Mineral Physics I
Chapter 3. Lattice vibration
Section 6. Dispersion relation of lattice vibration

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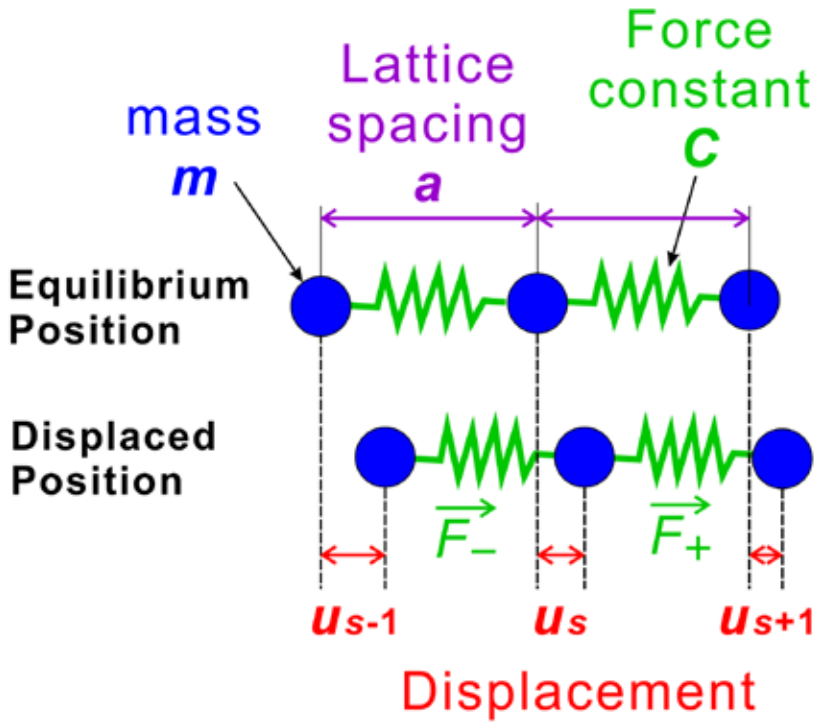
Forces on an atom by surrounding atoms -1

Ø One dimensionally aligned crystal.
- ü Composed of only one kind of atom
- ü The atomic mass: m
- ü The lattice spacing: a
- ü Bounded by springs with a force constant C

Ø The atom of interest: the number s
- u The position from the original point: $s \cdot a$
- ü The left neighboring atom: $s - 1$
  - u The position with respect to the original point: $(s - 1) \cdot a$
- ü The right neighboring atom: $s + 1$
  - u The position with respect to the original point: $(s + 1) \cdot a$



Forces on an atom by surrounding atoms -2

Ø Consider the net force on the atom of interest when the atoms are displaced

ü Caused by interaction with the neighboring atoms $s-1$ and $s+1$

ü Proportional to the difference in displacements (Hooke's law, harmonic approximation)

u Force by the left spring:

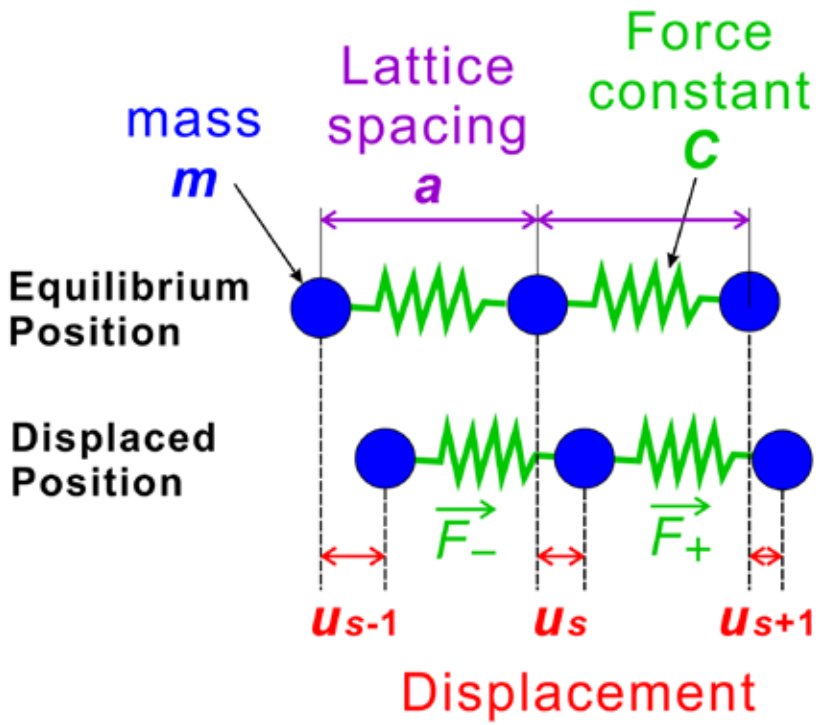
○ $F_- = C(u_{s-1} - u_s)$ (3.6.1)

u Force by the right spring:

○ $F_+ = C(u_{s+1} - u_s)$ (3.6.2)

u The net force to the s_{th} atom:

○ $F_s = F_- + F_+ = C(u_{s+1} - 2u_s + u_{s-1})$ (3.6.3)



Equation of motion of an atom in a 1D crystal

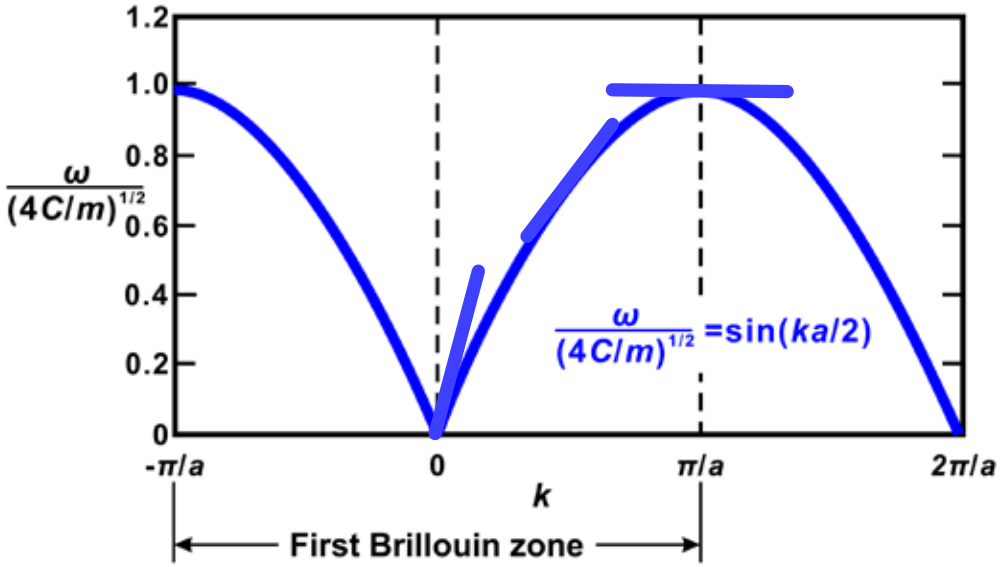
- The equation of motion of the s_{th} atom
  - $m\frac{\mathrm{d}^2u_s}{\mathrm{d}t^2} = F_s = C(u_{s-1} - 2u_s + u_{s+1})$ (3.6.4)
- Atomic vibration in a periodic lattice ⇒ ensemble of waves
  - ⇒ the solution in the form of a wave function:
    - $u_s = A\exp(\pm ikx)\exp(i\omega t) = A\exp(\pm iksa)\exp(i\omega t)$ (3.6.5)
      - sa: the distance from the original point, or the position of the oscillation
- By substituting (3.2.4) to (3.2.5), we have
  - $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}[A\exp(\pm iksa)\exp(i\omega t)]$
    $= C[A\exp(\pm ik(s-1)a)\exp(i\omega t) - 2A\exp(\pm iksa)\exp(i\omega t) + A\exp(\pm ik(s +$

Dispersion relation

Ø By simplifying Eq. (3.6.6) $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}[A\exp(\pm iksa)\exp(i\omega t)] = C[A\exp(\pm ik(s -$

Shape of dispersion relation

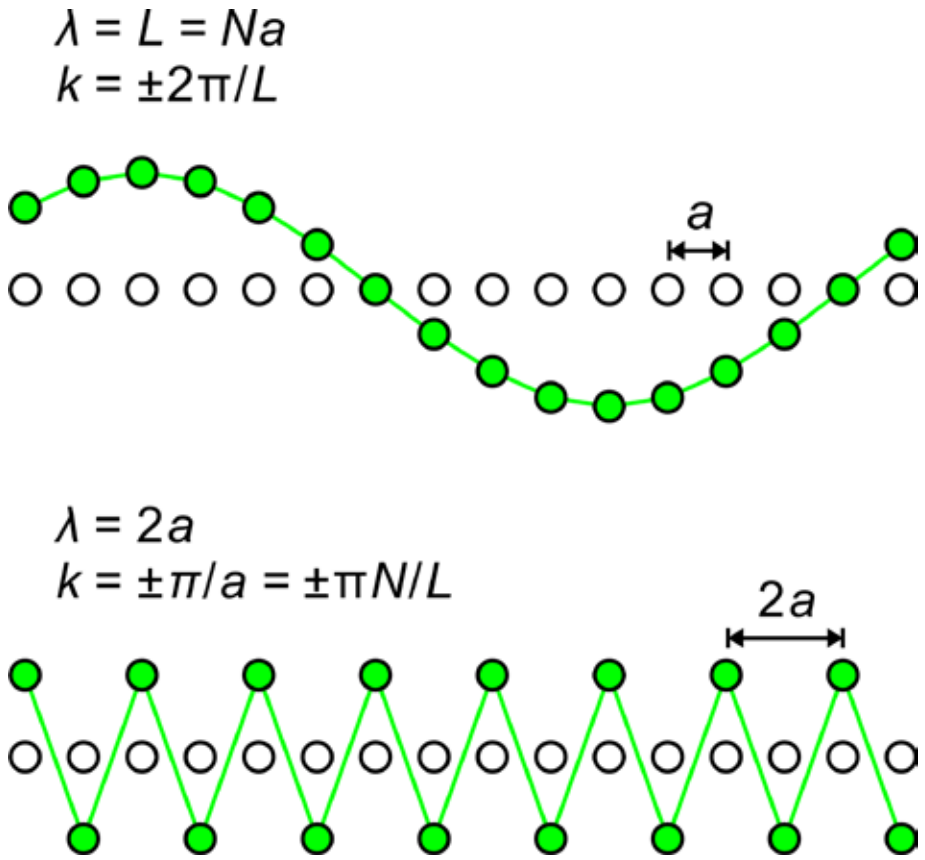
- Group velocity of lattice waves: $v_g = d\omega/dk$
  - At low ω and k, or long T and λ
    - high v_g
      - Macroscopic elastic waves are faster than lattice vibration waves
    - Nearly linear ($\sin x \cong x$)
      - $v_g = d\omega/dk \cong \omega/k = v_P$
      - The group velocity = the phase velocity
  - Very low v_g at high ω and k
    - $v_g = 0$ at $\omega = \pi/a$ (3.6.8)
      - What situation?



$$\omega = \sqrt{4C/m}\,\sin(ka/2)$$

Waves in a discrete lattice

- A 1D crystal is a collection of atoms
  - Ø Limited number of atoms à limited size
    - ü The dimension of a *N*-atom crystal: $L = (N-1)a$
    - ü The longest wave length: $\lambda_{\max} = L$
    - ü The smallest wave number:
      - § $|k_{\min}| = 2\pi/L$ (3.6.9)
  - Ø Consists of discretely distributed atoms
    - ü Atomic spacing: a
    - ü The shortest wave length: $\lambda_{\min} = 2a$
    - ü The largest wave number:
      - § $|k_{\max}| = 2\pi/2a = \pi/a$ (3.6.10)
      - § $v_g = 0$, The wave is standing.



First Brillouin zone

q Two directions of wave propagation in 1D-lattice,

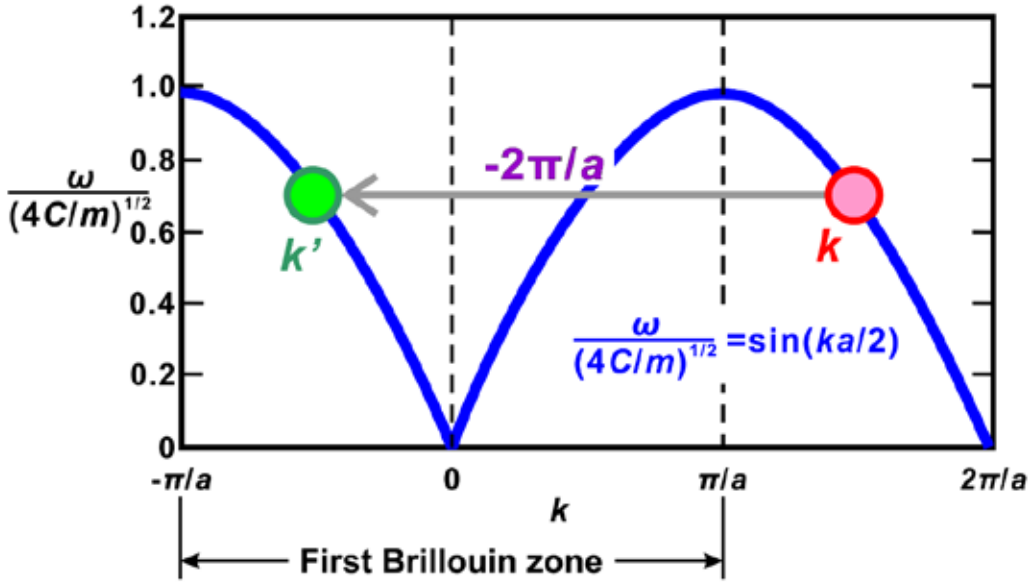
Ø $-\frac{\pi}{a} \leq k \leq +\frac{\pi}{a}$ (3.6.11)

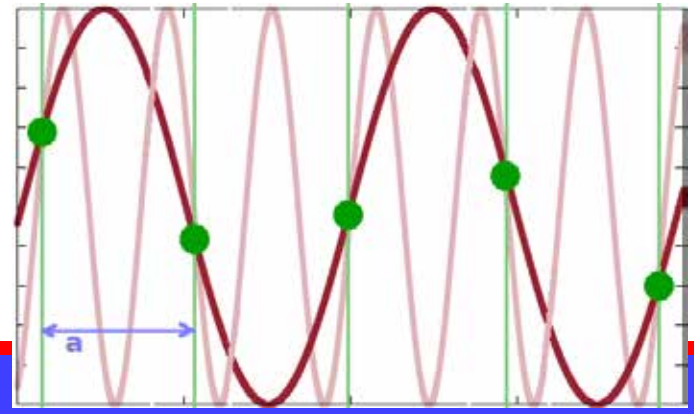
ü First Brillouin zone

q k out of the 1st BZ: identical to k' within the 1st BZ by $2\pi n/a$ shift (n: integer)

Ø $k' = k - 2\pi n/a$

$$A\exp(iksa)\exp(i\omega t) = A\exp(i(k' +$$





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