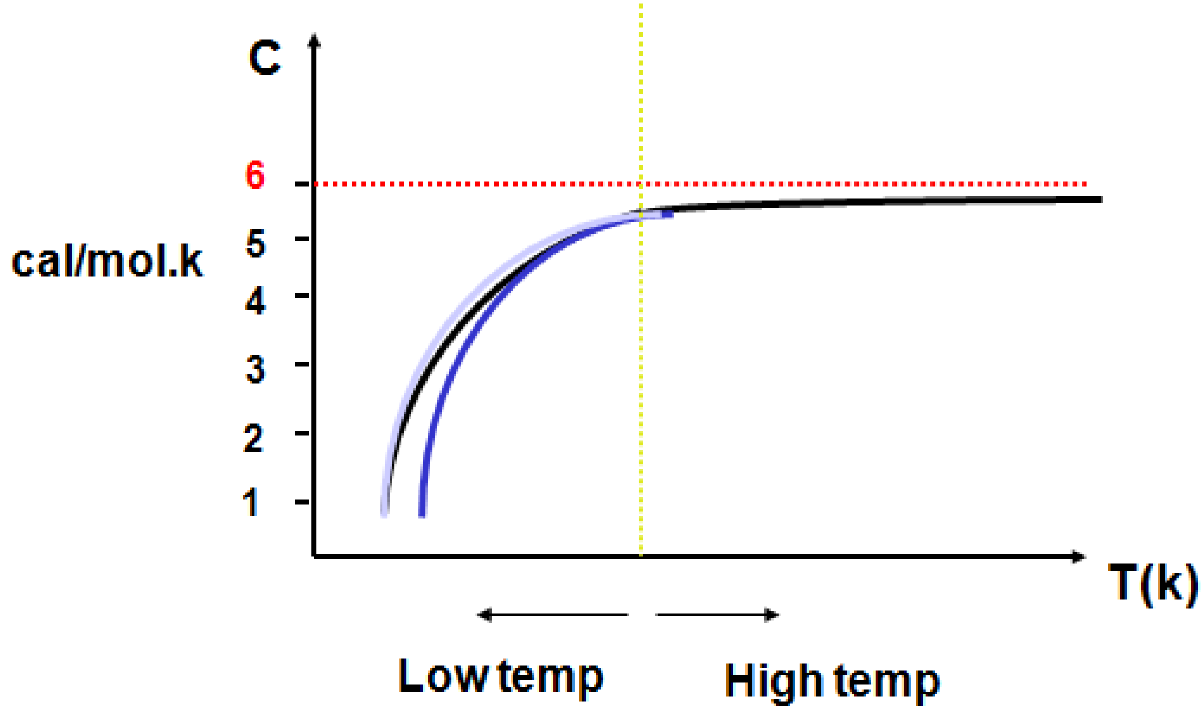
- Three models

➢ Dulong-Petit model

➢ Bose-Einstein model

➢ Debye model

Three models



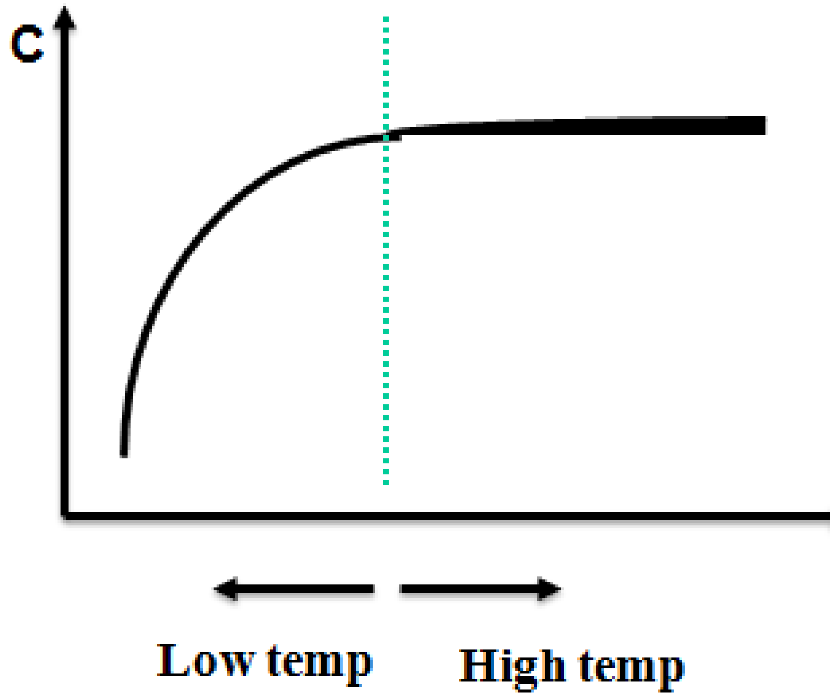
— 實驗值

······ Law of Dulong –Petit, based on Maxwell-Boltzmann distribution

— Bose-Einstein model

— Debye model

Q: why specific heat of solid behaves differently at low and high temp?



A: Quantum effect emerges at low temp, and this effect is disturbed by thermal energy at high temp.

Dulong and Petit

- Maxwell-Boltzman distribution function

$E = k_B T$.... (k_B: Boltzman const)

three dimension, $E = 3k_B T$

$C_v = \partial E/\partial T = \partial Q/\partial T$

$C_v = 3k_B$

only valid at high temp regime!

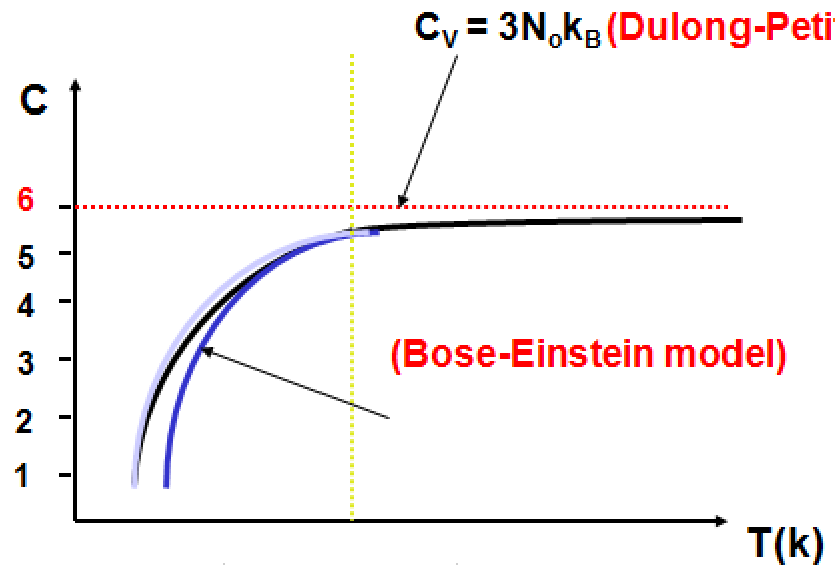
specific heat of solid must be calculated in different ways at low and high temps respectivel

Bose-Einstein model

- **Assumption**

- Three dimension harmonic oscillator
- Vibrate independently
- same frequency

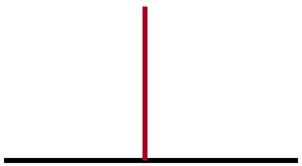
Deviation



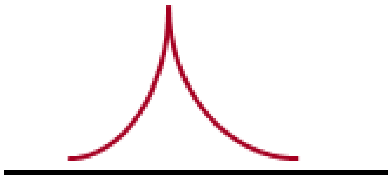
- Fail to valid in low temp
- Mistake 1: only one atomic vibration frequency (ω_E)
- Mistake 2: no interaction between individual phonons.

Debye model

- **Assumption**
- Similar to black body
- Vibrate dependently as elastic standing waves (differ from Bose-Einstein model)
- Frequency 0~ν



frequency (Einstein model)



Frequency distribution (Debye model)

Debye model

- atomic vibrations as phonons in a box

$$\lambda_n = \frac{L}{2n}$$

$$E_n = \hbar\omega_n = \frac{hv}{\lambda_n} = \frac{2nhv}{L}$$

- Bose-Einstein statistics

$$\overline{N}(E_n) = \frac{1}{e^{E/kT} - 1}$$

Debye model

- The energy in solid

$$U = \sum E_n \overline{N(E_n)}$$

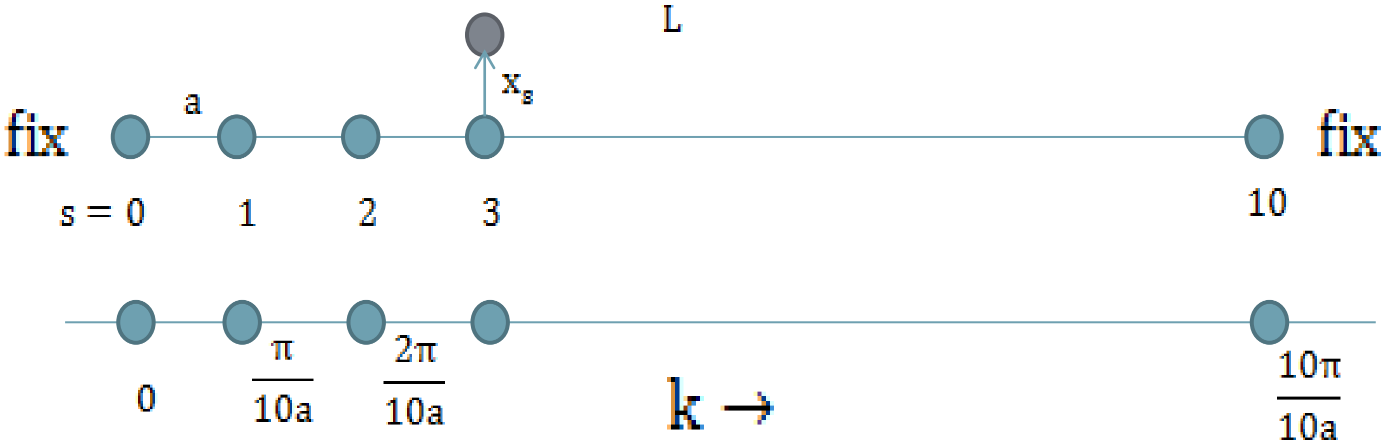
$$U = \sum_K \sum_P \frac{\hbar\omega_{K,P}}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

$$U = \sum_P \int \frac{\hbar\omega_{K,P}}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} D_P(\omega) d\omega \qquad D(\omega) = \text{density of modes/states}$$

Debye model-

frequency distribution

1-D normal vibration mode

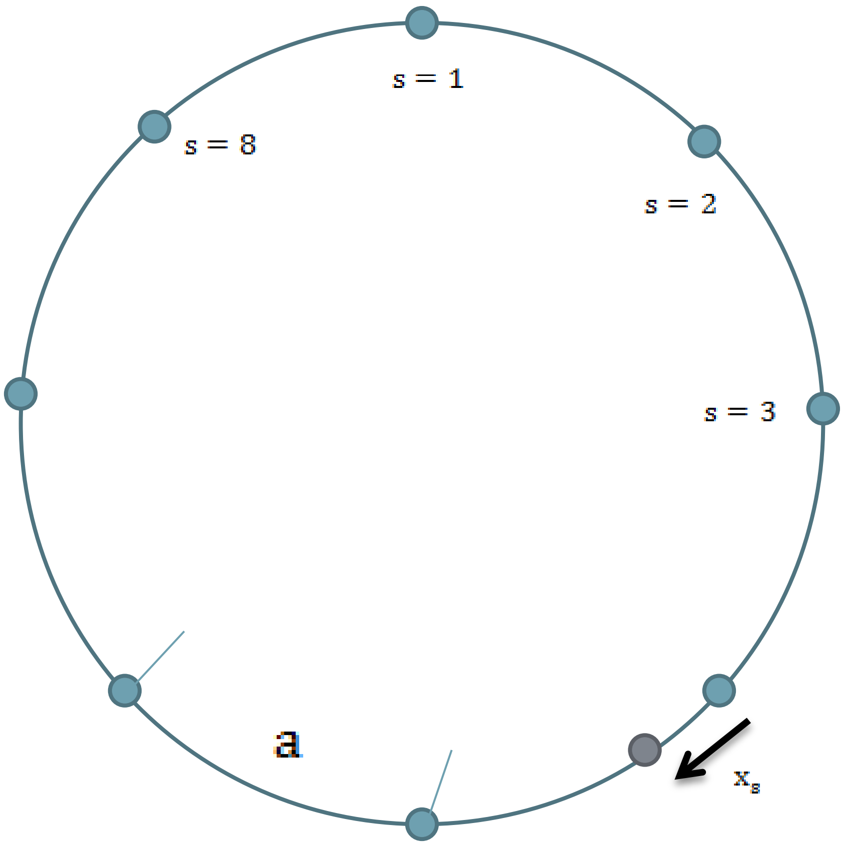


$$x_s = x(0)\exp\left(-i\omega_{K,p}t\right)\sin sKa$$

$$K = \frac{\pi}{L}\ ,\ \frac{2\pi}{L}\ ,\ \ldots.\frac{(N-1)\pi}{L}$$

Debye model-
frequency distribution

periodic boundary



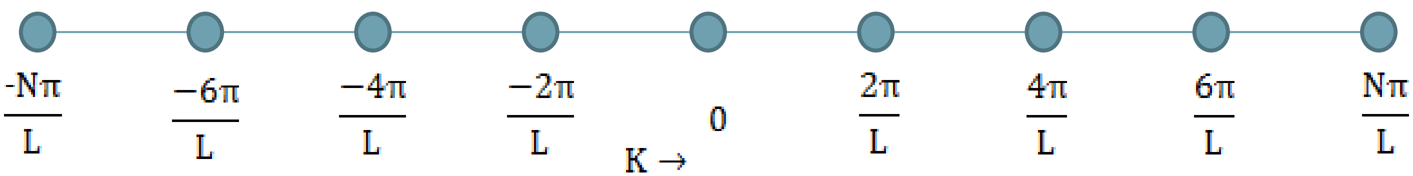
$$x(sa) = x(sa + L)$$

- sin(sKa),cos(sKa)
- boundary conditions
  NKa = 2nπ
- For K=0，K=8π/8a，
  sin(sKa) is meaningless

Debye model-

frequency distribution

periodic boundary condition



$$K = 0\ ,\ \pm\frac{2\pi}{L}\ ,\ \pm\frac{4\pi}{L}\ ,\ \ldots\ ,\ \frac{N\pi}{L}\quad ,\quad \Delta K = \frac{2\pi}{L}$$

Debye model-
frequency distribution

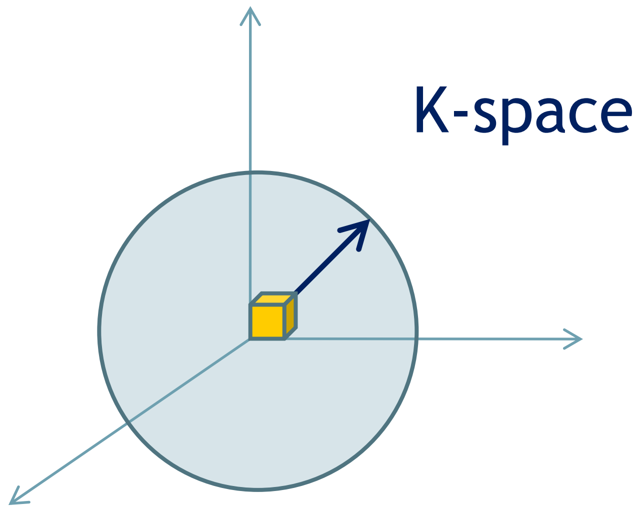
3-D normal vibration density of states

- The allowed K is $(\frac{2\pi}{L})^3$

- The number of allowed states

$$N = (\frac{4\pi K^3}{3})/(\frac{2\pi}{L})^3$$

$$D(\omega) = \frac{dN}{d\omega} = \left(\frac{VK^2}{2\pi^2}\right)(\frac{dK}{d\omega})$$



Debye model- frequency distribution

- The approximation of Debye model

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

- Debye frequency

$$\omega_D{}^3 = \frac{6\pi^2 v^3 N}{V}$$

Debye model

- The energy in solid

$$U = 3 \times \int_0^{\omega_D} \left(\frac{V\omega^2}{2\pi^2 v^3}\right) \left(\frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}\right) d\omega$$

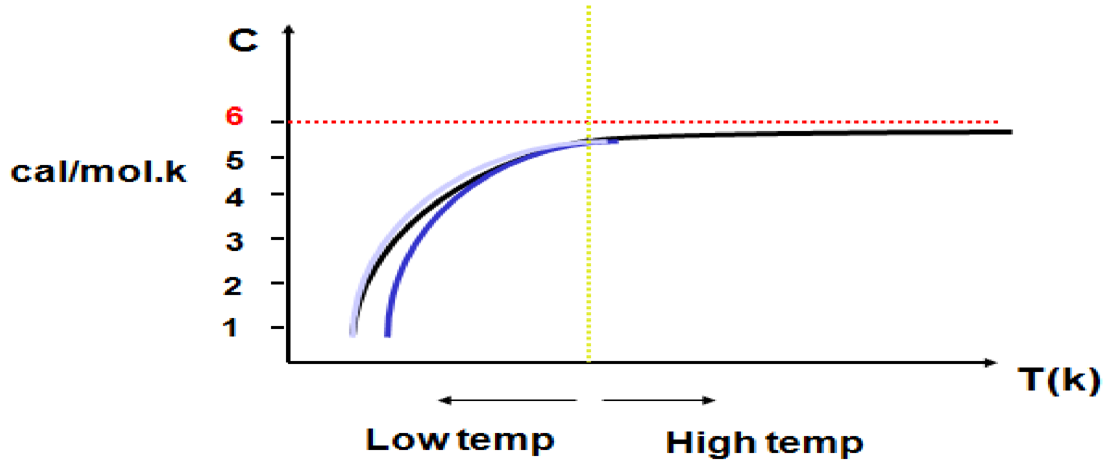
- Debye temperature is defined as θ

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

- **The energy in solid (Debye model)**

$$U = 3Nk_B T D_3\left(\frac{\theta}{T}\right) \qquad C_V = 9Nk_B\left(\frac{\theta}{T}\right)^3 \int_0^{x_D} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

Conclusion



Lattice thermal transport:
(wave-particle duality description)

Classical mechanics: wave-like phenomena
Quantum mechanics: particle-like properties

Thanks for your attention!!

Q and A