Chapter 3

Lattice Vibrations and Phonons
(晶格振动与声子)

Outline

- **Chapter 3.1** Classical Lattice Vibrations (晶格振动的经典理论)
- **Chapter 3.2** Phonons (声子)
- **Chapter 3.3** Phonon Heat Capacity (声子热容)
- **Chapter 3.4** Anharmonicity (非谐效应)

Outline

- **Chapter 3.1** Classical Lattice Vibrations (晶格振动的经典理论)
- **Chapter 3.2** Phonons (声子)
- **Chapter 3.3** Phonon Heat Capacity (声子热容)
- **Chapter 3.4** Anharmonicity (非谐效应)

Objectives

- To understand the concept of “**lattice wave**”.
- To understand the characteristics of lattice vibrations in 1D.
- To learn the characteristics of lattice vibrations in 3D.

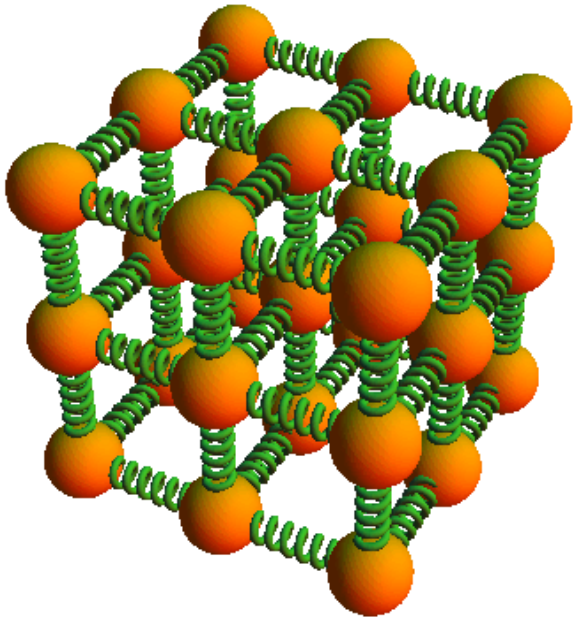
A Model of Lattice Vibrations
(晶格振动模型)

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ A Model of Lattice Vibrations (晶格振动模型)

- In real crystals, the atoms (or molecules) DO NOT remain static at the lattice points. Instead, **they always vibrate around the equilibrium positions (lattice points) at both finite and zero temperatures**.

- Lattice vibrations play a key role in accounting for many physical properties of solids, such as **thermal capacity**, **thermal conductivity**, **thermal expansion**, **electrical conductivity**, and **superconductivity**.



Schematic Diagram of a Model of Lattice Vibrations in 3D

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ A Model of Lattice Vibrations (晶格振动模型)

❖ Lattice vibrations can be understood by a simplified model adopting the following appropriate approximations:

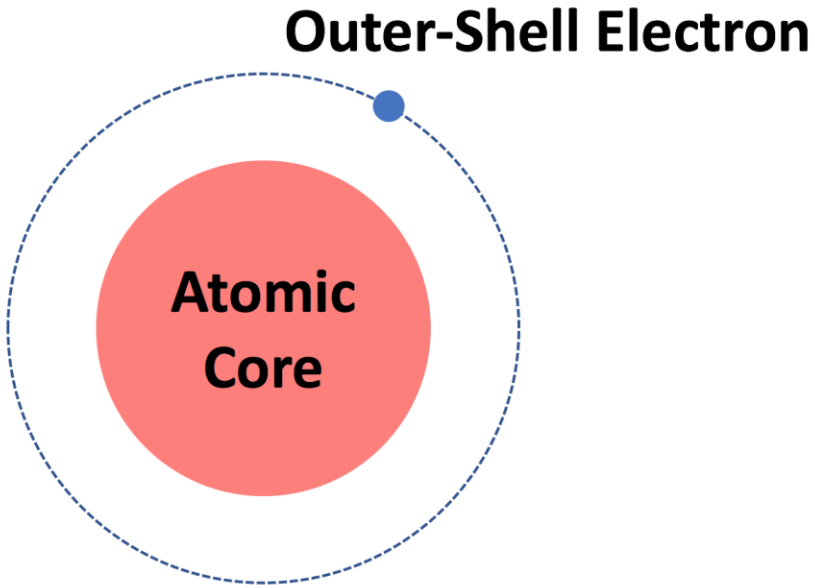
- ❑ **Adiabatic Approximation (绝热近似)**
- ❑ **Nearest-Neighbor Approximation (最近邻近似)**
- ❑ **Harmonic Approximation (简谐近似)**
- ❑ **Born-von Karman Approximation (玻恩-冯卡门近似)**

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ A Model of Lattice Vibrations (晶格振动模型)

❑ Adiabatic Approximation (绝热近似)

- The atoms (or molecules) at the lattice points can be treated as a combination of **atomic core** (原子实) and **outer-shell electrons** (外层电子), the motion of which is separable.



Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ A Model of Lattice Vibrations (晶格振动模型)

❑ Adiabatic Approximation (绝热近似)

- The mass of atomic core is much (3-5 orders of magnitude) larger than that of the outer-shell electrons such that the electrons move fast enough to follow the atomic core motion. The electrons remain at the **ground stat**e (**基态**) at every moment of the atomic core motion.

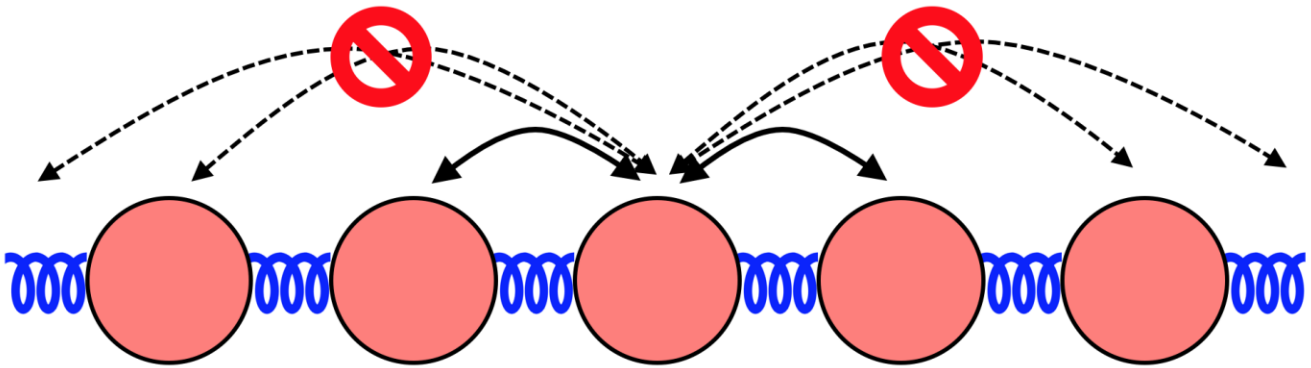
- This approximation is also called **Born-Oppenheimer approximation (玻恩-奥本海默近似)**.

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ A Model of Lattice Vibrations (晶格振动模型)

❑ Nearest-Neighbor Approximation (最近邻近似)

- Only the interactions between nearest-neighbor lattice points are considered, and those between next-nearest-neighbor points and beyond are omitted.



Schematic Diagram of Nearest-Neighbor Approximation

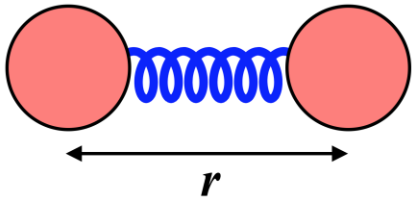
Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ A Model of Lattice Vibrations (晶格振动模型)

❑ Harmonic Approximation (简谐近似)

- The potential energy between interacting atoms can be expressed in terms of **Taylor series (泰勒级数)** around the equilibrium positions:

$$V(r) = V(a+\delta)$$
$$= V(a) + \left(\frac{\mathrm{d}V}{\mathrm{d}r}\right)_a \delta + \frac{1}{2}\left(\frac{\mathrm{d}^2V}{\mathrm{d}r^2}\right)_a \delta^2 + \frac{1}{3!}\left(\frac{\mathrm{d}^3V}{\mathrm{d}r^3}\right)_a \delta^3 +$$



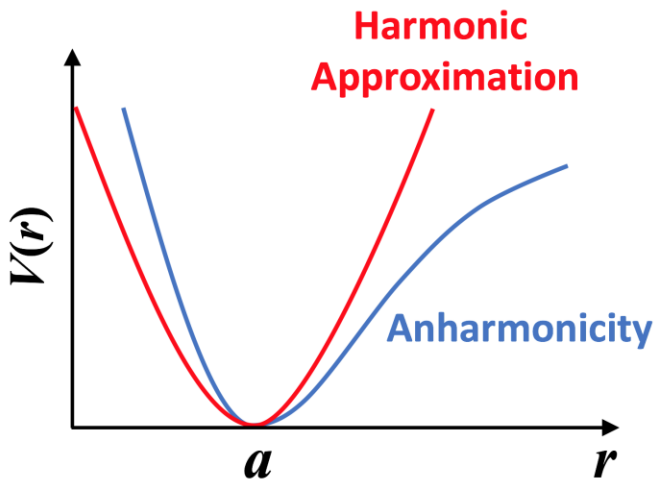
Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ A Model of Lattice Vibrations (晶格振动模型)

❑ Harmonic Approximation (简谐近似)

- The **harmonic approximation** is such that only the terms up to δ^2 are kept and those associated with δ^3 and beyond are omitted.

$$V(r) = V(a+\delta)$$
$$= V(a) + \left(\frac{\mathrm{d}V}{\mathrm{d}r}\right)_a \delta + \frac{1}{2}\left(\frac{\mathrm{d}^2V}{\mathrm{d}r^2}\right)_a \delta^2 + \frac{1}{3!}\left(\frac{\mathrm{d}^3V}{\mathrm{d}r^3}\right)_a \delta^3 +$$

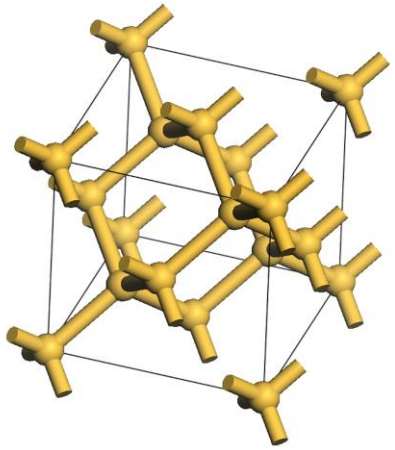


Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

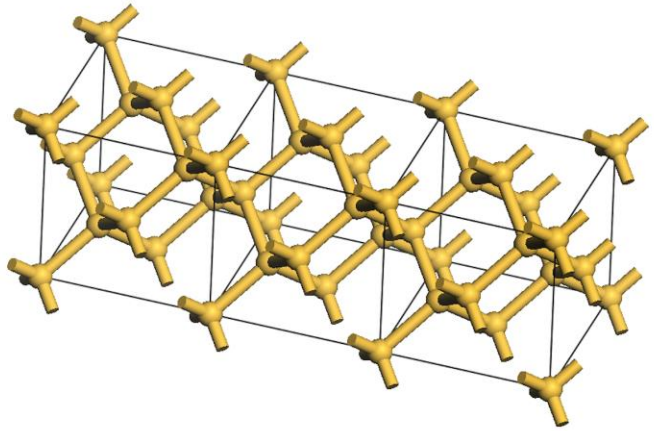
➢ A Model of Lattice Vibrations (晶格振动模型)

❑ Born-von Karman Approximation (玻恩-冯卡门近似)

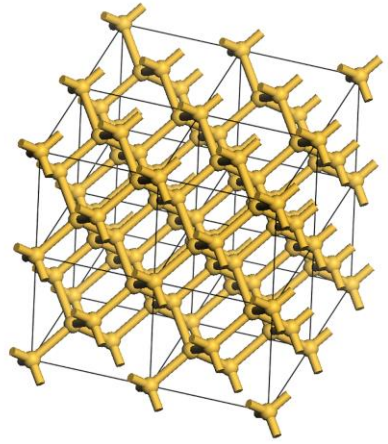
- **Born-von Karman approximation** is to impose the restriction that the spatial distribution of crystal properties (e.g., potential energy, wave function) must be periodic at multiple cells of a Bravais lattice.



1 unit cell of Si crystal



3 unit cells of Si crystal



8 unit cells of Si crystal

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ A Model of Lattice Vibrations (晶格振动模型)

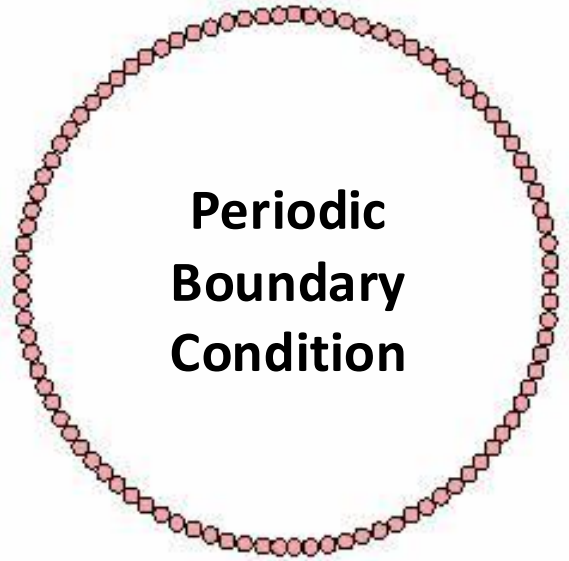
❑ Born-von Karman Approximation (玻恩-冯卡门近似)

- This approximation is also called **Born-von Karman boundary condition** (玻恩-冯卡门边界条件) or **periodic boundary condition** (周期性边界条件).

- Mathematically, the approximation can be stated as:

$$\psi(\boldsymbol{r} + \boldsymbol{N_i a_i}) = \psi(\boldsymbol{r})$$

where $\boldsymbol{i}$ runs over the dimensions of the Bravais lattice, $\boldsymbol{a_i}$ are the basis vectors, and $\boldsymbol{N_i}$ are integers (assuming the lattice has $\boldsymbol{N = N_1 N_2 N_3}$ cells).

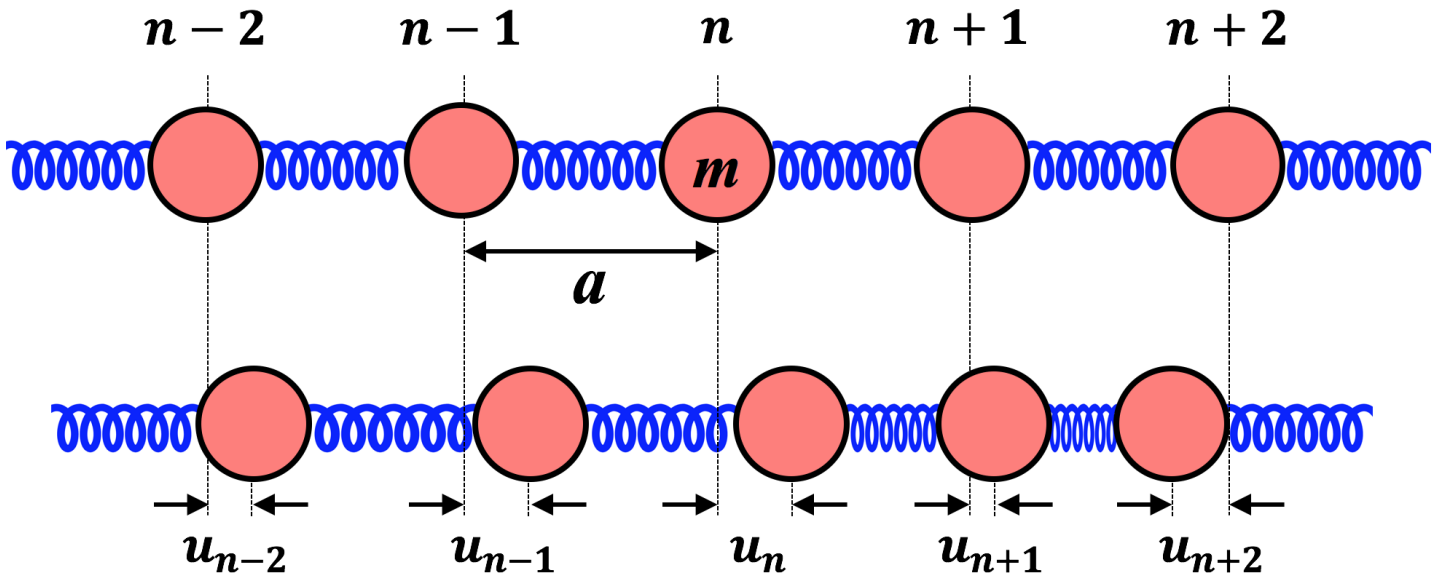


Vibrations of a 1D Monoatomic Chain
(一维单原子链的振动)

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ We consider a 1D monoatomic chain (one atom per primitive cell) consisting of N identical atoms with mass m.



Here, a is the lattice constant and u_n is the displacement of the nth atom from its equilibrium position at time t.

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ In the **harmonic approximation**, the interatomic potential V_n between atoms n and $n+1$ as a function of the atomic displacement can be written as:

$$V_n(r) = V_n(a+\delta) \approx V_n(a) + \left(\frac{dV_n}{dr}\right)_a \delta + \frac{1}{2}\left(\frac{d^2V_n}{dr^2}\right)_a \delta^2 = V_n(a) + \frac{1}{2}K\delta^2$$

Here, $\delta = u_n - u_{n+1}$ and $K = \left(\frac{d^2V_n}{dr^2}\right)_a$ represents the **force constant (力常数)**.

Note that, at the equilibrium position, $\left(\frac{dV_n}{dr}\right)_a = 0$.

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ In the **nearest-neighbor approximation**, the elastic force (defined as $f = -\frac{dV}{dr} = -K\delta$) on atom n can be expressed as:

$$f_n = f_1 + f_2 = -K(u_n - u_{n+1}) - K(u_n - u_{n-1}) = K(u_{n+1} + u_{n-1} - 2u_n)$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ The **Newtonian equation of motion (牛顿运动方程)** for atom n is:

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

❖ The solutions to the set of equations have the form of "**lattice waves**":

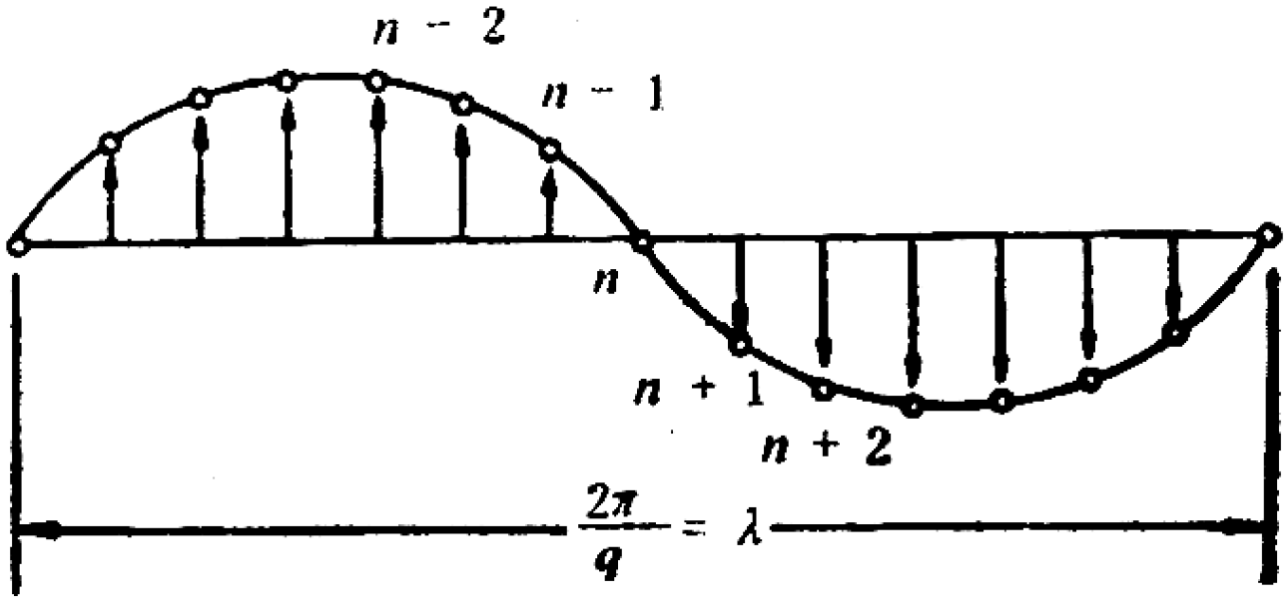
$$u_{nq} = A_q \mathrm{e}^{i(\omega t - naq)}$$

Here, A_q is the amplitude, ω the angular frequency, $q = 2\pi/\lambda$ the wave vector, and λ the wave length.

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ A **lattice wave** (格波) is the collective vibrations of all atoms in the chain.



Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

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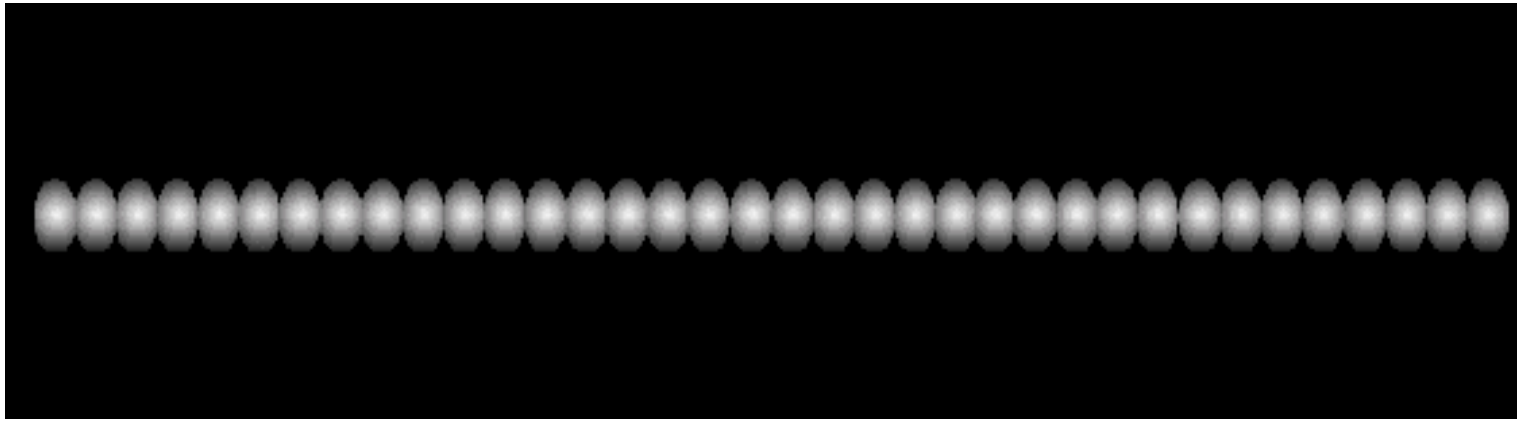
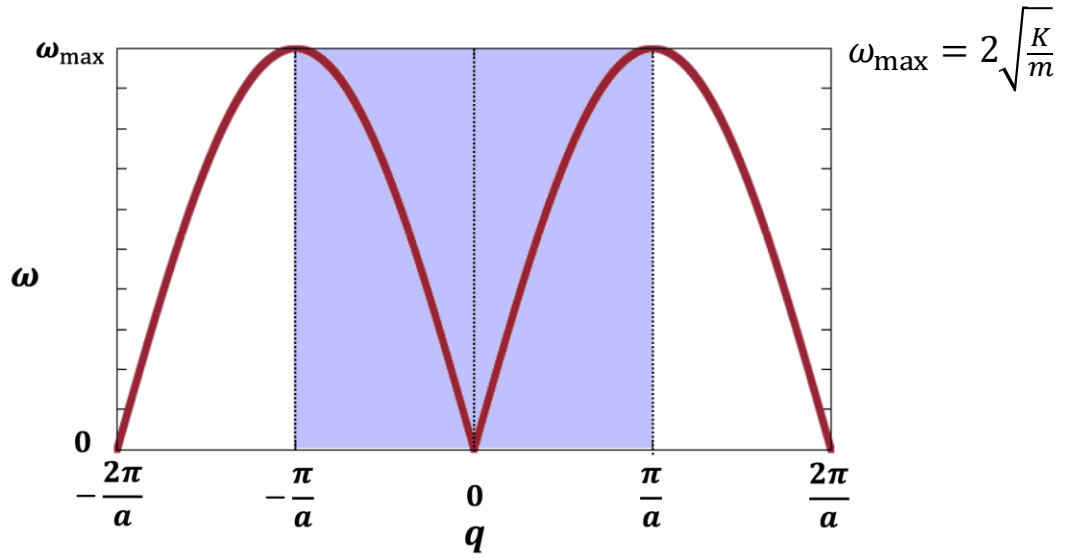


Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ By applying $\boldsymbol{u_{nq}}$ to the Newtonian equations of motion, it is obtained:

$$\boldsymbol{\omega = 2\sqrt{\frac{K}{m}}\left|\sin\left(\frac{1}{2}aq\right)\right|}$$



❖ The $\omega \sim q$ relation is also called "**dispersion relation**" (色散关系).

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ The range of **wave vector q** is physically significant **only in the first Brillouin zone**.

$$\frac{u_{n+1,q}}{u_{nq}} = \mathrm{e}^{-iaq} \rightarrow -\pi \le aq < \pi \quad \text{or} \quad -\pi < aq \le \pi$$

$$\rightarrow \boxed{-\frac{\pi}{a} \le q < \frac{\pi}{a}} \quad \text{or} \quad \boxed{-\frac{\pi}{a} < q \le \frac{\pi}{a}}$$

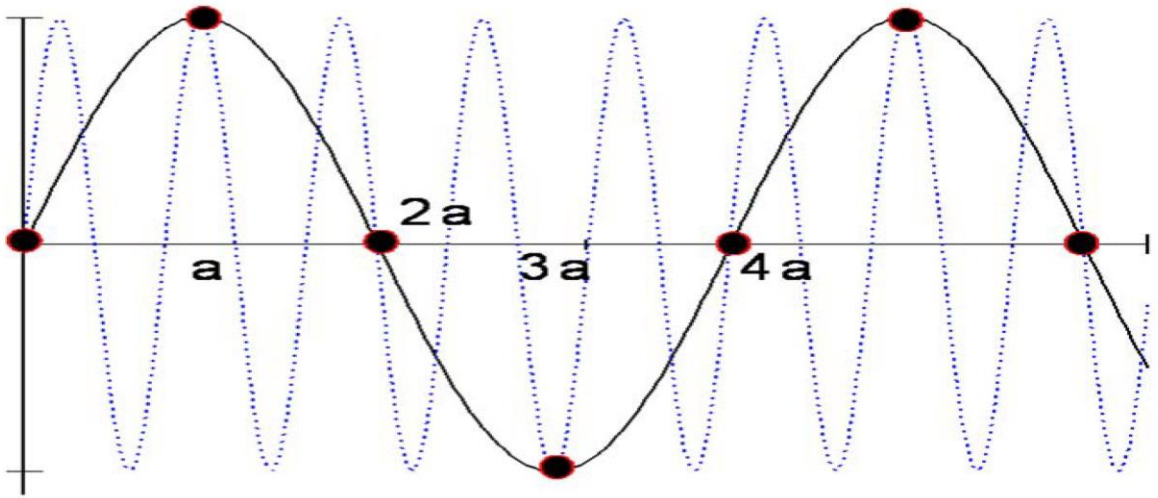
$$\rightarrow \omega(q + G_n) = \omega(q) \qquad (G_n = n\frac{2\pi}{a} \text{ is a reciprocal lattice vector})$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ The range of **wave length λ** is physically significant **only in the case of $\lambda \geq 2a$**.

$$-\frac{\pi}{a} < q \leq \frac{\pi}{a} \quad \text{and} \quad \lambda = \frac{2\pi}{q} \quad \Rightarrow \quad \lambda \geq 2a$$



Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ By applying the **periodic boundary condition**, it is obtained:

$$u_{n+N,q} = u_{nq} \quad \Rightarrow \quad q = l\frac{2\pi}{Na}$$ (l is an integer and N the number of primitive cells)

❖ For a monoatomic chain with $\boldsymbol{N}$ atoms (primitive cells), the number of wave vectors $\boldsymbol{q}$ in the first (or each) Brillouin zone is also $\boldsymbol{N}$. One $\boldsymbol{q}$ corresponds to one **vibration mode** (振动模).

$$-\frac{\pi}{a} \le q < \frac{\pi}{a} \quad \Rightarrow \quad -\frac{N}{2} \le l < \frac{N}{2} \qquad (l_1, l_2, \cdots, l_N)$$

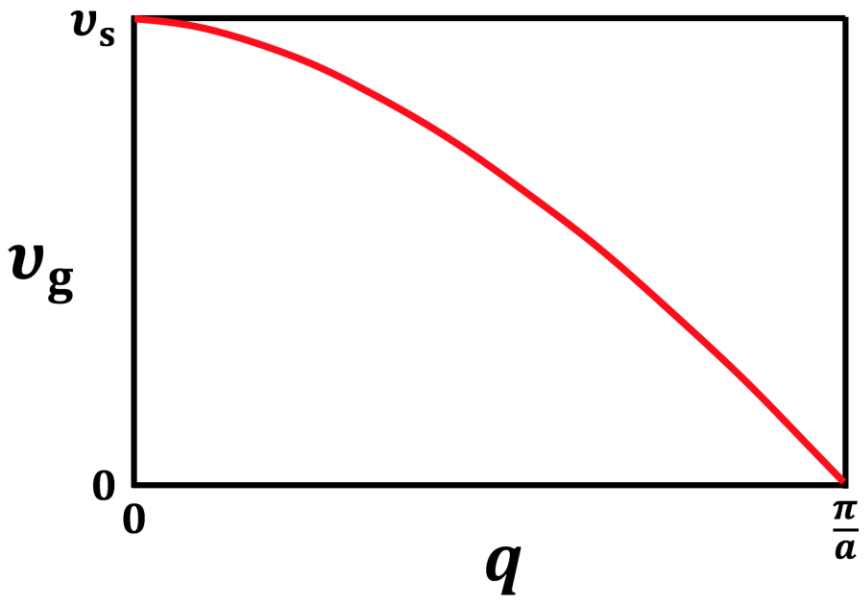
Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ **Group velocity (群速度)** of the lattice waves:

$$v_g = \frac{d\omega}{dq} = v_s \cos\left(\frac{1}{2}aq\right)$$

$v_s = a\sqrt{\frac{K}{m}}$ is the **velocity of sound (声速)**



Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

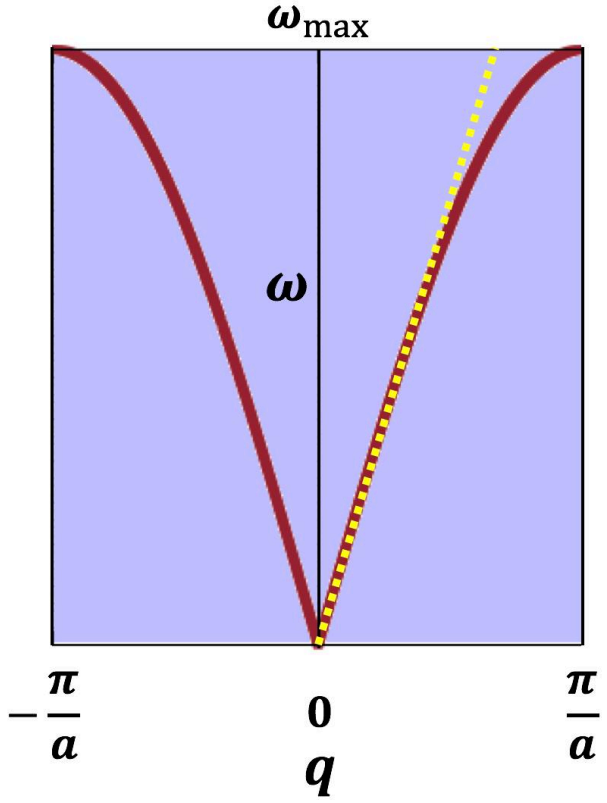
➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ Acoustical waves (声学波) in the long wavelength limit (长波极限 $q \to 0$):

$$\omega = 2\sqrt{\frac{K}{m}}\left|\sin\left(\frac{1}{2}aq\right)\right|$$

$$q \to 0 \quad \Rightarrow \quad \omega \to a\sqrt{\frac{K}{m}}|q| = v_s|q| \to 0$$

$$\frac{u_{n+1,q}}{u_{nq}} = \mathrm{e}^{-iaq} \to 1$$



Acoustical branch (声学支): $\omega \propto q \to 0$ when $q \to 0$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

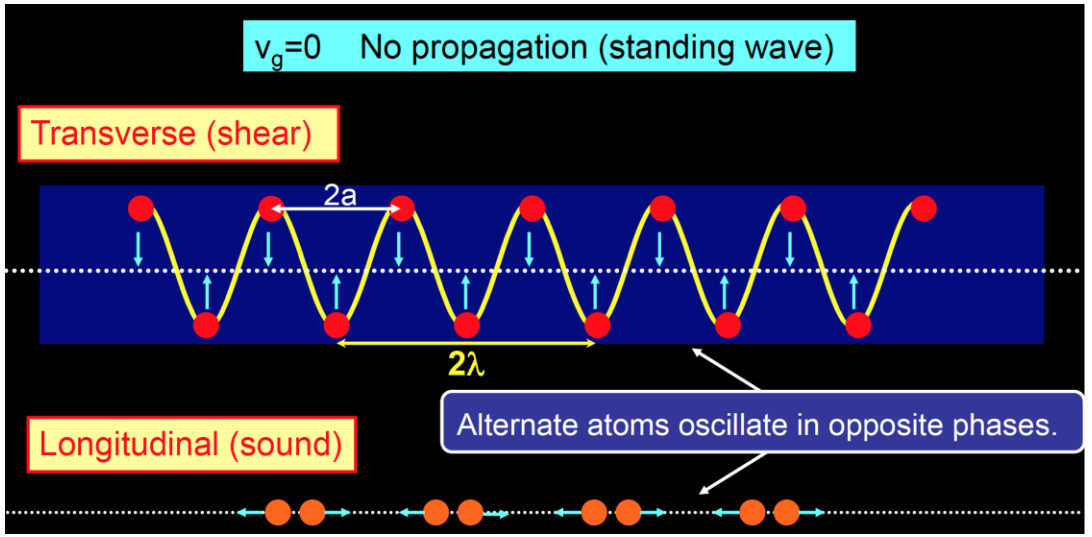
➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ Standing waves (驻波) at the boundary of the first Brillouin zone ($q = \pm\frac{\pi}{a}$):

$$v_g = v_s \cos\left(\frac{1}{2}aq\right)$$

$$q = \pm\frac{\pi}{a} \quad \Rightarrow \quad v_g = 0$$

$$\frac{u_{n+1,q}}{u_{nq}} = e^{-iaq} = -1$$

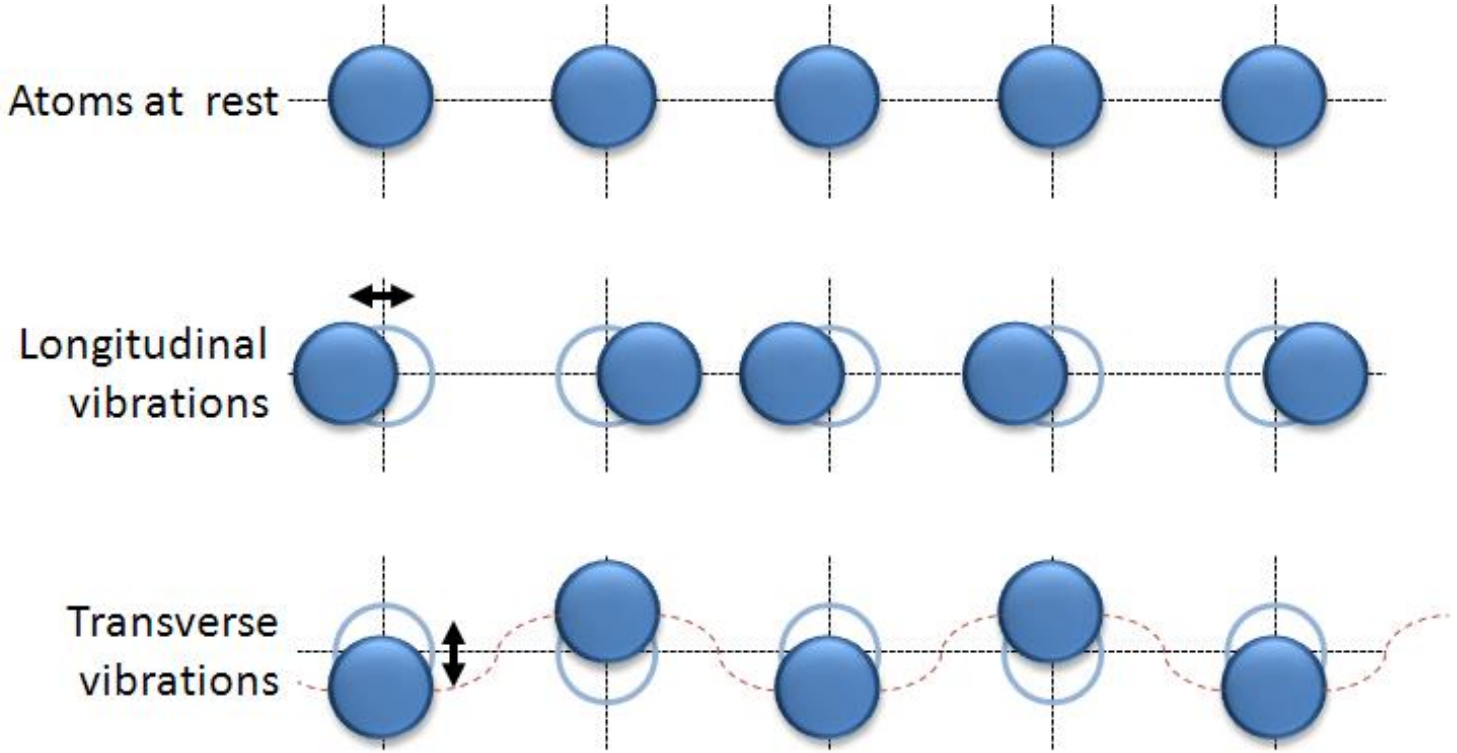


The standing waves are as a result of Bragg reflection (布拉格反射)!

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ Longitudinal Vibrations (纵振动/纵波) vs Transverse Vibrations (横振动/横波):



Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

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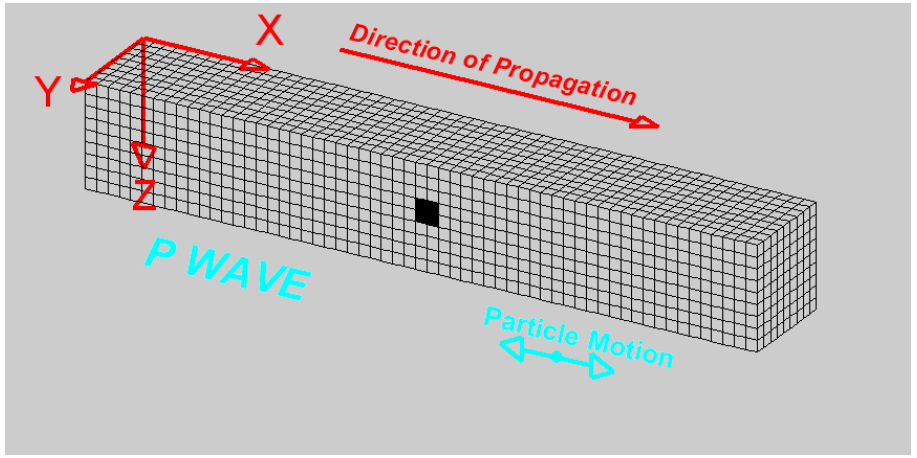
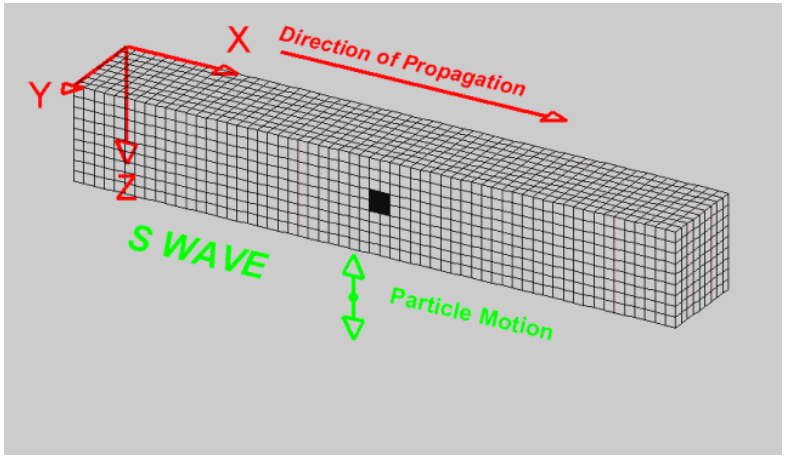




Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ **Total displacement** of atom n as a result of lattice vibrations:

$$u_n = \sum_q u_{nq} = \sum_q A_q \mathrm{e}^{i(\omega_q t - naq)}$$

Note:

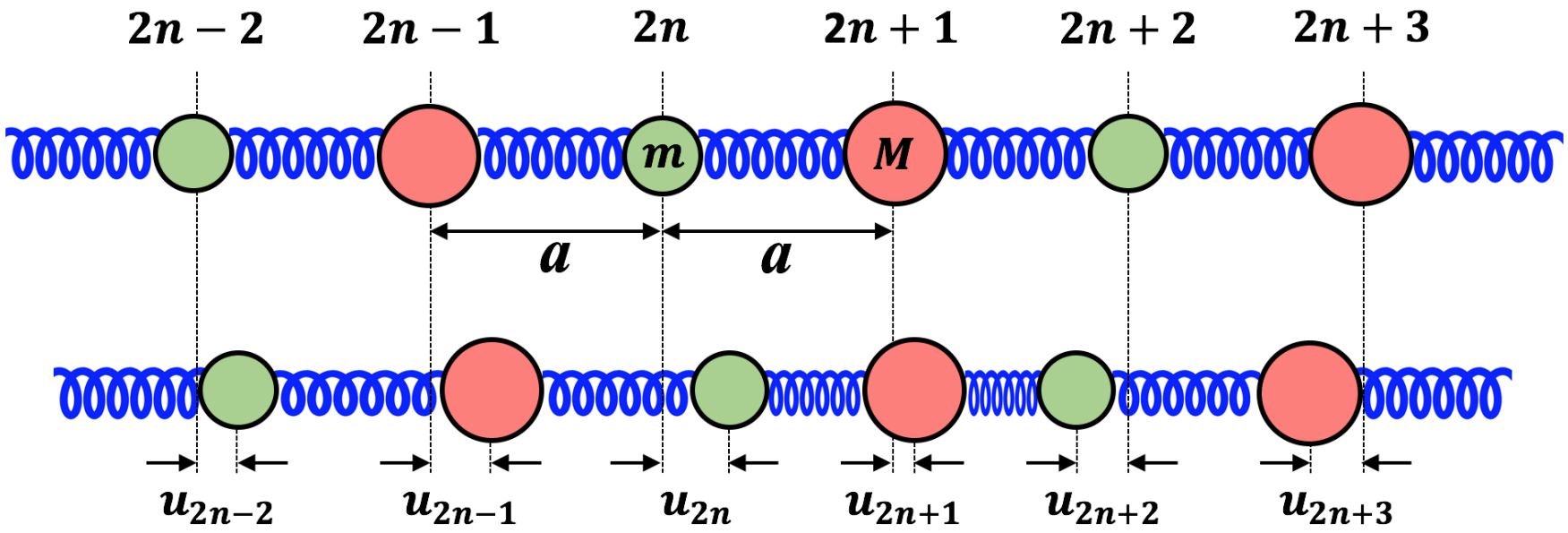
$\boldsymbol{u_{nq}}$ represents the displacement of atom n as a result of the $\boldsymbol{q}$**th vibration mode**.

Vibrations of a 1D Diatomic Chain
(一维双原子链的振动)

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ We turn to consider a 1D diatomic chain (two atoms per primitive cell) consisting of N primitive cells. The masses of the two atoms of each cell are m and M, respectively.



Note that the lattice constant is $2a$ instead of a!

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ By applying a procedure similar to that of the case of 1D monoatomic chain as well as assuming the **harmonic and nearest-neighbor approximations**, the **Newtonian equation of motion** for the 1D diatomic chain reads:

$$\begin{cases} m\dfrac{d^2u_{2n}}{dt^2} = K(u_{2n+1} + u_{2n-1} - 2u_{2n}) \\ M\dfrac{d^2u_{2n+1}}{dt^2} = K(u_{2n+2} + u_{2n} - 2u_{2n+1}) \end{cases}$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ The solutions to the coupled set of equations above also have the form of "**lattice waves**":

$$\begin{cases} u_{2n,q} = A_q \mathrm{e}^{i[\omega t-(2n)aq]} \\ u_{2n+1,q} = B_q \mathrm{e}^{i[\omega t-(2n+1)aq]} \end{cases}$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ By applying $\boldsymbol{u_{2n,q}}$ and $\boldsymbol{u_{2n+1,q}}$ to the Newtonian equations of motion, it is obtained:

$$\omega^2 = \begin{cases} \omega_+^2 = \dfrac{K}{\mu}\left[1 + \sqrt{1 - \dfrac{4\mu^2}{mM}\sin^2(aq)}\right] & \textbf{Optical Branch (光学支)} \\ \omega_-^2 = \dfrac{K}{\mu}\left[1 - \sqrt{1 - \dfrac{4\mu^2}{mM}\sin^2(aq)}\right] & \textbf{Acoustical Branch (声学支)} \end{cases}$$

$\mu = \frac{mM}{m+M}$ represents the reduced mass (约化质量) of a primitive cell.

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

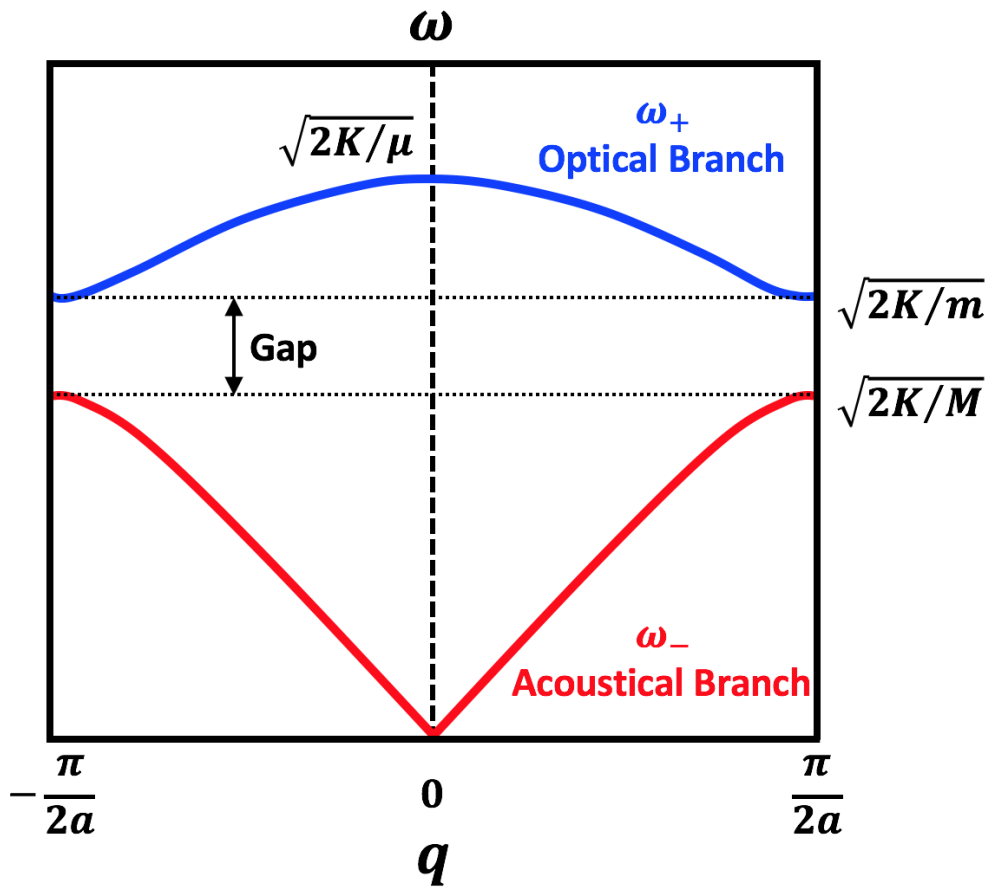
❖ **Dispersion relation** of a 1D diatomic chain:

The first Brillouin zone:

$$-\frac{\pi}{2a} \leq q < \frac{\pi}{2a}$$

or

$$-\frac{\pi}{2a} < q \leq \frac{\pi}{2a}$$



➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ Ratio between the displacement amplitudes of the two atoms in a primitive cell:

$$\begin{cases} \left(\frac{B}{A}\right)_{+} = \frac{2K - m\omega_{+}^{2}}{2K\cos(aq)} \\ \left(\frac{B}{A}\right)_{-} = \frac{2K - m\omega_{-}^{2}}{2K\cos(aq)} \end{cases}$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ The acoustical branch: $\omega_- \propto q \to 0 \quad \text{when } q \to 0$

$$\left(\frac{B}{A}\right)_- = \frac{2K - m\omega_-^2}{2K\cos(aq)} > 0$$

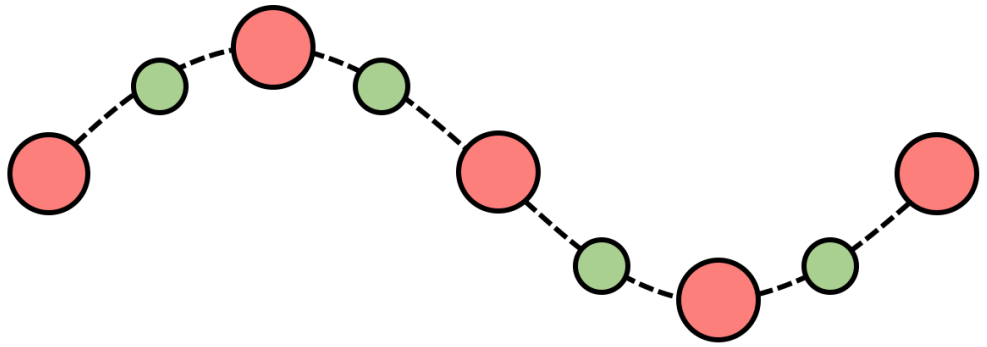
$$\Rightarrow \quad \left(\frac{\boldsymbol{B}}{\boldsymbol{A}}\right)_- = \mathbf{1}, \ \ \textbf{when } \boldsymbol{q} = \mathbf{0}$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ The acoustical branch: $\omega_{-} \propto q \to 0$ when $q \to 0$

In the long wavelength limit ($q \to 0$) of **acoustical branch**, the vibrations of the two atoms in a cell are **exactly the same in both phase and amplitude**!



An Example of Acoustical Vibration Mode
(Transverse Wave)

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ The optical branch: $\omega_+ \to \sqrt{2K/\mu} \neq 0$ when $q \to 0$

$$\left(\frac{B}{A}\right)_+ = \frac{2K - m\omega_+^2}{2K\cos(aq)} < 0$$

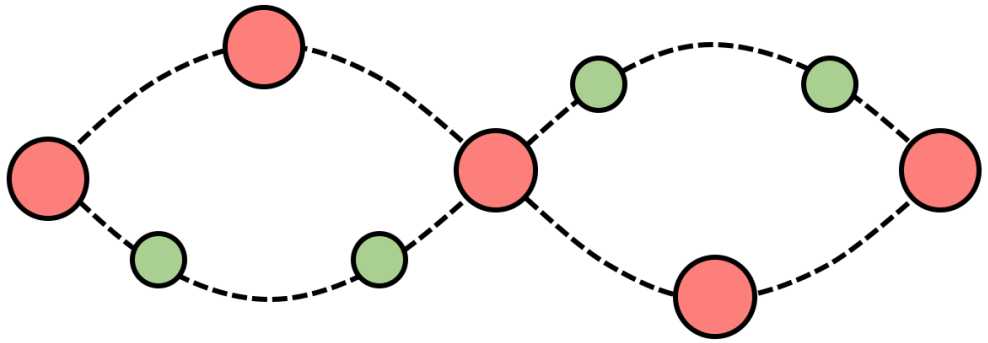
$$\Rightarrow \quad \left(\frac{\boldsymbol{B}}{\boldsymbol{A}}\right)_+ = -\frac{\boldsymbol{m}}{\boldsymbol{M}}, \quad \textbf{when } \boldsymbol{q = 0}$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ The optical branch: $\omega_+ \to \sqrt{2K/\mu} \neq 0$ when $q \to 0$

In the long wavelength limit ($q \to 0$) of **optical branch**, the vibrations of the two atoms in a cell are **opposite in phase, and the center of mass remains still**!



An Example of Optical Vibration Mode
(Transverse Wave)

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ Periodic boundary condition:

$$u_{2(n+N),q} = u_{2n,q} \longrightarrow q = l\frac{\pi}{Na}$$ (l is an integer and N the number of primitive cells)

❖ For a diatomic chain with $\boldsymbol{N}$ primitive cells, the number of wave vectors $\boldsymbol{q}$ in the first (or each) Brillouin zone is also $\boldsymbol{N}$. Since one $\boldsymbol{q}$ corresponds to two vibration modes (one acoustical and one optical), the **total number of vibration modes is $2\boldsymbol{N}$.**

$$-\frac{\pi}{2a} \le q < \frac{\pi}{2a} \longrightarrow -\frac{N}{2} \le l < \frac{N}{2} \quad (l_1, l_2, \cdots, l_N)$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ **Total displacements** of the two atoms in a primitive cell:

$$u_{2n} = \sum_q u_{2n,q} = \sum_q A_q \mathrm{e}^{i[\omega_q t - (2n)aq]}$$

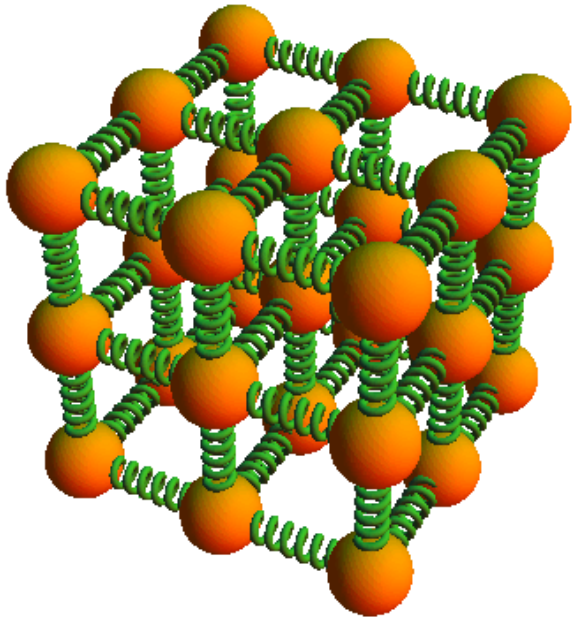
$$u_{2n+1} = \sum_q u_{2n+1,q} = \sum_q B_q \mathrm{e}^{i[\omega_q t - (2n+1)aq]}$$

Vibrations of a 3D Lattice
(三维晶格的振动)

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 3D Lattice (三维晶格的振动)

❖ Most real crystals have 3D lattices. In general, the vibrations of a 3D lattice can be described in a way similar to the case of 1D chains as discussed above.



Schematic Diagram of a Model of Lattice Vibrations in 3D

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 3D Lattice (三维晶格的振动)

❖ We consider a 3D lattice with $\boldsymbol{N = N_1 N_2 N_3}$ primitive cells (with $\boldsymbol{N_j}$ the number of primitive cells along the direction of the basis vector $\boldsymbol{\vec{a}_j}$, $j = 1, 2, 3$). Each primitive cell has $\boldsymbol{n}$ atoms with mass $\boldsymbol{m_k}$ $(k = 1, 2, \cdots, n)$.

❖ For a lattice vector $\vec{R}(l) = l_1\vec{a}_1 + l_2\vec{a}_2 + l_3\vec{a}_3$, the coordinates of the $\boldsymbol{n}$ atoms in the primitive cell are:

$$\vec{R}_{lk} \quad k = 1, 2, \cdots, n$$

The corresponding **displacements** of the $\boldsymbol{n}$ atoms from their equilibrium positions are:

$$\vec{u}_{lk} \quad k = 1, 2, \cdots, n$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 3D Lattice (三维晶格的振动)

❖ The **Newtonian equations of motion** for the n atoms in the primitive cell are:

$$m_k \frac{d^2}{dt^2} \vec{u}_{lk} = -\nabla_{\vec{u}_{lk}} V_l$$

V_l denotes the total interatomic potential energy of the primitive cell.

❖ The solutions to the equations above have the form of "**lattice waves**":

$$\vec{u}_{lkq} = \vec{A}_{kq} \mathbf{e}^{i(\omega t - \vec{R}_{lk} \cdot \vec{q})}$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 3D Lattice (三维晶格的振动)

❖ **Total displacement** of the atoms in a primitive cell:

$$\vec{u}_{lk} = \sum_{q} \vec{u}_{lkq} = \sum_{q} \vec{A}_{kq} \mathbf{e}^{i\left(\omega_q t - \vec{R}_{lk} \cdot \vec{q}\right)}$$

$\vec{u}_{lkq}$ represents the atomic displacement as a result of the q**th vibration mode**.

➢ Vibrations of a 3D Lattice (三维晶格的振动)

❖ The **periodic boundary condition** requires:

$$\vec{u}\left(\boldsymbol{R_l} + \boldsymbol{N_j a_j}\right) = \vec{u}(\boldsymbol{R_l}) \qquad \boldsymbol{j = 1, 2, 3}$$

$$\rightarrow \quad \boldsymbol{N_j \vec{a}_j \cdot \vec{q} = h_j 2\pi} \qquad \boldsymbol{j = 1, 2, 3}$$

$$\rightarrow \quad \vec{\boldsymbol{q}} = \frac{\boldsymbol{h_1}}{\boldsymbol{N_1}}\vec{\boldsymbol{b}}_{\boldsymbol{1}} + \frac{\boldsymbol{h_2}}{\boldsymbol{N_2}}\vec{\boldsymbol{b}}_{\boldsymbol{2}} + \frac{\boldsymbol{h_3}}{\boldsymbol{N_3}}\vec{\boldsymbol{b}}_{\boldsymbol{3}}$$

$\vec{b}_j$ $(j = 1, 2, 3)$ denote the basis vectors of the reciprocal lattice.

➢ Vibrations of a 3D Lattice (三维晶格的振动)

❖ The volume occupied by each $\boldsymbol{q}$ in the reciprocal space:

$$\frac{\vec{\boldsymbol{b}}_1}{\boldsymbol{N}_1} \cdot \left(\frac{\vec{\boldsymbol{b}}_2}{\boldsymbol{N}_2} \times \frac{\vec{\boldsymbol{b}}_3}{\boldsymbol{N}_3} \right) = \frac{\boldsymbol{\Omega}^*}{\boldsymbol{N}}$$

$\boldsymbol{\Omega}^*$ denotes the volume of a primitive cell in the reciprocal lattice.

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 3D Lattice (三维晶格的振动)

❖ The **distribution density** of $\boldsymbol{q}$ in the reciprocal space:

$$\frac{\boldsymbol{N}}{\boldsymbol{\Omega}^*} = \frac{\boldsymbol{N\Omega}}{(\boldsymbol{2\pi})^3} = \frac{\boldsymbol{V}}{(\boldsymbol{2\pi})^3}$$

$\boldsymbol{\Omega}$ denotes the volume of a primitive cell and $\boldsymbol{V}$ the total volume of the direct lattice .

❖ The number of $\boldsymbol{q}$ per primitive cell in the reciprocal lattice:

$$\frac{\boldsymbol{N}}{\boldsymbol{\Omega}^*} \times \boldsymbol{\Omega}^* = \boldsymbol{N}$$

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 3D Lattice (三维晶格的振动)

❖ For all $\boldsymbol{q}$,

- the number of **acoustical branches** is $\mathbf{3}$ (corresponding to $\mathbf{1}$ branch of **longitudinal wave** and $\mathbf{2}$ branches of **transverse waves**);

- the number of **optical branches** is $\mathbf{3}\boldsymbol{n} - \mathbf{3}$.

❖ The **total number of vibration modes** is $\mathbf{3}\boldsymbol{n}\boldsymbol{N}$, which is equal to the total number of **degrees of freedom (自由度)** in the 3D crystal.

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 3D Lattice (三维晶格的振动)

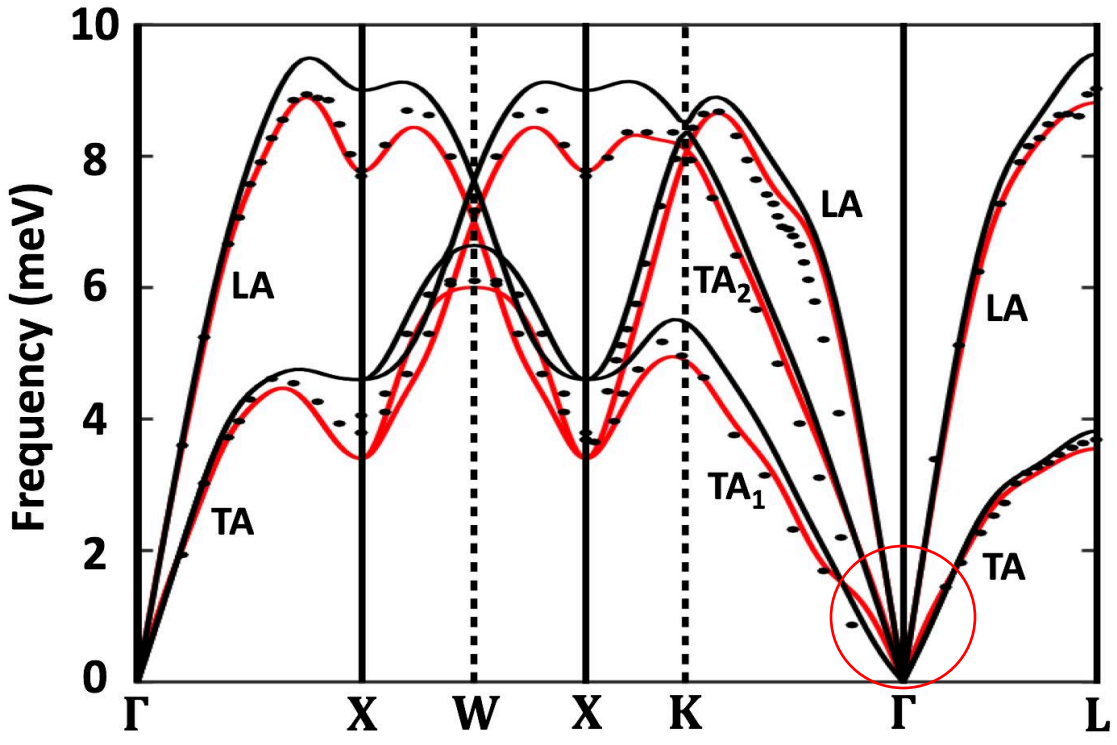
❖ Characteristics of lattice vibrations **in 3D**:

	Number of Primitive Cells 原胞数	Number of Atoms per Primitive Cell 原胞内原子数
	N	n
Number of Wave Vectors in Each BZ 布里渊区内波矢数	N	
Total Number of Branches 格波总支数	$3n$	
Number of Acoustical Branches 声学支数	3 (1 longitudinal and 2 transverse)	
Number of Optical Branches 光学支数	$3n-3$	
Total Number of Vibration Modes 振动模总数	$3nN$	
Number of Acoustical Modes 声学模数	$3N$	
Number of Optical Modes 光学模数	$3nN-3N$	

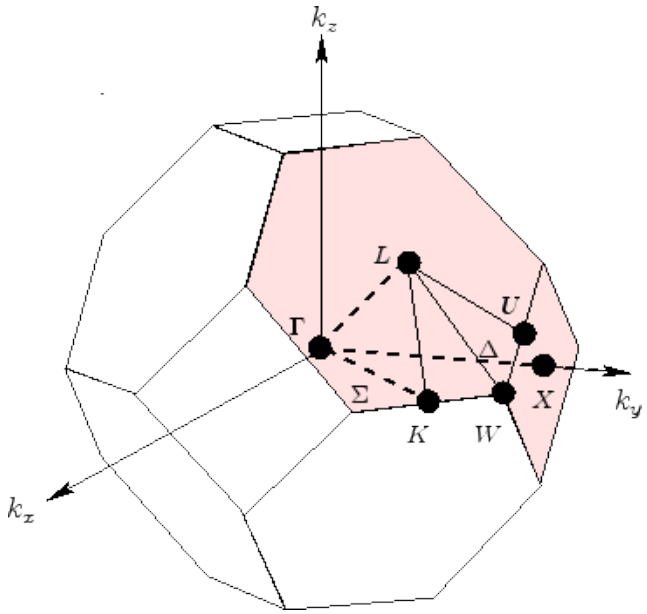
Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 3D Lattice (三维晶格的振动)

❖ Examples of **lattice vibration spectrum (晶格振动谱)** in real crystals:



Pb (1 atom per primitive cell)



bcc reciprocal lattice

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Vibrations of a 3D Lattice (三维晶格的振动)

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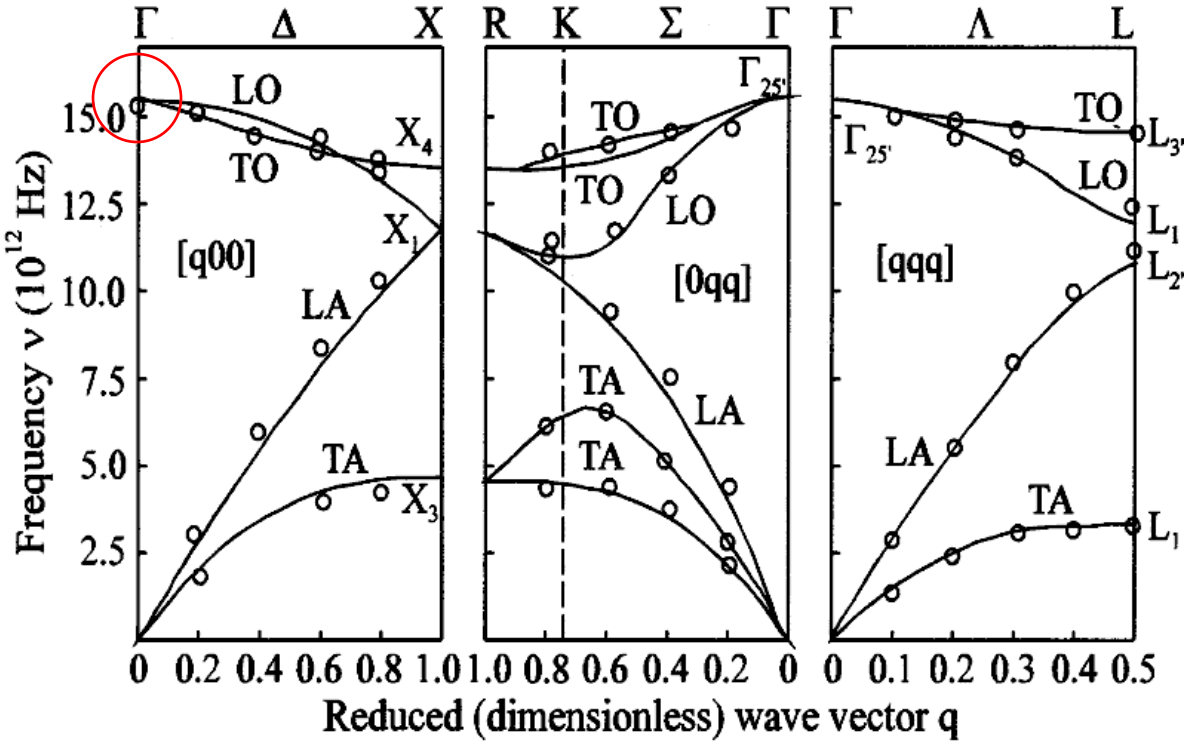
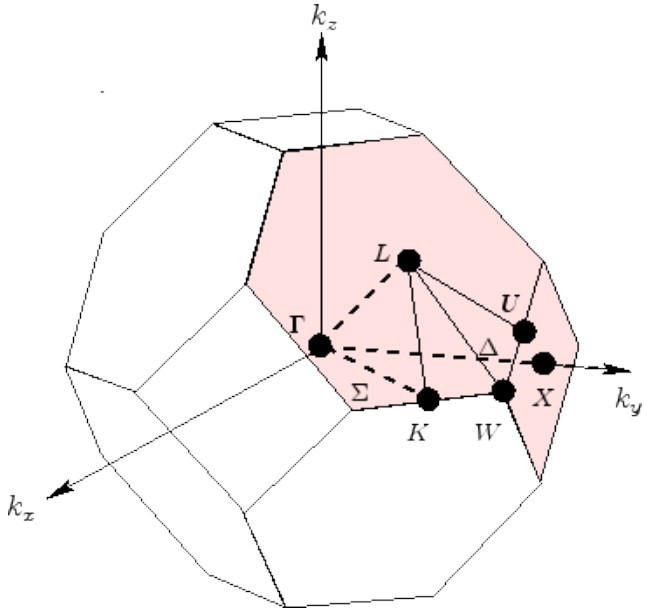


Si (2 atoms per primitive cell)



bcc reciprocal lattice

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

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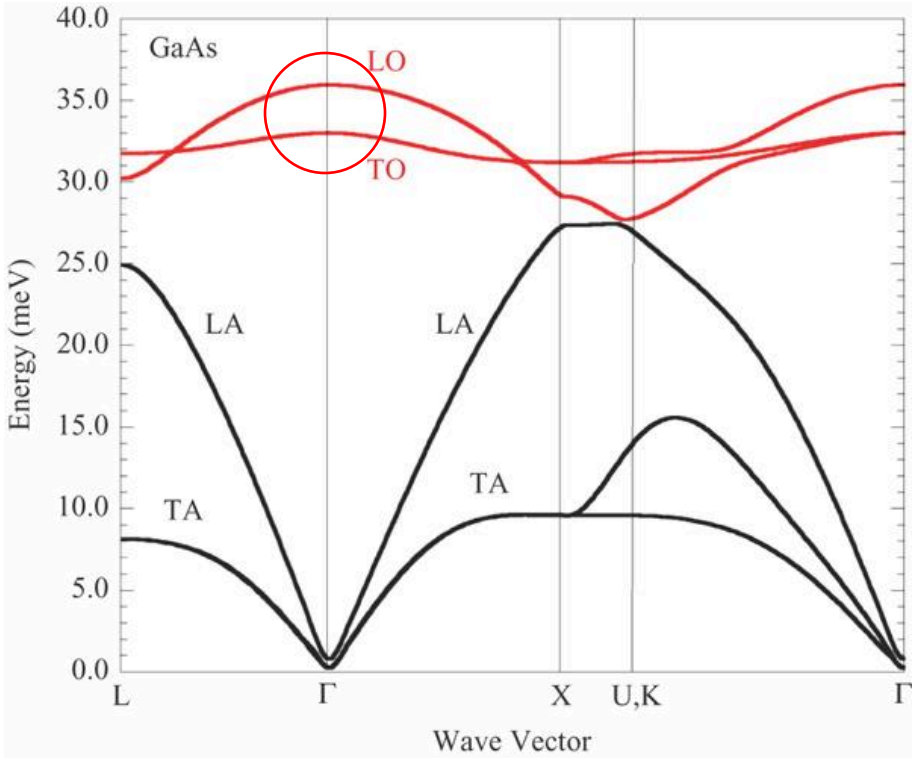
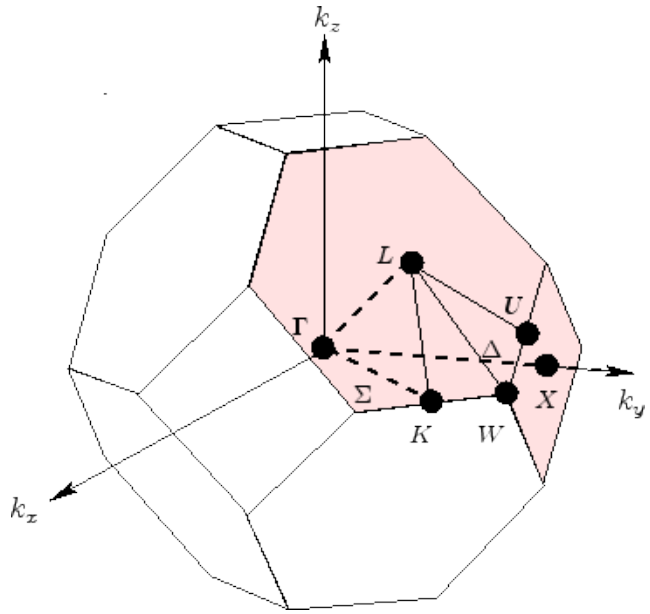


GaAs (2 atoms per primitive cell)



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Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

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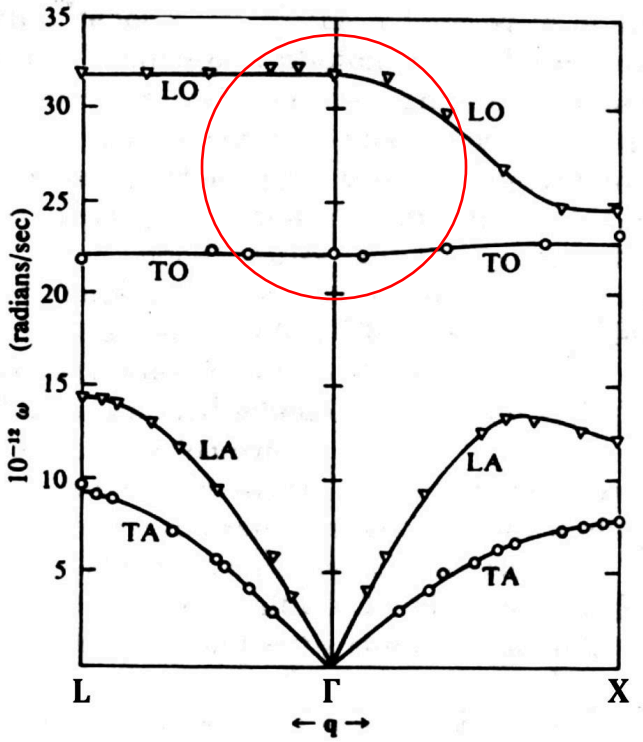
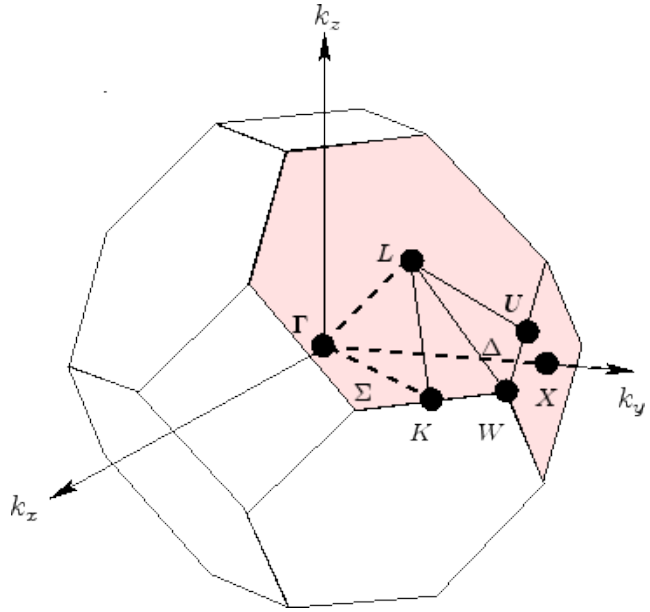


NaCl (2 atoms per primitive cell)



bcc reciprocal lattice

Summary (总结)

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

➢ Summary (总结)

- ❖ The **4 approximations** made for modeling lattice vibrations.
- ❖ Lattice vibrations in a 1D **monoatomic** chain: **acoustical branch only.**
- ❖ Lattice vibrations in a 1D **diatomic** chain: **both acoustical and optical branches.**
- ❖ Lattice vibrations in a 3D lattice.

Chapter 3.1: 课后作业

考虑一维双原子链(1D diatomic chain):

1) 计算长波极限($q \to 0$)下声学支和光学支格波的色散关系$\omega \sim q$;

2) 分析第一布里渊区边界处的振动特点;

3) 当$m = M$时, 画出第一布里渊区内的色散关系$\omega \sim q$, 并与一维单原子链 (1D monoatomic chain) 的情形进行比较.

提交时间： **3月17日之前**

提交方式： **手写（写明姓名学号）后拍照，通**过本班课代表统一提交电子版