Subgroup meeting-09/07

Introduction of thermal transport

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OUTLINE

- 2010.08.24
- brief introduction of thermal conductivity
- Phonons
- Debye model

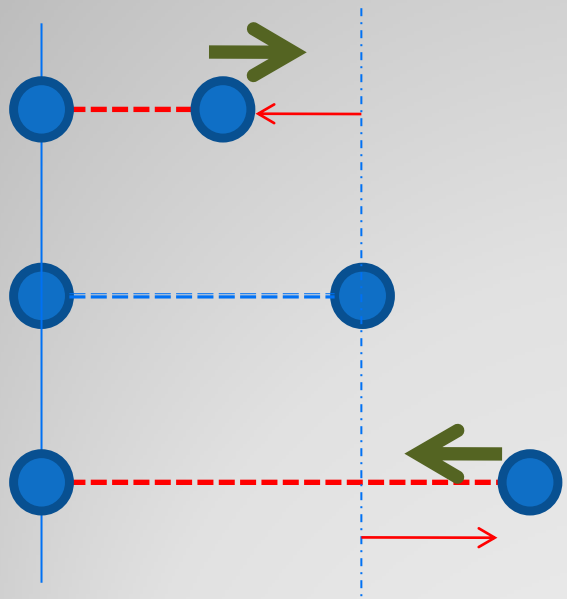
- 2010.09.07
- Questions
- K-space and reciprocal space
- Brillouin zone

Outline 2010.09.07

- review questions
- K-space
- Reciprocal lattice
- Brillouin zone
- Future work

Review questions

- How do atoms oscillate? Hooke's law



壓縮　|U|=max　K=0

平衡位置　U=0　K=max

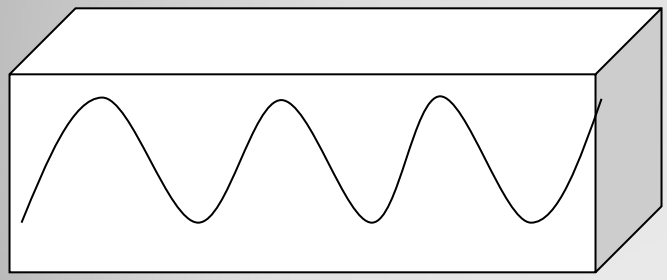
伸長　|U| =max　K=0

$$U = -\int kxdx = \frac{1}{2}kx^2$$

Review questions

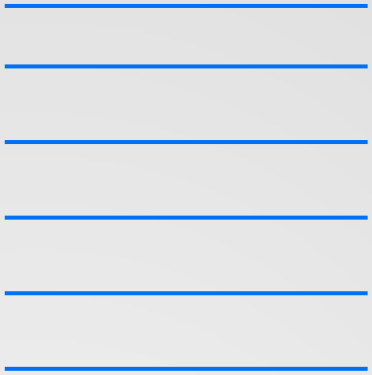
- Why the energy of phonon is not continuous?

Wave in a box

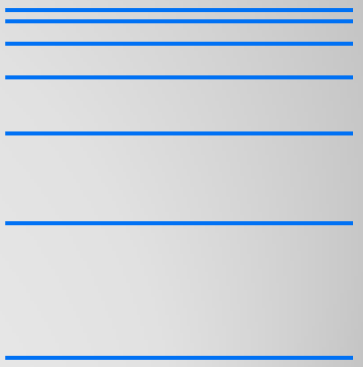


Energy levels

Oscillator

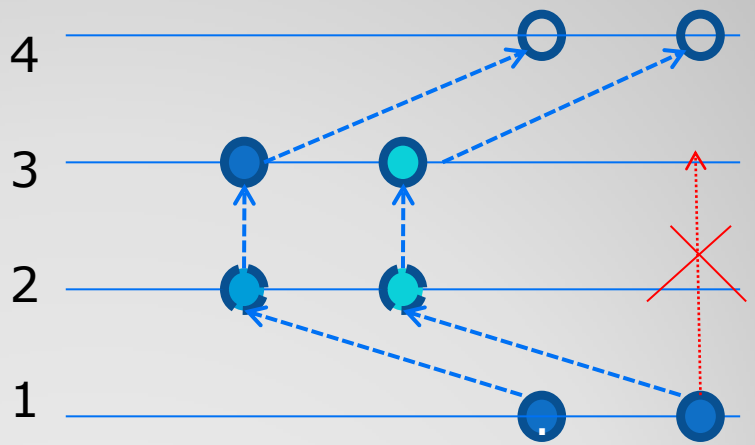


Particle in a box



Review questions

- Why we can ignore electron effect at specific heat of solid ?
- Electron → fermions obey the exclusion principle



- we should consider the contribution of electrons at very low temperature

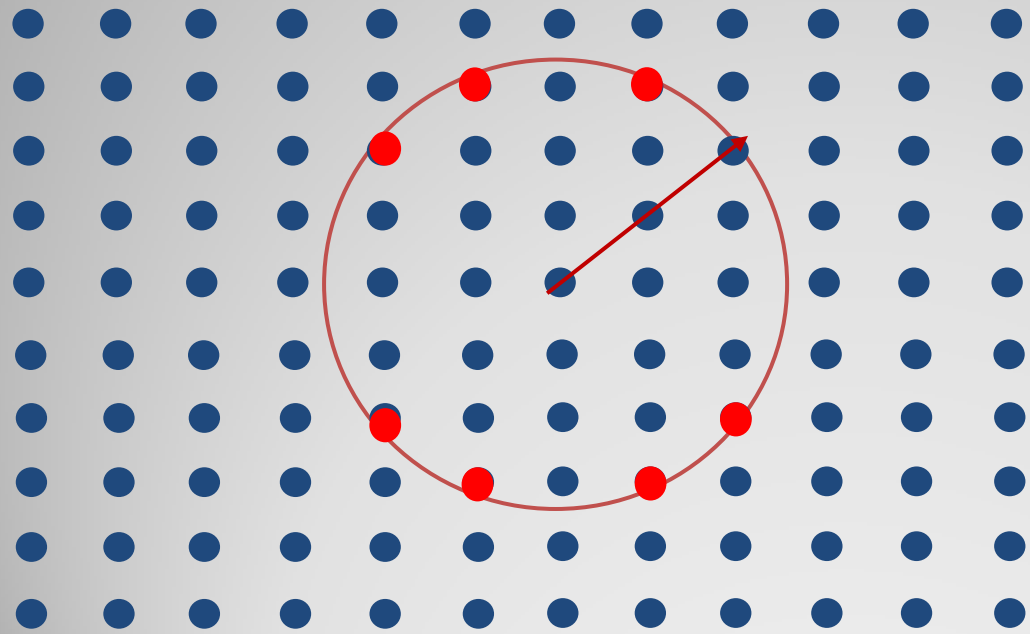
K-space

Blue point

$$K = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \ldots\ldots + \frac{2n\pi}{L}$$

Red circle

$$K = \left|\frac{2\pi}{\lambda}\right| = \left|\frac{\pi}{na}\right|$$



Reciprocal lattice

- **Definition**

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}, \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}, \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}$$

- **Unit**

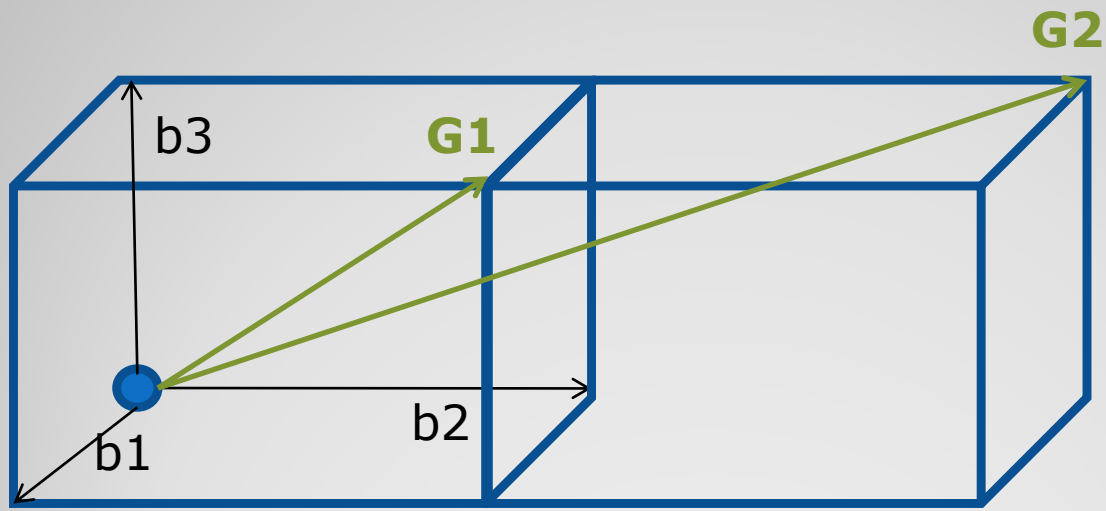
Lattice: length

Reciprocal lattice: 1/length

Reciprocal lattice

- Reciprocal vector

$$G = v_1 b_1 + v_2 b_2 + v_3 b_3$$



Reciprocal lattice

- points in reciprocal space can be corresponded with collective vectors pointing from the origin → G

- Common lattices comparison

lattice	Reciprocal lattice	Description
SC	SC	Lattice constant a Reciprocal lattice constant $2\pi/a$
BCC	FCC	
FCC	BCC	

Fourier space

- The unit of the coordinate is (1/length)
- Fourier transform

- points in Fourier space can describe the character of waves
  → **wave constant K**
- Reciprocal lattice points are the correspondence of lattice points in Fourier space
  → **reciprocal lattice vector G**

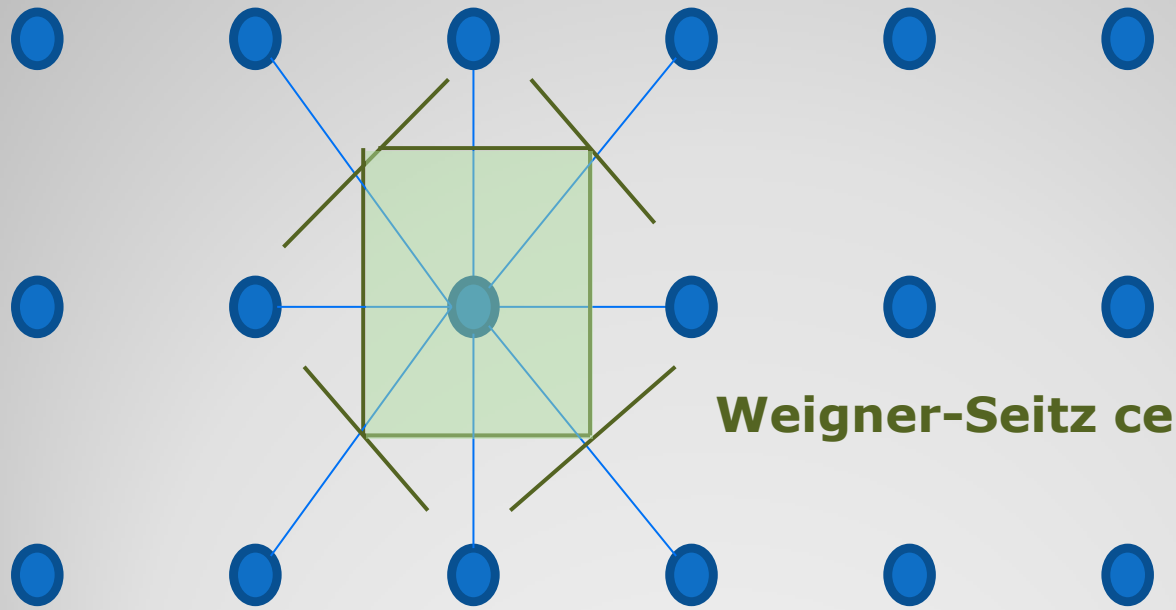
Brillouin zone

- The Wigner-Seitz cell in reciprocal space
- K can only be valid in First Brillouin zone for elastic wave
- First Brillouin zone

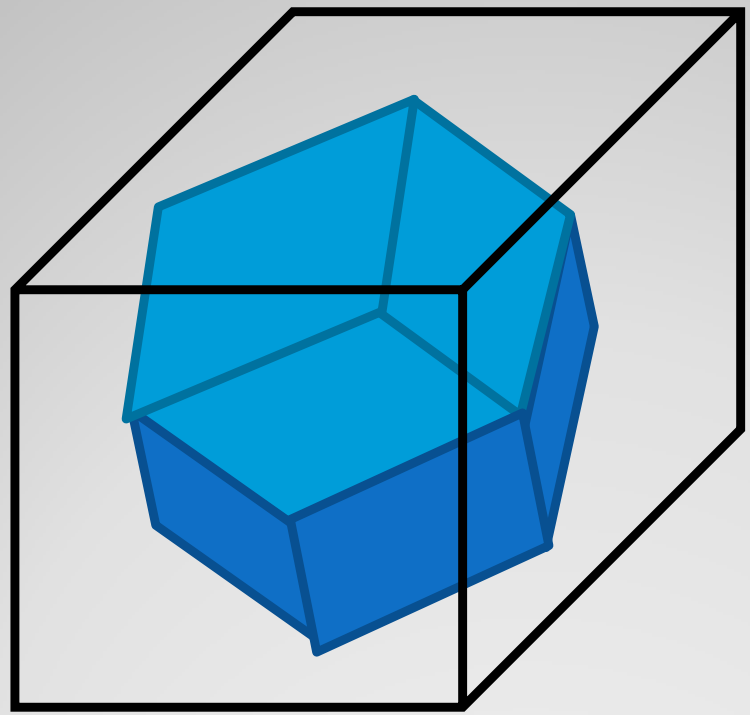
  $-\pi/a < K < \pi/a$

Brillouin zone

- How to get Brillouin zone?



Brillouin zone



FUTURE WORK

- 1.The mean free path of phonon
- 2.Thermal conductivity, density, heat capacity and mean free path
- 3.The scale of phonon engineering
- 4.Debye temperature of different material
- *The transport of phonons*
- *The thermal effect of electrons*

Thanks for your attention