Subgroup meeting -2010/11/02
Introduction of thermal transport

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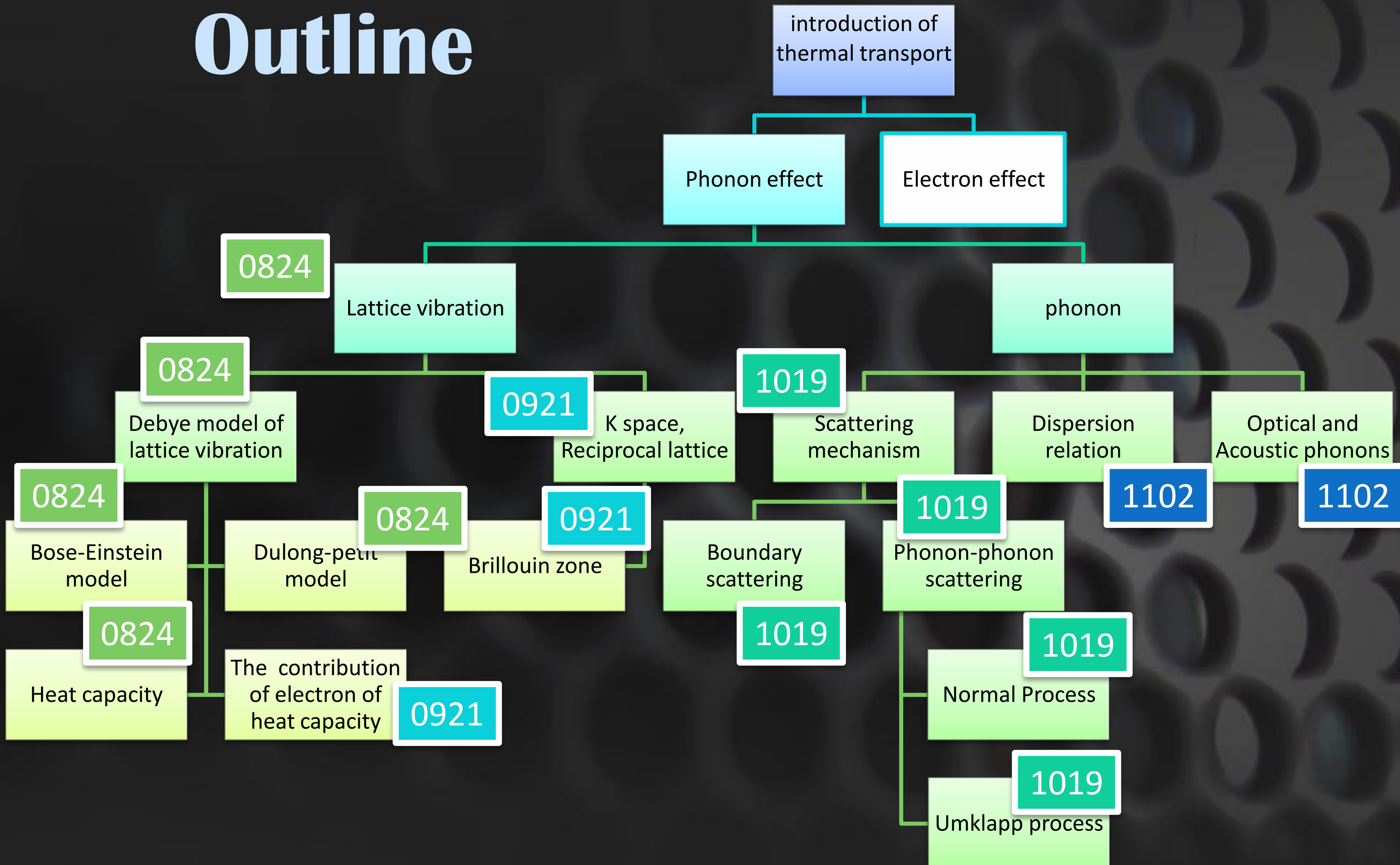
Outline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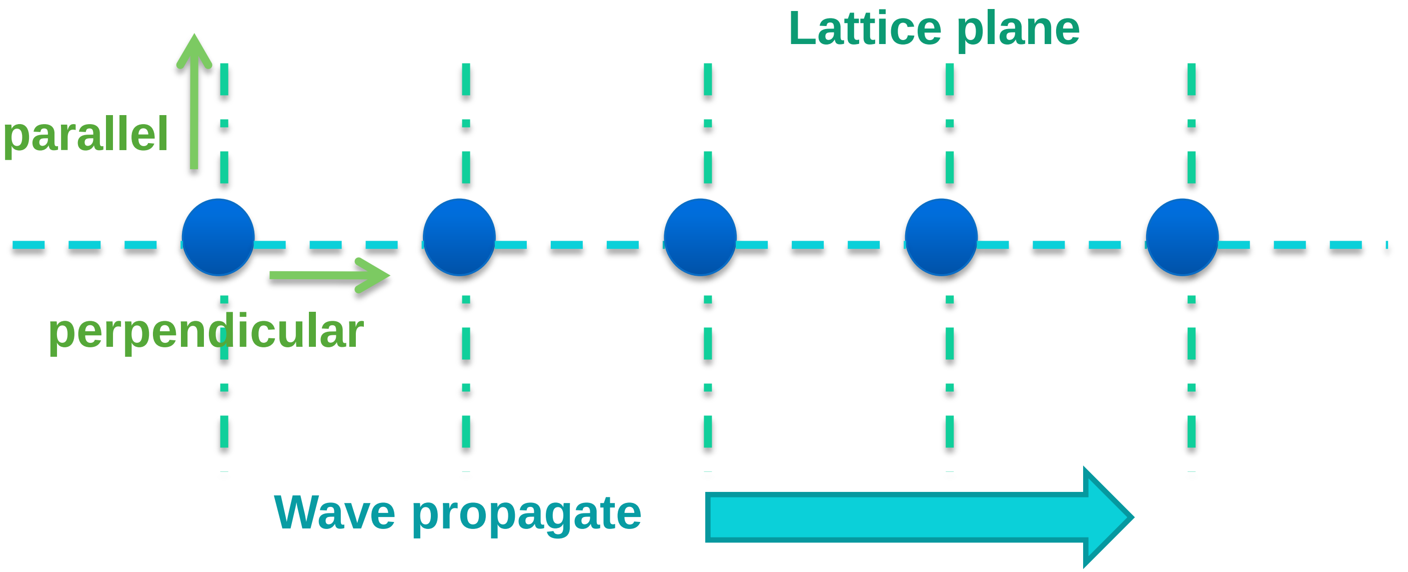
Outline 2010/11/02

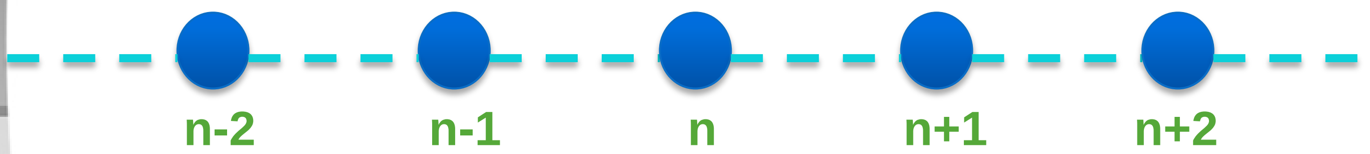
- Monatomic basis
  - dispersion relation
- Two kinds of atom basis
  - dispersion relation
  - two kinds of assumption
  - optical and acoustic phonons

Monatomic basis



- Directions of simplest mathematical solution
- [100] [110] [111]

Monatomic basis



- One Dimensional
- Consider only neighbor interactions

$$F_n = C(x_{n+1} - x_n) + C(x_{n-1} - x_n)$$

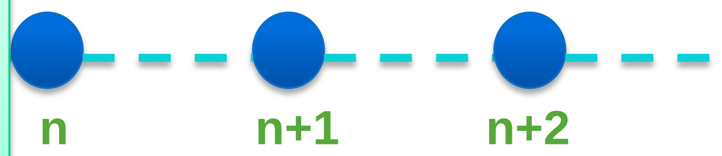
$$M\frac{d^2x}{dt^2} = C(x_{n+1} + x_{n-1} - 2x_n)$$

Monatomic basis

$$x_s = x\exp(isKa)\exp(+i\omega t)$$

$$x_{s+1} = x\exp(isKa + iKa)\exp(+i\omega t)$$

$$x_{s-1} = x\exp(isKa - iKa)\exp(+i\omega t)$$



$$\exp(iKa) + \exp(-iKa) = 2\cos Ka$$

- Solve the diff

$$-M\omega^2 x_s = C[\exp(iKa) + \exp(-iKa) - 2]x_s$$

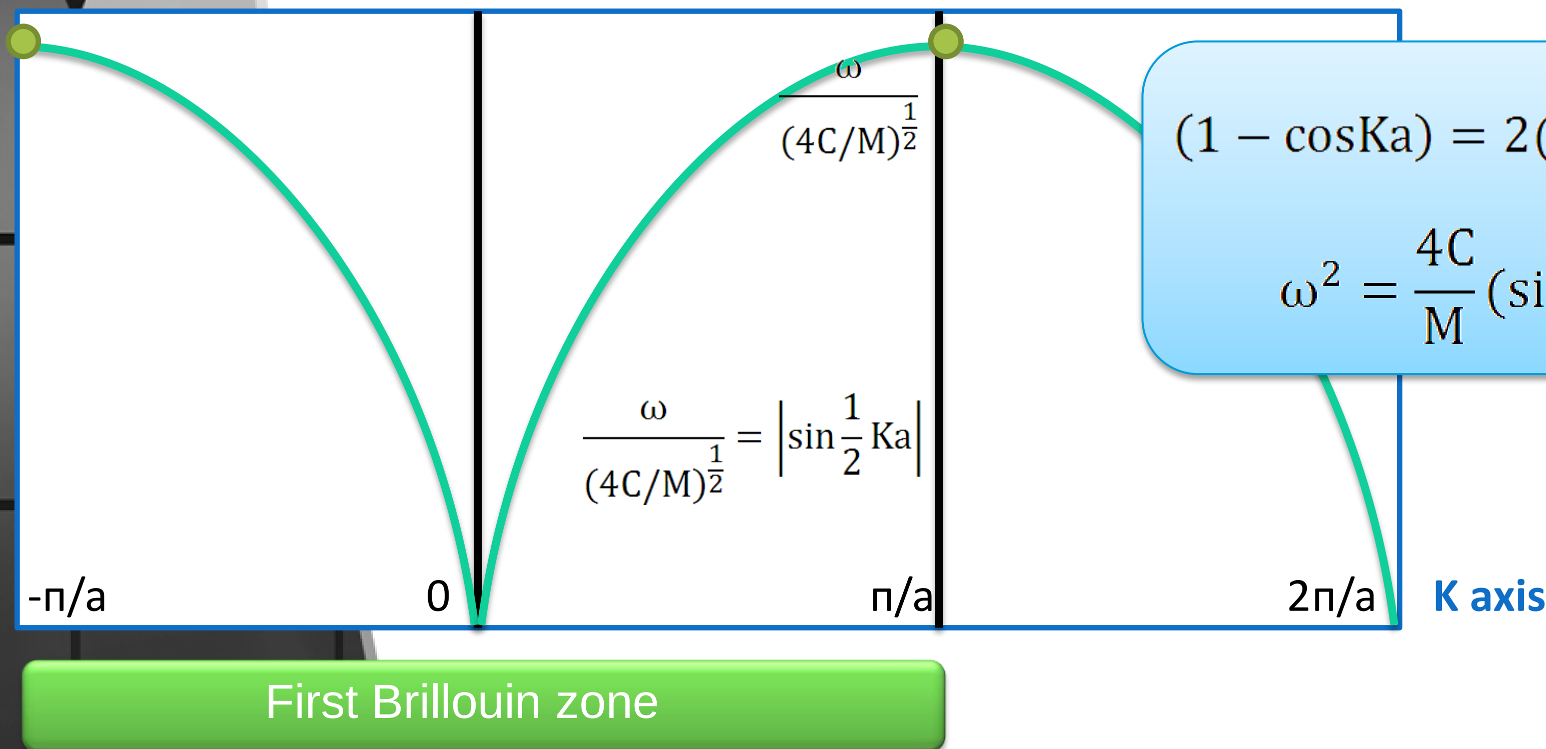
- We can get Dispersion Relation

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

Monatomic basis

- Plot the ω versus K

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



$$\frac{\omega}{(4C/M)^{\frac{1}{2}}}$$

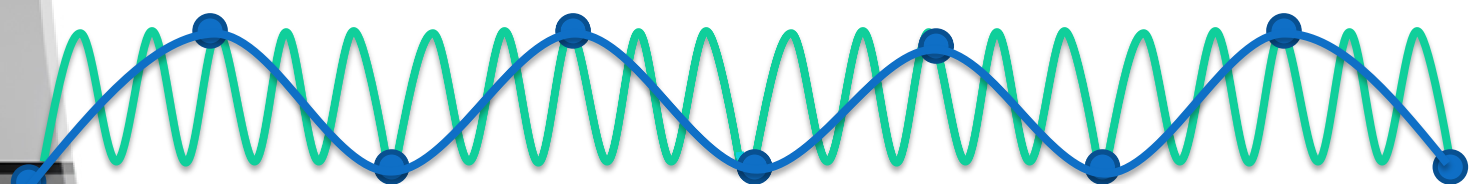
$$\frac{\omega}{(4C/M)^{\frac{1}{2}}} = \left|\sin\frac{1}{2}Ka\right|$$

$$(1 - \cos Ka) = 2(\sin^2\frac{1}{2}Ka)$$

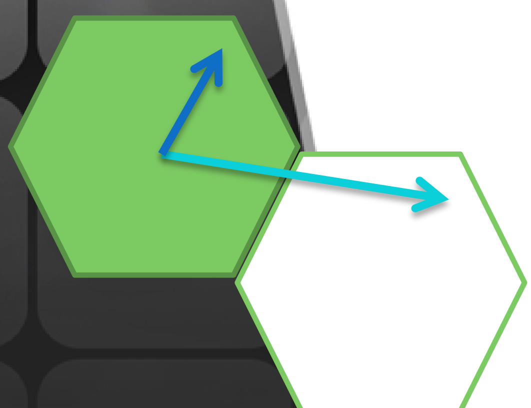
$$\omega^2 = \frac{4C}{M}(\sin^2\frac{1}{2}Ka)$$

Reminder of Brillouin zone

- Only when **-π/a <K< π/a**, K is valid

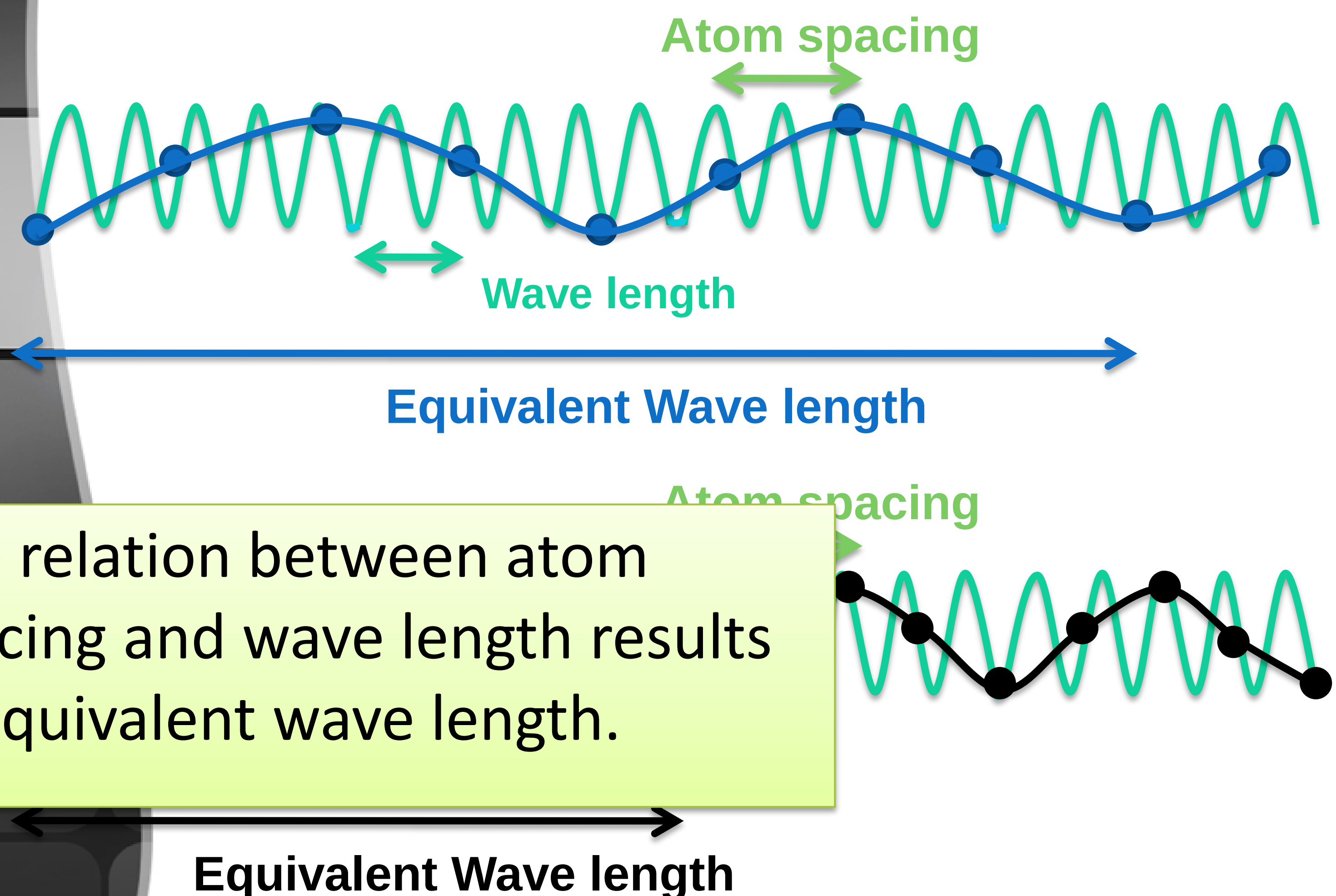


K is lager then π/a
The wave length is small then the spacing of atoms → meaning less



K’ is the valid equivalent of K

Reminder of Brillouin zone



- The relation between atom spacing and wave length results in equivalent wave length.

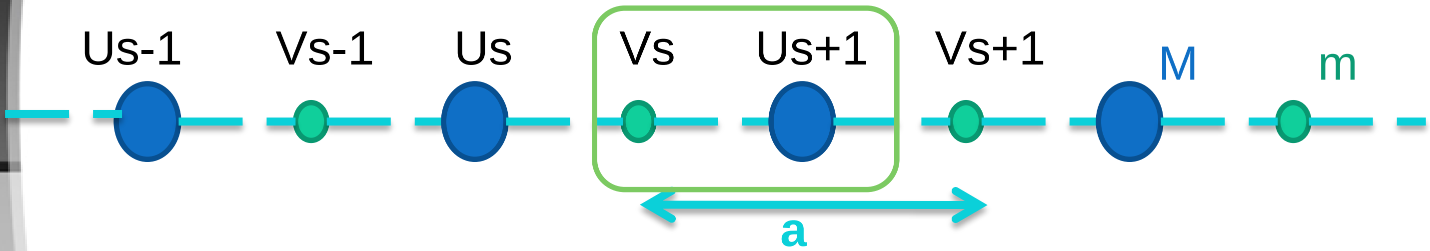
Two atoms basis

- One Dimension
- Two kinds of assumption

1. Different masses (M>>m)

2. Different springs (ions) (K,G)

Mass difference case



- Different masses M and m

$$M\frac{d^2u_s}{dt^2} = C(v_s + v_{s+1} - 2u_s)$$

$$m\frac{d^2v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$$

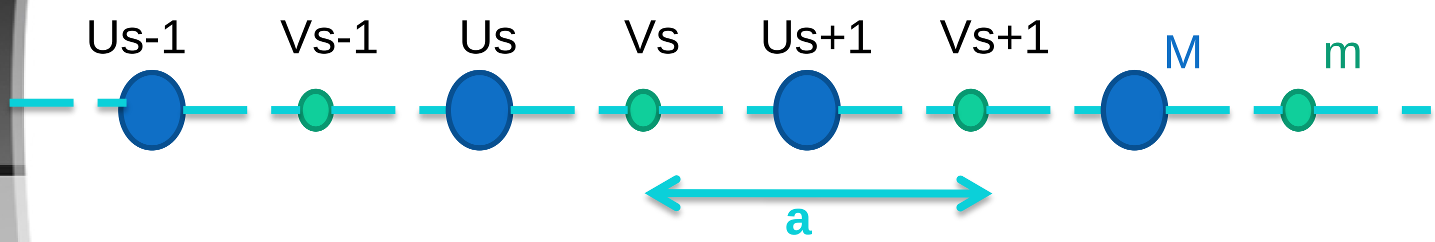
$$u_s = u\exp(isKa)\exp(-i\omega t)$$

$$v_s = v\exp(isKa)\exp(-i\omega t)$$

$$Mu = Cv[1 + \exp(-iKa)] - 2Cu$$

$$mv = Cu[\exp(iKa) + 1] - 2Cv$$

Mass difference case



$$(2C - \omega^2 M)u - Cv[1 + \exp(-iKa)] = 0$$

$$-Cu[\exp(iKa) + 1] + (2C - \omega^2 m)v = 0$$

- The homogeneous linear equation have a solution only if

$$\begin{vmatrix} (2C - \omega^2 M) & -C[1 + \exp(-iKa)] \\ -C[\exp(iKa) + 1] & (2C - \omega^2 m) \end{vmatrix} = 0$$

Mass difference case

Solve $$Mm\omega^4 - 2C(M+m)\omega^2 + 2C^2(1-\cos Ka) = 0$$

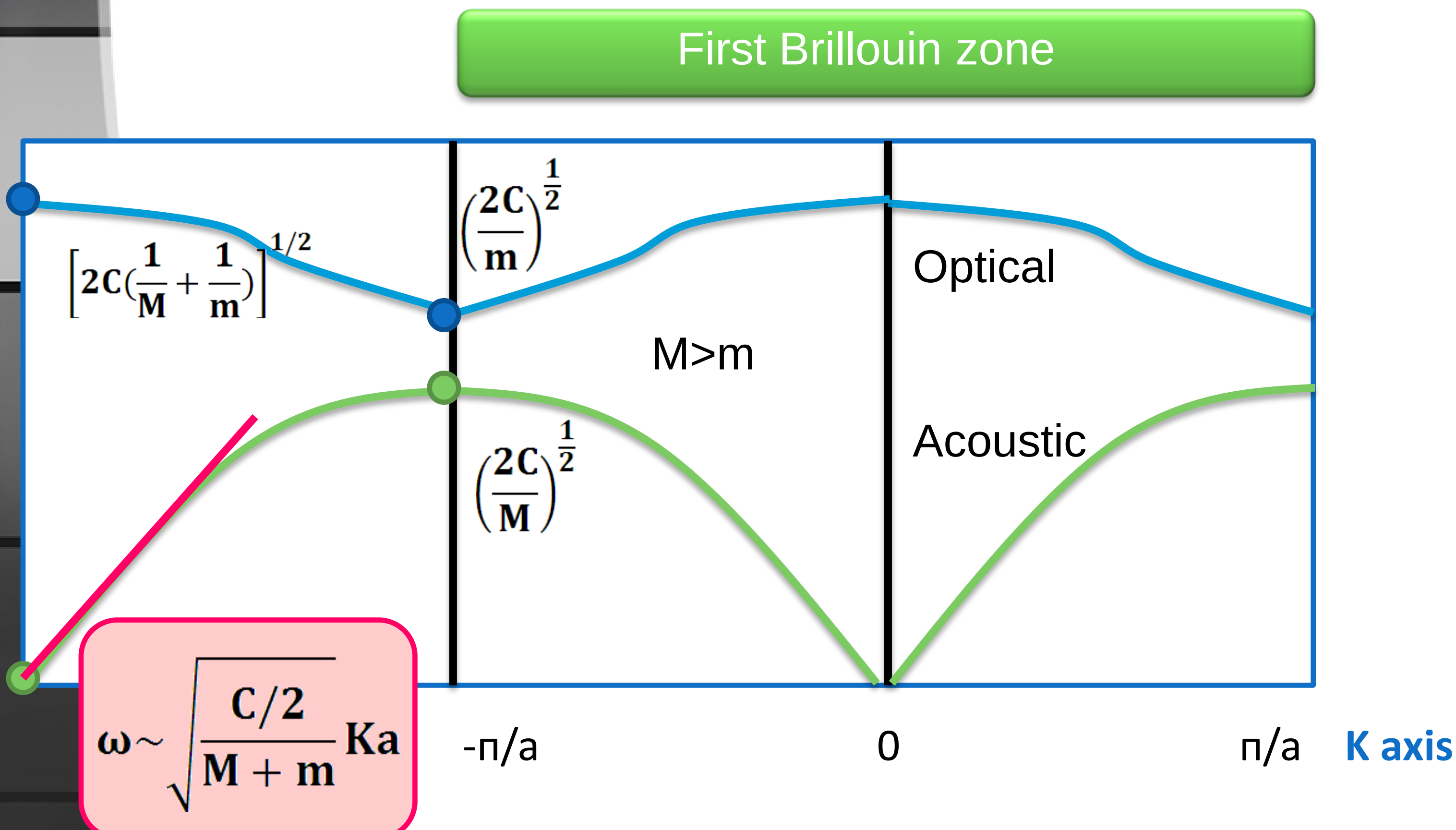
Get $$\omega^2 = \frac{C(M+m)}{Mm} \pm \frac{C\sqrt{(M+m)^2 - 2Mm(1-\cos Ka)}}{Mm}$$

- Simpler limiting case
- K=+π/a ,-π/a
- Ka<<1

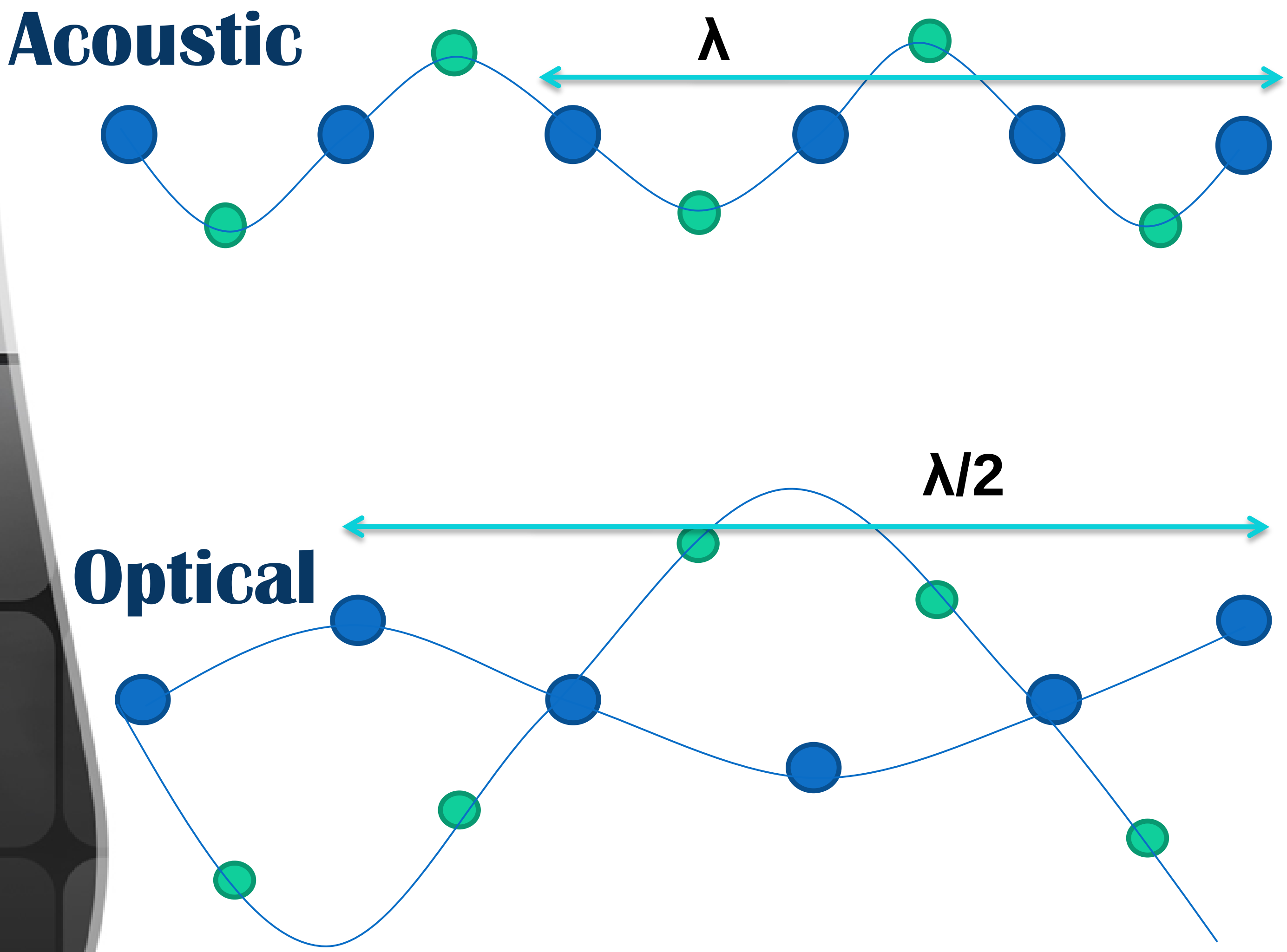
	Optical branch	Acoustic branch
$K = \pm\frac{\Pi}{a}$	$\omega^2 = \frac{2C}{m}$	$\omega^2 = \frac{2C}{M}$
$Ka \ll 1$	$\omega^2 \sim 2C(\frac{1}{M} + \frac{1}{m})$	$\omega^2 \sim \frac{\frac{1}{2}C}{M+m}K^2a^2$

Mass difference case

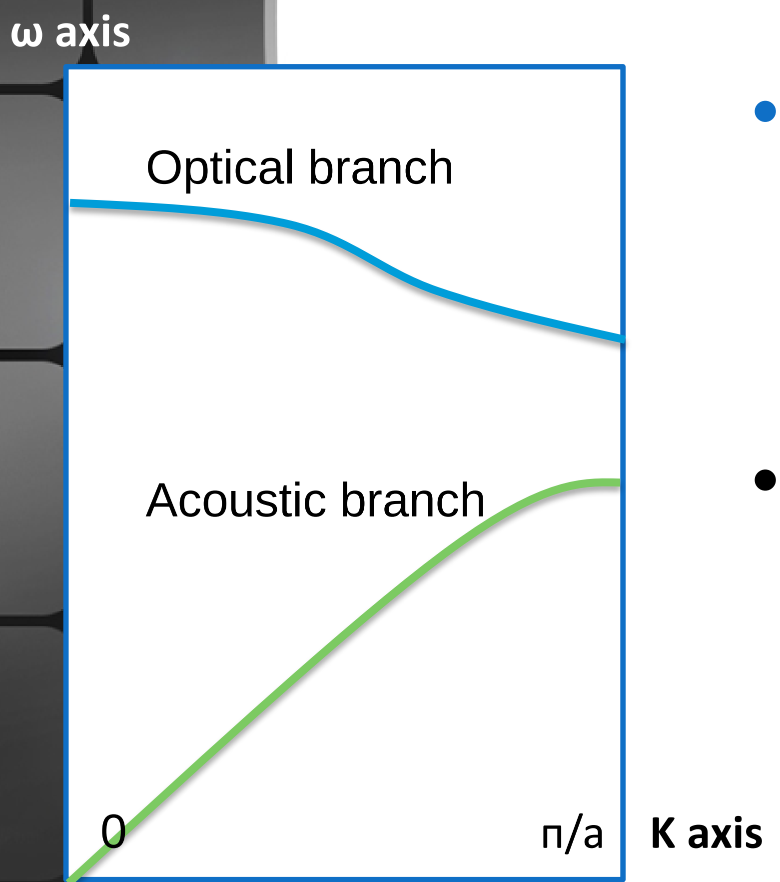
- Plot the ω versus K



Optical and Acoustic phonons



Optical phonon

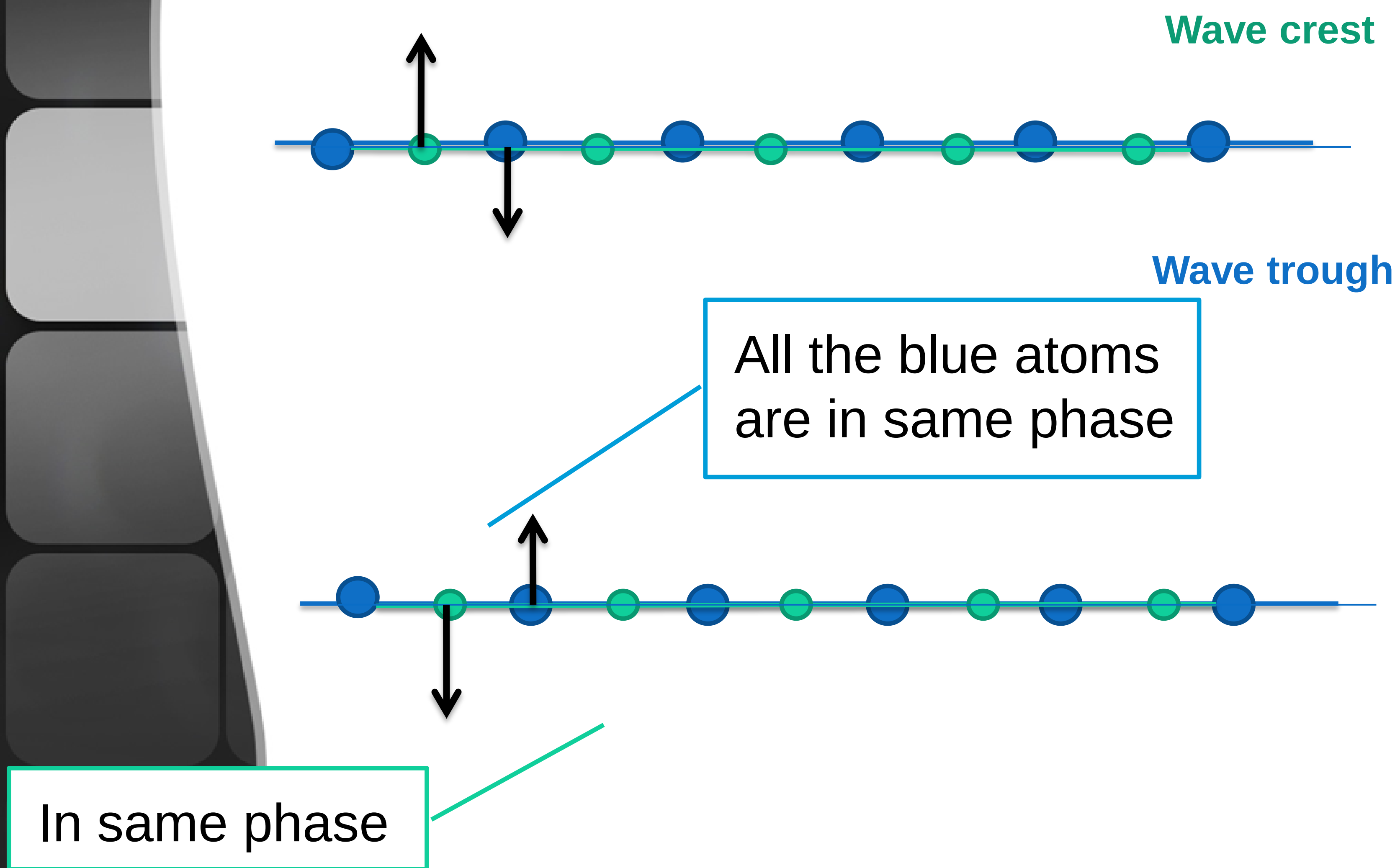


- **Optical phonon branch**

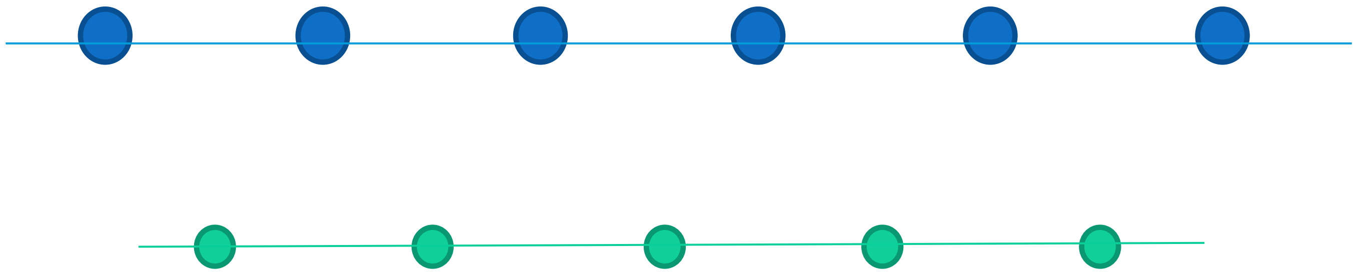
  K=2π/λ=0 → λ=∞

- How can the wave length of optical phonon be infinite?

Optical phonon



Optical phonon

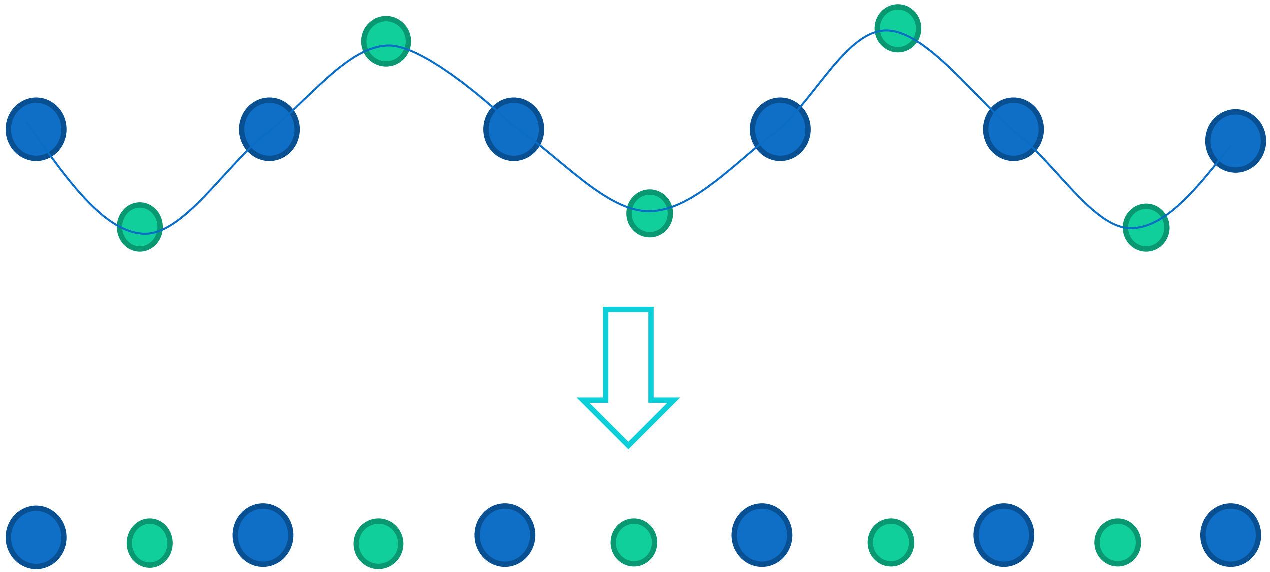


- All atoms in the same kind are in same phase →$\lambda=\infty$
- A time period(T) is from wave crest to next wave crest

  Frequency is 1/T → $\omega\neq0$

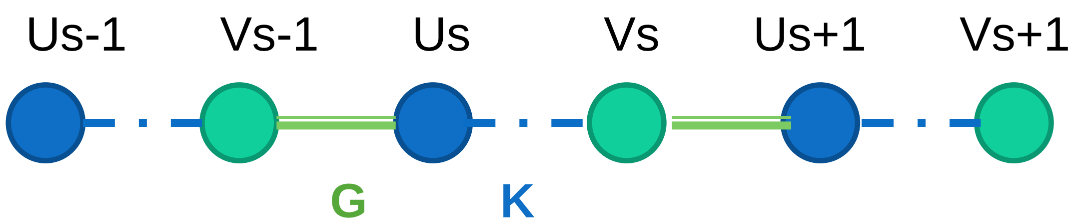
- $\omega\neq0$ (max) and $\lambda=\infty$

Acoustic phonon



- For acoustic phonon
- $\lambda=\infty \quad \omega=0$

Spring difference case



- Different springs G and K

$$M\frac{d^2u_s}{dt^2} = K(v_s - u_s) + G(v_{s-1} - u_s)$$

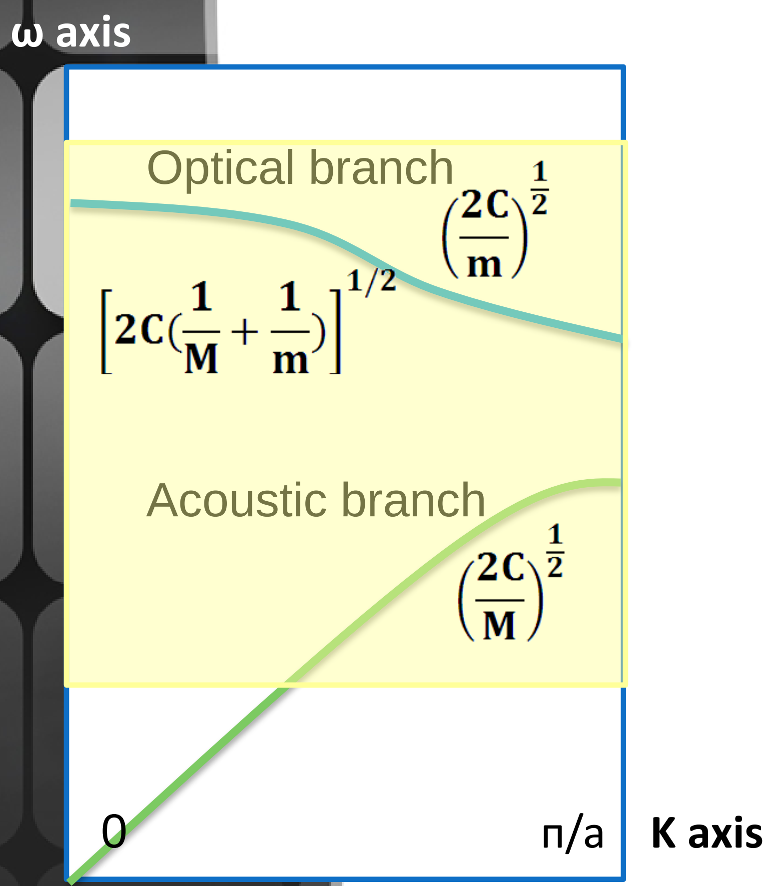
$$M\frac{d^2v_s}{dt^2} = K(u_s - v_s) + G(u_{s+1} - v_s)$$

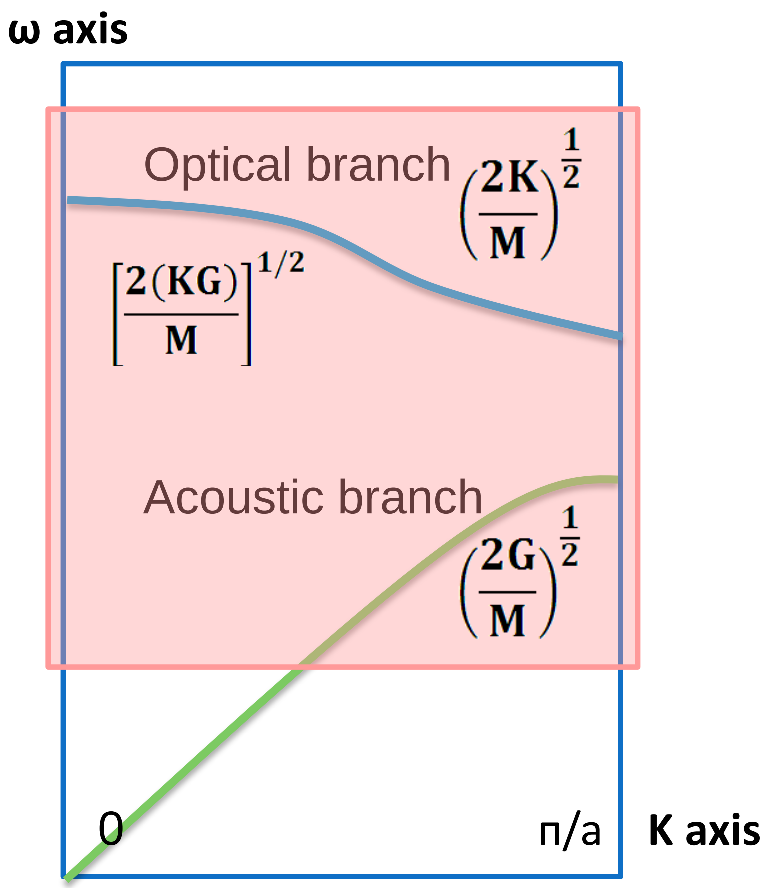
- Dispersion relation

$$\omega^2 = \frac{K+G}{M} \pm \frac{\sqrt{K^2 + G^2 + 2KG(\cos ka)}}{M}$$

Two atoms basis

- Compare ω versus k





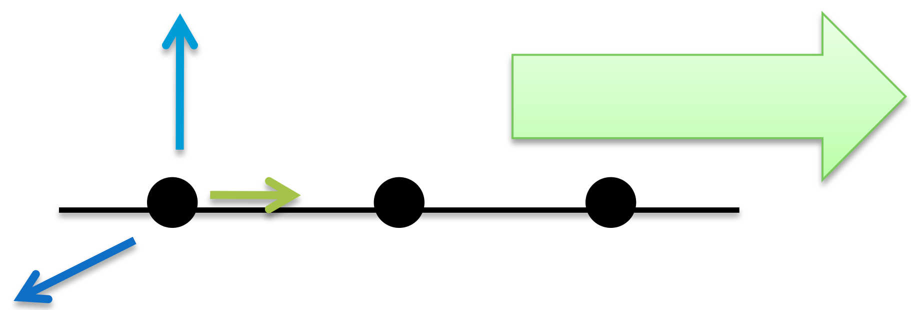
Two atoms basis

- Six kinds of phonons

  Acoustic : L_1A L_2A TA

  Optical: L_1O L_2O TO

  for different propagate direction



Thank you for your attention