

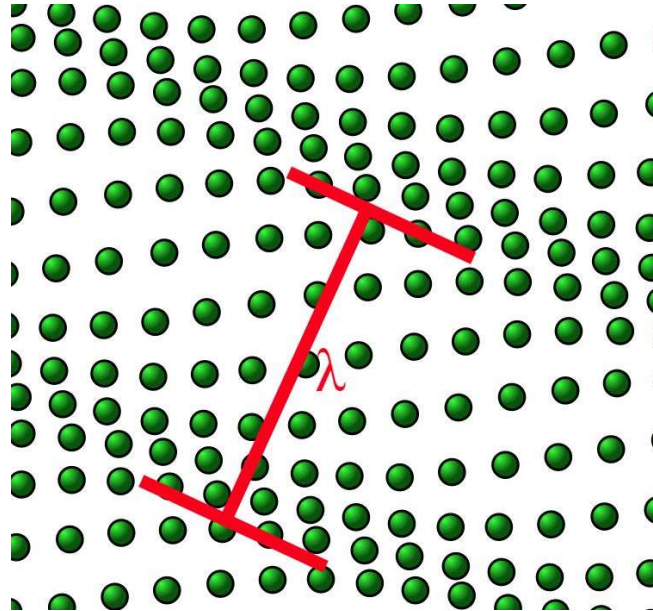
# Phonons I: Crystal vibrations

classical

- one-dimensional vibration
- one-dimensional vibration for a crystal with basis
- three-dimensional vibration

Q

- quantum theory of vibration



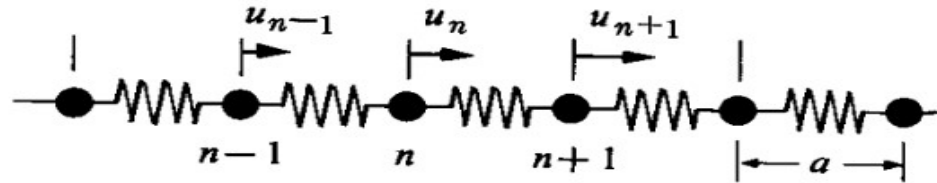
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## One-dimensional vibration (classical analysis)

- consider only *longitudinal* motion
- consider only nearest-neighbor (NN) coupling



$u_n$ : displacement

$\alpha$ : elastic constant

$$M \frac{d^2 u_n}{dt^2} = \alpha(u_{n+1} - u_n) - \alpha(u_n - u_{n-1})$$

Consider a motion in which all atoms vibrate sinusoidally with the same frequency  $\omega$  (a **steady state**)

let  $u_n(t) = v_n e^{-i\omega t}$  take real part only

$\Rightarrow M\omega^2 v_n = \alpha(2v_n - v_{n+1} - v_{n-1})$  ← a difference equation

$$\Rightarrow \begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & \ddots & 0 \\ 0 & \ddots & \ddots & -1 \\ -1 & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} = \frac{M}{\alpha} \omega^2 \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}$$

Periodic  
Boundary  
Condition

The equation remains invariant when  $n \rightarrow n+1$

- For a system with translation symmetry, there is a plane wave solution.

Assume  $v_n = Ae^{ikX_n}$ , where  $X_n = na$ ,

*i.e.*  $u_n = Ae^{ikna} e^{-i\omega t}$

then we'll get

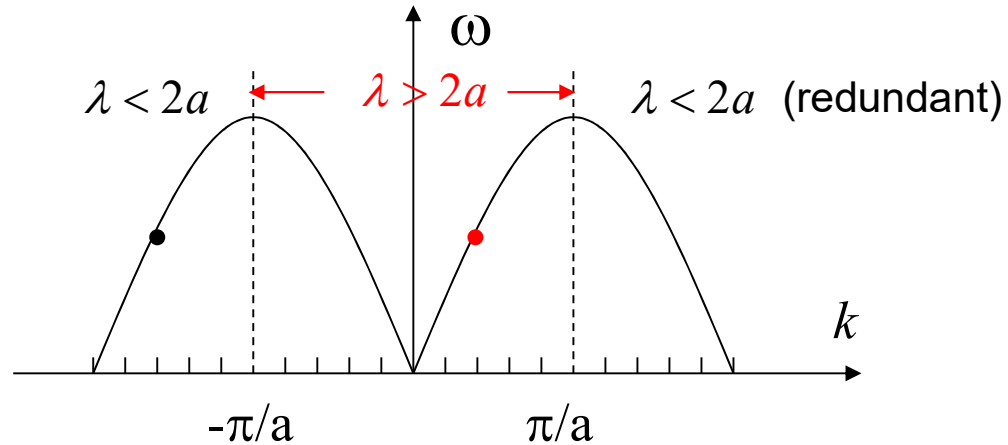
$$M\omega^2 e^{ikna} = \alpha \left[ 2e^{ikna} - e^{ik(n+1)a} - e^{ik(n-1)a} \right],$$

which leads to

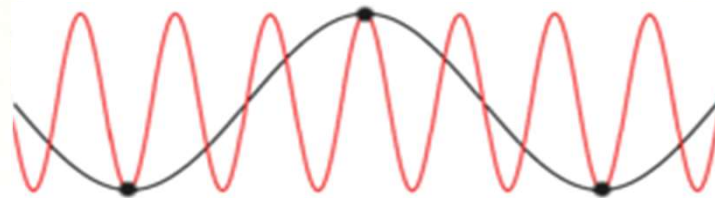
$$\omega(k) = \omega_M |\sin(ka/2)|, \quad \omega_M = 2\sqrt{\alpha/M}$$

↑  
dispersion relation (色散關係)

Dispersion curve  $\omega(k) = \omega_M |\sin(ka/2)|$



- The wave outside the  $[-\pi/a, \pi/a]$  is unphysical, so we restrict  $k$  to the first BZ



- The waves with wave numbers  $k$  and  $k+2\pi/a$  describe the same atomic displacement

## Displacement of the $n$ -th atom

$$u_n(t) = Ae^{i(kX_n - \omega t)}, \quad X_n = na$$

### Pattern of vibration:

- $k \sim 0$ ,  $\exp(ikX_n) \sim 1$ .

Every atom move in unison. Little restoring force.

- $k \sim \pi/a$ ,  $\exp(ikX_n) \sim (-1)^n$ .

Adjacent atoms move in opposite directions. Maximum restoring force.

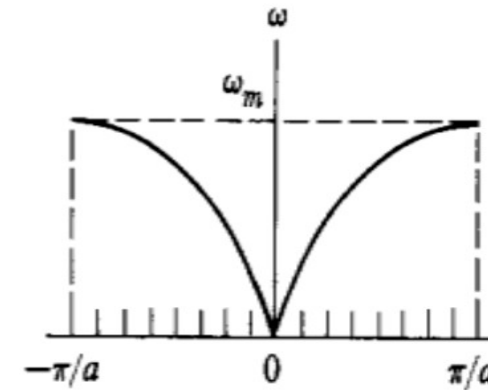
### Phase velocity $v_p$ and Group velocity $v_g$

- $k \sim 0$ ,  $\omega = (\omega_M a/2)k$ ,

$$v_p = v_g = \omega_M a/2$$

(For linear dispersion, phase velocity = group velocity)

- $k \sim \pi/a$ , group velocity  $\sim 0$



$$v_p = \frac{\omega}{k}$$

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

The values of  $k$  are **discrete** for a finite system.

For a 1-dim crystal with  $N$  atoms, consider

**Periodic boundary condition (PBC):**  $u_0(t) = u_N(t)$

(Note: PBC allows travelling wave, while open BC gives standing wave)

$$u_n = A \exp[i(kX_n - \omega t)],$$

$$u_N = u_0 \Rightarrow \exp(ikNa) = 1$$

$$\therefore k = \frac{m}{N} \frac{2\pi}{a}, m = 1, 2, \dots, N$$

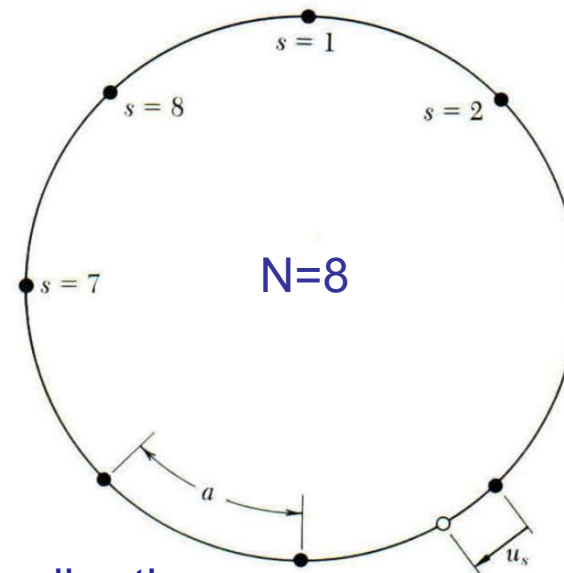
or 
$$m = -\frac{N}{2} + 1, \dots, \frac{N}{2}$$

$$\Delta k = 2\pi/Na$$

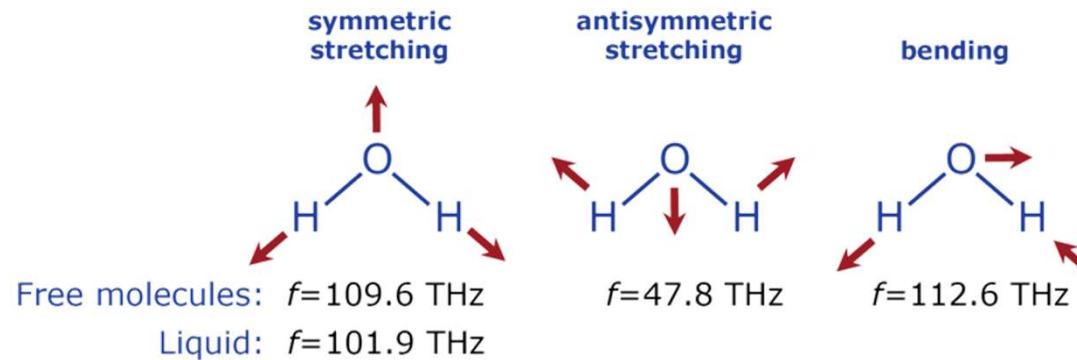
- Each  $k$  describes a **normal mode** of the vibration

簡正模

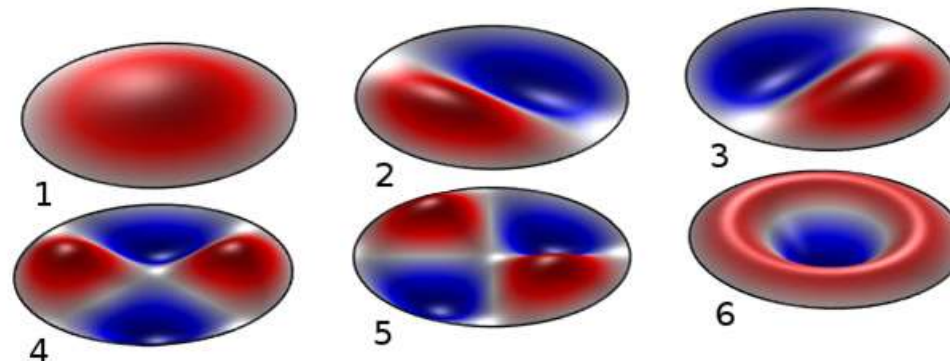
- Number of  $k$ 's = number of atoms  $N$   
(or, the number of unit cells)



## Normal mode (ref: wiki) ~ energy eigenstate



- A pattern of vibration in which all parts of the system move sinusoidally with the same frequency (called **natural frequency**).
- Normal mode can vibrate independently. That is, the excitation of one mode will not cause the motion of a different normal mode.
- A general vibration can be considered as a superposition of normal modes.



• • • • •  
1D lattice

• • • • •  
1D lattice with basis

• • •  
3D lattice

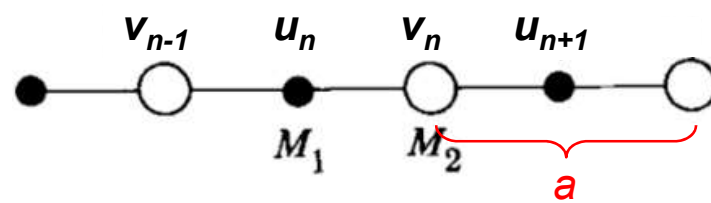
• • • • •  
quantized vibration

• • • • •  
optional

- one-dimensional vibration
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## Vibration of a crystal with 2 atoms in a unit cell



$$\begin{cases} M_1 \frac{d^2 u_n}{dt^2} = \alpha(v_n + v_{n-1} - 2u_n), \\ M_2 \frac{d^2 v_n}{dt^2} = \alpha(u_{n+1} + u_n - 2v_n). \end{cases}$$

$$\text{Assume } \begin{pmatrix} u_n \\ v_n \end{pmatrix} = \begin{pmatrix} A_1 e^{ikna} \\ A_2 e^{ik(n+1/2)a} \end{pmatrix} e^{-i\omega t}$$

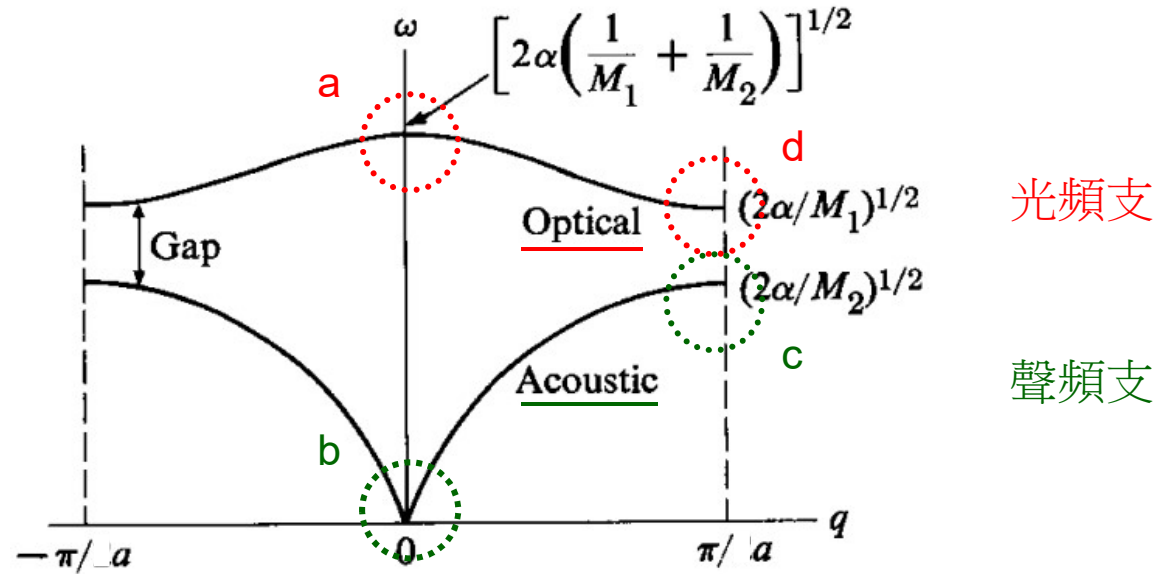
$$\Rightarrow \begin{pmatrix} 2\alpha - M_1 \omega^2 & -2\alpha \cos(ka/2) \\ -2\alpha \cos(ka/2) & 2\alpha - M_2 \omega^2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = 0,$$

$$\Rightarrow \det \begin{pmatrix} 2\alpha - M_1 \omega^2 & -2\alpha \cos(ka/2) \\ -2\alpha \cos(ka/2) & 2\alpha - M_2 \omega^2 \end{pmatrix} = 0.$$

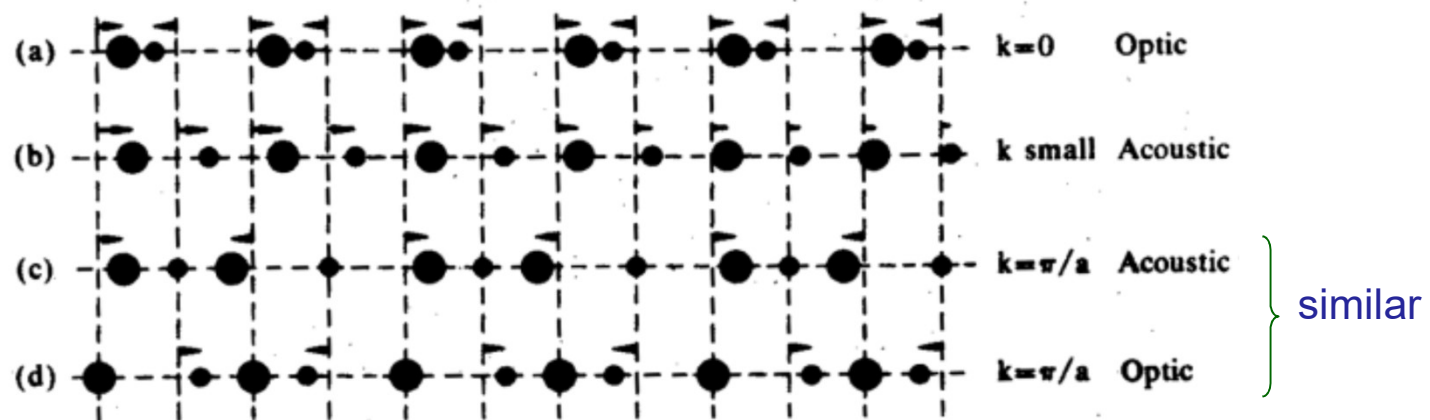
$$\Rightarrow \omega_{\pm}^2 = \alpha \left( \frac{1}{M_1} + \frac{1}{M_2} \right) \pm \alpha \sqrt{\left( \frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2(ka/2)}{M_1 M_2}}.$$

important

Two branches of dispersion curves (assuming  $M_2 > M_1$ )



Patterns of vibration: (Prob.3)



See a nice demo at <http://www.ph2.uni-koeln.de/505.html>

How many **normal modes** ( $k$  points) in each branch?

$$\text{Imposing PBC on } \begin{pmatrix} u_n \\ v_n \end{pmatrix} = \begin{pmatrix} A_1 e^{ikna} \\ A_2 e^{ik(n+1/2)a} \end{pmatrix} e^{-i\omega t}$$

$$\begin{pmatrix} u_N \\ v_N \end{pmatrix} = \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \Rightarrow \exp(ikNa) = 1$$

$$\therefore k = \frac{m}{N} \frac{2\pi}{a}, m = 1, 2, \dots, N$$

$$\text{or } m = -\frac{N}{2} + 1, \dots, \frac{N}{2} \quad \text{Same as before (a lattice with no basis)}$$

- There are 2 branches, so the total number of  $k$  points (normal modes) is  $2N$ , same as the total DOF of the atoms.
- This equality remains true for complex crystals in higher dimensions.

Q: what happens if the two atoms in a basis are of the same type?

• • • • •  
1D lattice

• • • •  
1D lattice with basis

• • •  
**3D lattice**

• • • •  
quantized vibration

• • • •  
optional

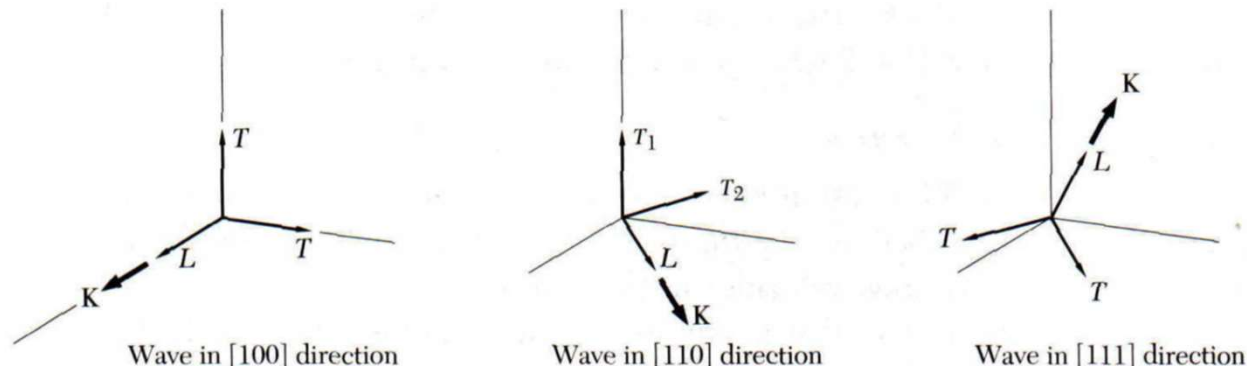
- one-dimensional vibration
- one-dimensional vibration for a crystal with basis
- **three-dimensional vibration**
- quantum theory of vibration

## Three-dimensional vibration

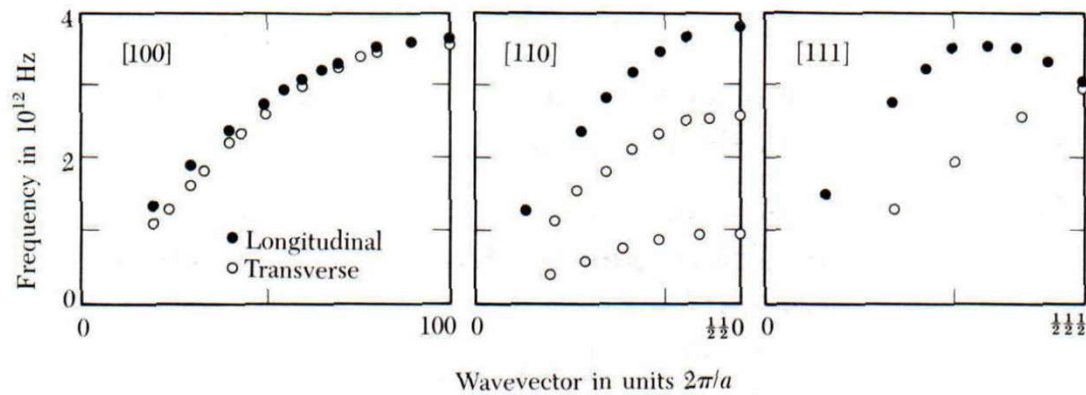
Along a given direction of propagation, there are

1 longitudinal wave and 2 transverse waves,

each may have different velocities



Sodium (BCC)



**Figure 11** The dispersion curves of sodium for phonons propagating in the [001], [110], and [111] directions at 90 K, as determined by inelastic scattering of neutrons, by Woods, Brockhouse, March and Bowers. *Na*

1D lattice

1D lattice with basis

3D lattice

quantized vibration

optional

important

## 3D crystal with *basis*

Rules of thumb:

• For a 3-dim crystal, if each unit cell has  $p$  atoms, then there are

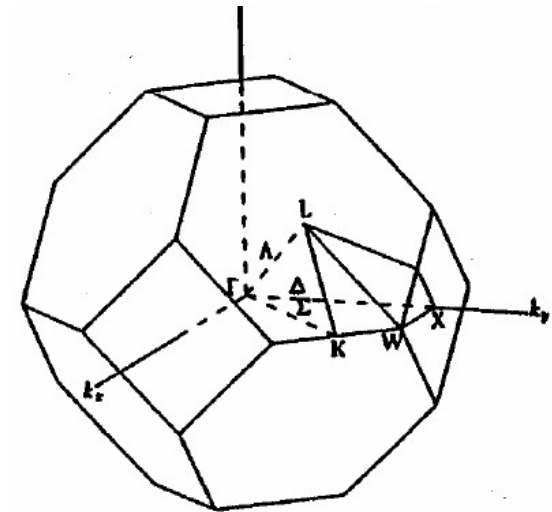
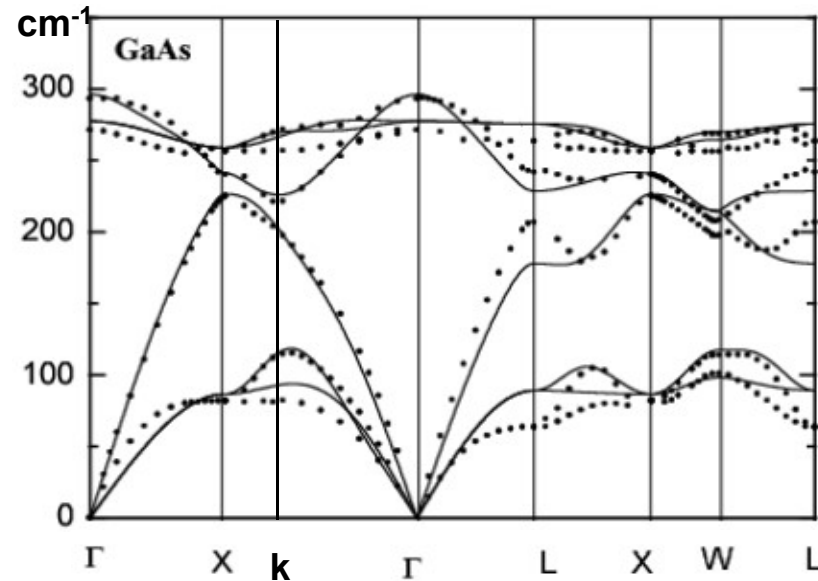
3 acoustic branches,

$3(p-1)$  optical branches

• If a crystal has  $N$  unit cells, then each branch has  $N$  normal modes (number of  $k$ -points for each dispersion curve).

• As a result, the total number of normal modes of the whole crystal is  $3pN$  (= total DOF of atoms in this crystal).

## FCC lattice with 2-atom basis



• • • • •  
1D lattice

• • • •  
1D lattice with basis

• • •  
3D lattice

• • • •  
quantized vibration

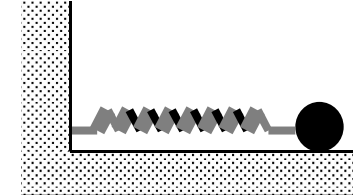
• • • •  
optional

- one-dimensional vibration
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- *quantum* theory of vibration

## Quantum theory of vibration

### Review: 1D simple harmonic oscillator (DOF=1)

$$H = \frac{p^2}{2m} + \frac{\alpha}{2} x^2$$



- Classically, it oscillates with a single freq  $\omega = (\alpha/m)^{1/2}$

Quantization:  $[x, p] = i\hbar$

define 
$$a = \frac{1}{\sqrt{2\hbar}} \left( \sqrt{m\omega} x + \frac{i}{\sqrt{m\omega}} p \right)$$

then 
$$[a, a^\dagger] = 1$$

$$H = \left( a^\dagger a + \frac{1}{2} \right) \hbar\omega$$

$$\Rightarrow H|n\rangle = \left( n + \frac{1}{2} \right) \hbar\omega |n\rangle$$

Creation and annihilation operators:

if  $|n\rangle$  is an energy eigenstate, then

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

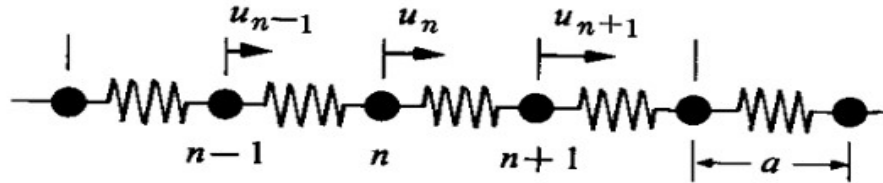
- After quantization, the energy becomes discrete

$$\varepsilon_n = \left( n + \frac{1}{2} \right) \hbar\omega$$

$$n = 0, 1, 2, \dots$$



## Quantization of a 1-dim vibrating crystal (see Kittel App. C)



- Energy dispersion of a normal mode (a given  $k$ ):  $\hbar\omega_k$
- Suppose the number of energy quanta (called **phonons**, 聲子) being excited is  $n_k$ , then the **total vibration energy**

$$U = \sum_k \left( n_k + \frac{1}{2} \right) \hbar\omega_k$$

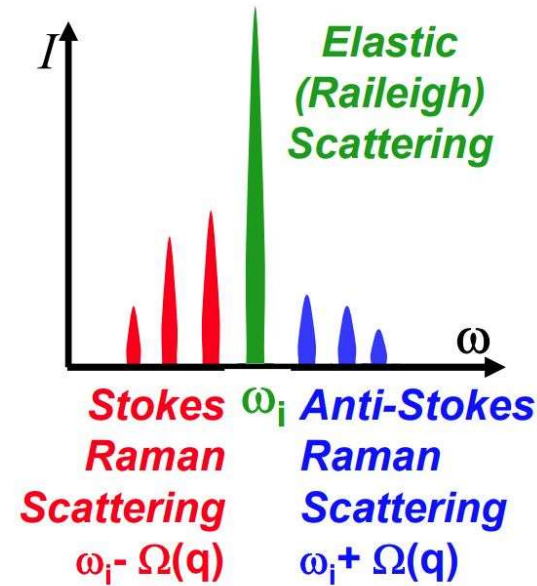
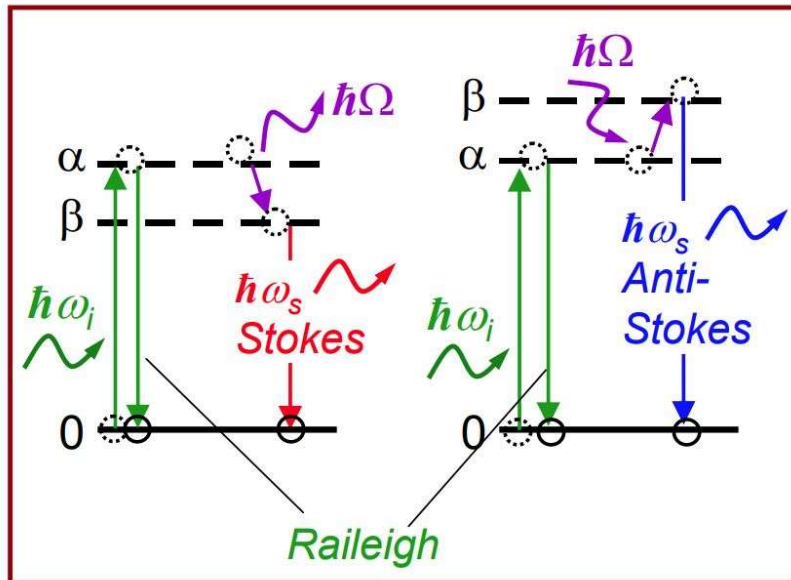
- There are no interaction between phonons, so the vibrations can be treated as a “free” phonon gas.  
(this is no longer true if the elastic force is nonlinear.)
- In general, for a 3D crystal with atom basis

$$U = \sum_{\vec{k}, s} \left( n_{\vec{k}, s} + \frac{1}{2} \right) \hbar\omega_{\vec{k}, s}, \quad s = 1 \cdots 3p \quad (\text{L/T, A/O...})$$

A  $\mathbf{k}$ -mode phonon acts as if it has momentum  $\hbar\mathbf{k}$  in a scattering process (for a math proof, see Ashcroft and Mermin, App. M)

Crystal recoils with momentum  $\hbar\vec{G}$

- Elastic scattering of photon:  $\hbar k' = \hbar k - \hbar G$  (Laue condition)
- Inelastic scattering of photon:  $\hbar k' = \hbar k \pm \hbar k_{\text{phonon}} - \hbar G$  (Raman scattering)



1930

From Sirenko's ppt

However, the physical momentum of a normal mode with wavevector  $\mathbf{k}$  is zero:

$$\begin{aligned}
 P &= M \sum_n \frac{du_n}{dt}, u_n = Ae^{i(kX_n - \omega t)} \\
 &= MA(-i\omega)e^{-i\omega t} \sum_{n=0}^{N-1} e^{ikna} \\
 &= MA(-i\omega)e^{-i\omega t} \frac{1 - e^{ikNa}}{1 - e^{ika}} \quad \text{uniform translation of the crystal} \\
 &= 0 \quad \text{since } k = 2\pi m / Na \quad (\neq 0 \text{ ONLY when } k=0) \\
 &\quad \uparrow \text{no center-of-mass motion of the crystal} \quad \downarrow
 \end{aligned}$$

Therefore, we call  $\hbar\mathbf{k}$  the **crystal momentum** (of the phonon), or **phonon momentum**, in order not to be confused with physical momentum.