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)

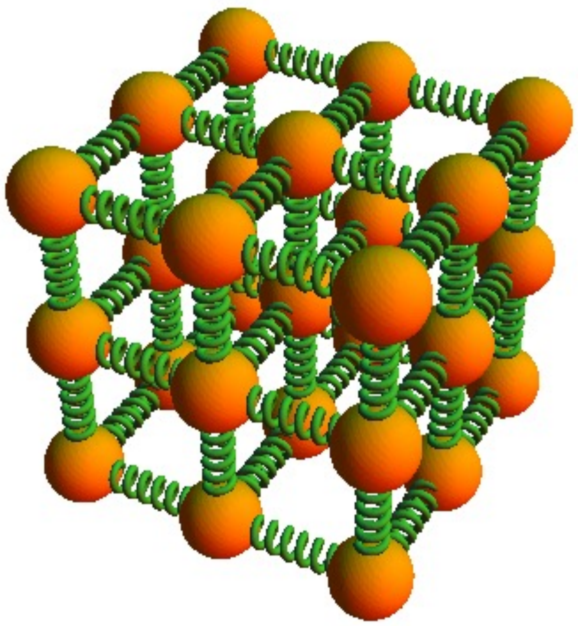
Objectives

- To learn the concept of **normal coordinates.**
- To understand the concept of **phonon** and its physical significance.
- To learn typical **quasi-particles**.

Normal Coordinates (简正坐标)

➢ Normal Coordinates (简正坐标)

❖ We consider a 3D lattice with $\boldsymbol{N}$ atoms. The equilibrium positions of the atoms are $\boldsymbol{R_n}$, and their displacements from the equilibrium positions at time $\boldsymbol{t}$ are $\boldsymbol{u_n}(\boldsymbol{t})$ $(n = 1, 2, \cdots, 3N)$.



Normal Coordinates (简正坐标)

- The interatomic potential energy $\boldsymbol{V}$ of the lattice can be expanded about the equilibrium positions in terms of **Taylor series (泰勒级数)**:

$$V = V_0 + \sum_{j=1}^{3N} \left(\frac{\partial V}{\partial u_j}\right)_0 u_j + \frac{1}{2}\sum_{i,j=1}^{3N} \left(\frac{\partial^2 V}{\partial u_i \partial u_j}\right)_0 u_i u_j + \cdots$$

Note that $\left(\frac{\partial V}{\partial u_j}\right)_0 = 0.$

➢ Normal Coordinates (简正坐标)

❖ In the harmonic approximation, the potential energy $\boldsymbol{V}$ of the lattice reads:

$$V = \frac{1}{2}\sum_{i,j=1}^{3N}\left(\frac{\partial^2 V}{\partial u_i \partial u_j}\right)_0 u_i u_j$$

❖ The kinetic energy $\boldsymbol{T}$ of the lattice can be expressed as:

$$T = \frac{1}{2}\sum_{j=1}^{3N} m_j\, \dot{u}_j^2$$

➢ Normal Coordinates (简正坐标)

❖ To simplify the forms of $\boldsymbol{V}$ and $\boldsymbol{T}$, we introduce **normal coordinates** $Q_1, Q_2, Q_3, \cdots, Q_{3N}$ that are connected with $u_1, u_2, u_3, \cdots, u_{3N}$ by an **orthogonal transformation (正交变换)**:

$$\sqrt{m_i}u_i = \sum_{j=1}^{3N} a_{ij}Q_j$$

➢ Normal Coordinates (简正坐标)

❖ We can always find a set of $\boldsymbol{a_{ij}}$ such that $\boldsymbol{V}$ and $\boldsymbol{T}$ are both **diagonalized** (对角化):

$$T = \frac{1}{2}\sum_{j=1}^{3N} \dot{Q}_j^2 \qquad\qquad V = \frac{1}{2}\sum_{j=1}^{3N} \omega_j^2 Q_j^2$$

➢ Normal Coordinates (简正坐标)

❖ The **generalized momenta** (广义动量) can be obtained as:

$$P_j = \frac{\partial L}{\partial \dot{Q}_j} = \dot{Q}_j$$

Here $L = T - V$ denotes the **Lagrangian** (拉格朗日量) of the system.

➢ Normal Coordinates (简正坐标)

❖ Thus, the **Hamiltonian (哈密顿量)** of the system reads:

$$H = T + V = \frac{1}{2}\sum_{j=1}^{3N}\left(P_j^2 + \omega_j^2 Q_j^2\right)$$

➢ Normal Coordinates (简正坐标)

❖ The equations of motion can be obtained through $\dot{\boldsymbol{P}}_{\boldsymbol{j}} = -\frac{\boldsymbol{\partial H}}{\boldsymbol{\partial Q_j}}$. Thus, we can obtain $3N$ **independent equations of motion:**

$$\ddot{Q}_j + \omega_j^2 Q_j = 0 \qquad j = 1,2,\cdots,3N$$

The solutions: $Q_j = A_j \mathrm{e}^{i(\omega_j t + \varphi)}$

❖ The normal coordinates describe **independent harmonic oscillations (独立简谐振动)!**

Normal Coordinates (简正坐标)

- The lattice displacements $\boldsymbol{u_n}$ can be expressed in terms of the normal coordinates as:

$$u_n = \sum_{j=1}^{3N} \frac{a_{nj}}{\sqrt{m_n}} Q_j$$

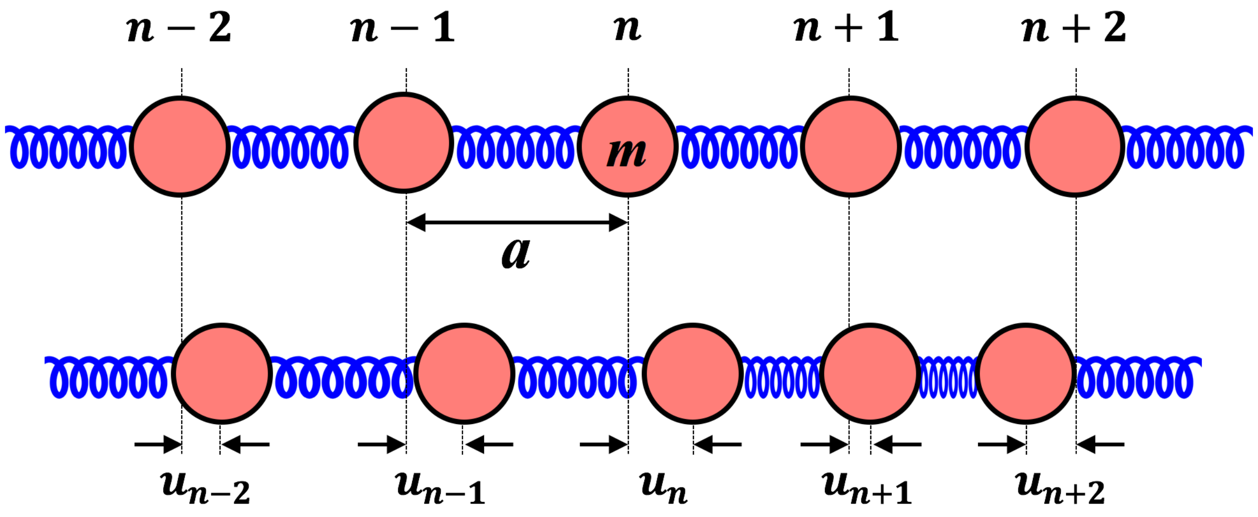
- Thus, $\boldsymbol{Q_j}$ essentially represents a **vibration mode (振动模)** of the lattice vibrations!

  The number of vibration modes is equal to the degrees of freedom!

Normal Coordinates (简正坐标)

The case of a 1D monoatomic chain:

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



➢ Normal Coordinates (简正坐标)

❖ The case of a 1D monoatomic chain:

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

The lattice displacements can also be expressed in terms of normal modes as:

$$u_n = \frac{1}{\sqrt{Nm}} \sum_q Q_q \mathrm{e}^{-inaq}$$

$$\longrightarrow \qquad Q_q = \sqrt{Nm} A_q \mathrm{e}^{i\omega_q t}$$

➢ Normal Coordinates (简正坐标)

❖ **The case of a 1D monoatomic chain:**

$$\sqrt{m_n} u_n = \sum_q a_{nq} Q_q$$

$$\rightarrow \quad a_{nq} = \frac{1}{\sqrt{N}} \mathrm{e}^{-inaq}$$

❖ The normal coordinates $\boldsymbol{Q_q}$ represent the **discrete Fourier transform (离散傅里叶变换)** of the lattice displacements $\boldsymbol{u_n}$!

- **Normal Coordinates (简正坐标)**

  - **The case of a 1D monoatomic chain:**

The normal coordinates $\boldsymbol{Q_q}$ require:

$$\begin{cases} Q_q^* = Q_{-q} \\ \dfrac{1}{N}\displaystyle\sum_{n=0}^{N-1} e^{ina(q-q')} = \delta_{qq'} \end{cases}$$

Quantization of Lattice Vibrations
(晶格振动的量子化)

➢ Quantization of Lattice Vibrations (晶格振动的量子化)

❖ The Hamiltonian of the lattice vibrations expressed in terms of **normal coordinates** (简正坐标) and **generalized momenta** (广义动量) reads:

$$\boldsymbol{H} = \frac{\mathbf{1}}{\mathbf{2}}\sum_{j=1}^{3N}\left(P_j^2 + \omega_j^2 Q_j^2\right)$$

Note that this represents the Hamiltonian of $3N$ **independent harmonic oscillators (**$3N$**个独立谐振子)**!

➢ Quantization of Lattice Vibrations (晶格振动的量子化)

- ❖ The stationary Schrodinger equation reads:

$$\hat{H}\psi = E\psi$$

Here, $\hat{H} = \frac{1}{2}\sum_{j=1}^{3N}\left(\hat{P}_j^2 + \omega_j^2\hat{Q}_j^2\right)$ denotes the **Hamiltonian operator (哈密顿量算符)**.

➢ Quantization of Lattice Vibrations (晶格振动的量子化)

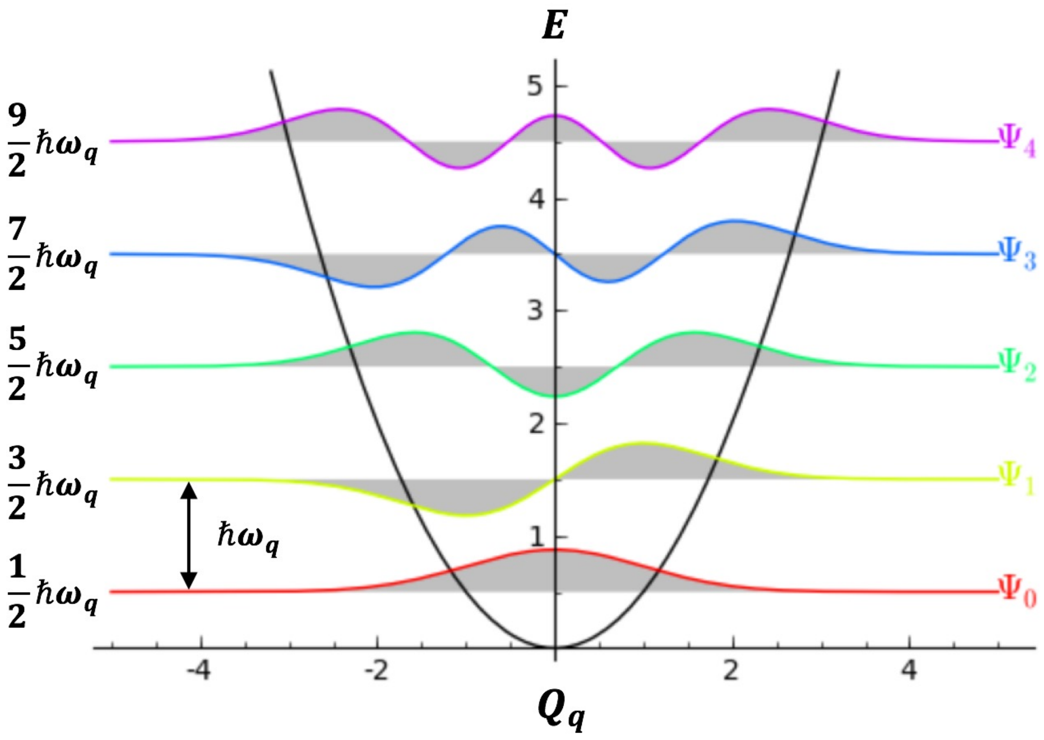
❖ The solutions to the Schrodinger equation:

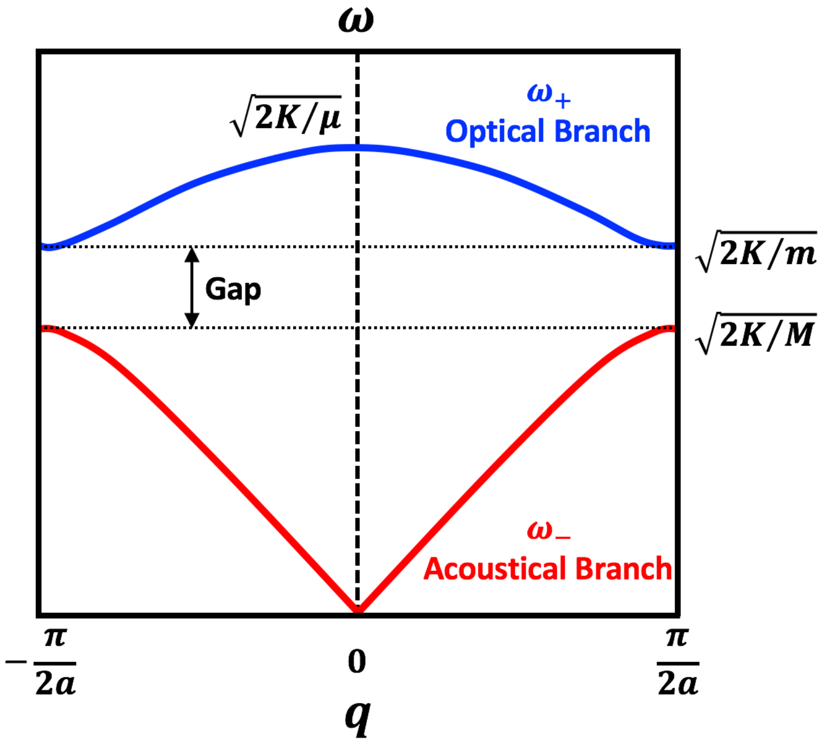
$$\boldsymbol{\psi_{n_q}} \qquad \boldsymbol{E_{n_q} = \left(n_q + \frac{1}{2}\right)\hbar\omega_q} \qquad \boldsymbol{n_q = 0, 1, 2, 3, \cdots}$$

$\boldsymbol{n_q}$ represents the number of phonons at stationary state $\boldsymbol{\psi_{n_q}}$.

Phonons (声子)

- A **phonon** represents a **quantum of lattice vibrations** (晶格振动的量子).





➢ Phonons (声子)

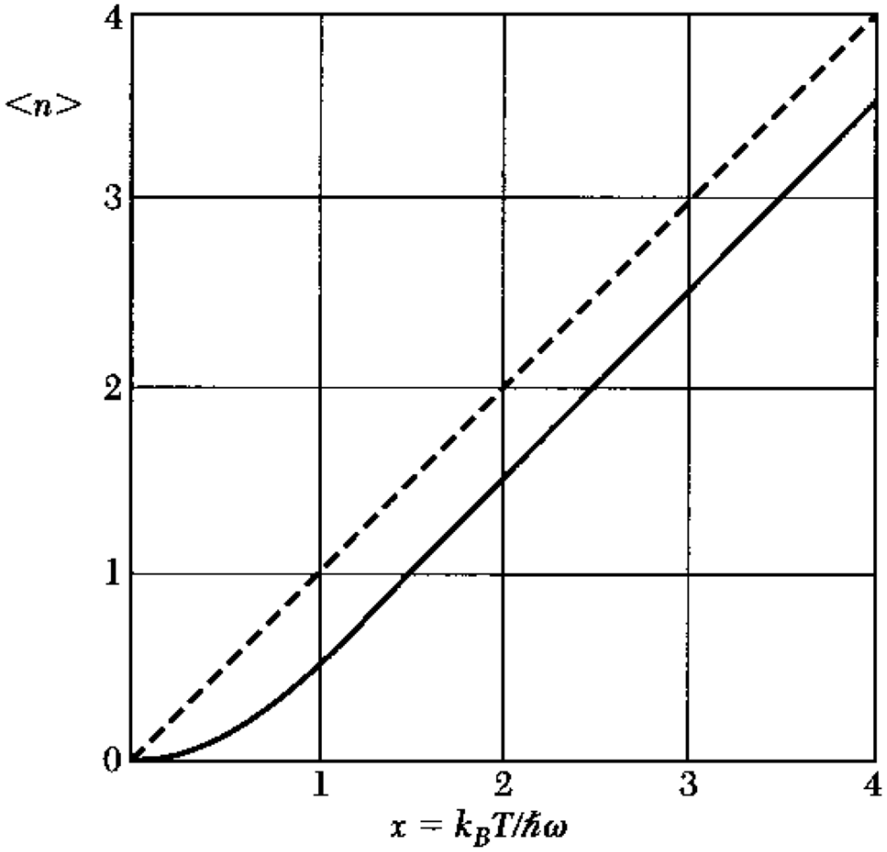
❖ A **phonon** represents a **quantum of lattice vibrations** (晶格振动的量子).

- Phonons can be regarded as **quasi-particles** (准粒子);
- The **energy** of a phonon is $\hbar\boldsymbol{\omega_q}$;
- The **quasi-momentum** (准动量) of a phonon is $\hbar\boldsymbol{q}$;
- Phonon belongs to **Bosons** (玻色子) and obeys **Bose-Einstein Statistics** (玻色-爱因斯坦统计):

$$\langle \boldsymbol{n} \rangle = \frac{\mathbf{1}}{\mathbf{e}^{\hbar\omega/k_\mathrm{B}T} - \mathbf{1}}$$

- **Phonons (声子)**
  - A **phonon** represents a **quantum of lattice vibrations** (晶格振动的量子).

$$\langle n \rangle = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$



➢ Phonons (声子)

❖ Experimental probe of phonon dispersion:

- Far-Infrared Spectroscopy (远红外光谱)
- Infrared Spectroscopy (红外光谱)
- Raman Spectroscopy (拉曼光谱)
- Brillouin Spectroscopy (布里渊散射谱)
- Diffuse X-Ray Scattering (X射线漫散射)
- Inelastic Neutron Scattering (非弹性中子散射)
- Inelastic Electron Tunneling Spectroscopy (非弹性电子隧道谱)
- Ultrasonic Methods (超声技术)

➢ Phonons (声子)

❖ Experimental probe of phonon dispersion:

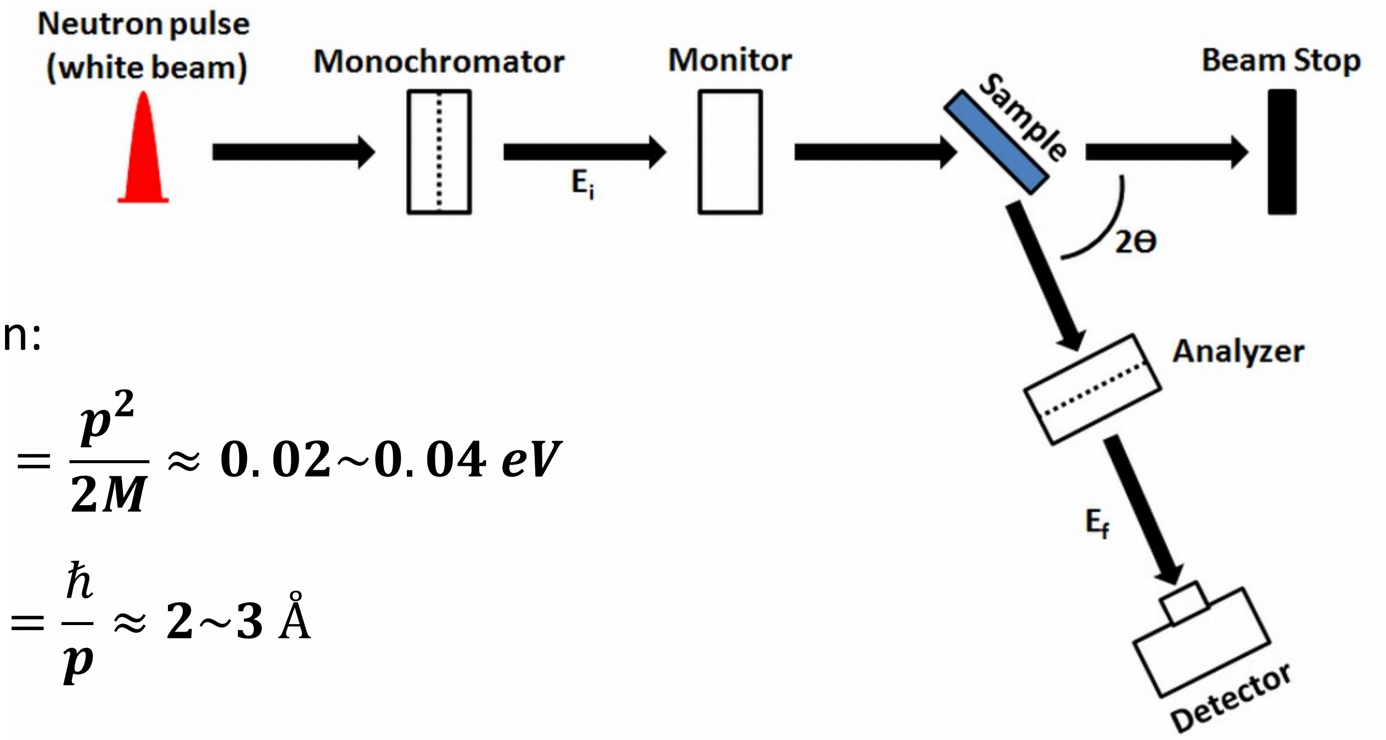
Conservation of Energy (能量守恒): $$\frac{\boldsymbol{p}'^2}{2\boldsymbol{M}} - \frac{\boldsymbol{p}^2}{2\boldsymbol{M}} = \pm\hbar\boldsymbol{\omega}_{\boldsymbol{q}}$$

Conservation of Momentum (动量守恒): $$\boldsymbol{p}' - \boldsymbol{p} = \pm\hbar\boldsymbol{q} + \hbar\boldsymbol{G}_{\boldsymbol{n}}$$

Phonons (声子)

- Experimental probe of phonon dispersion:

Inelastic Neutron Scattering (非弹性中子散射)



For a neutron:

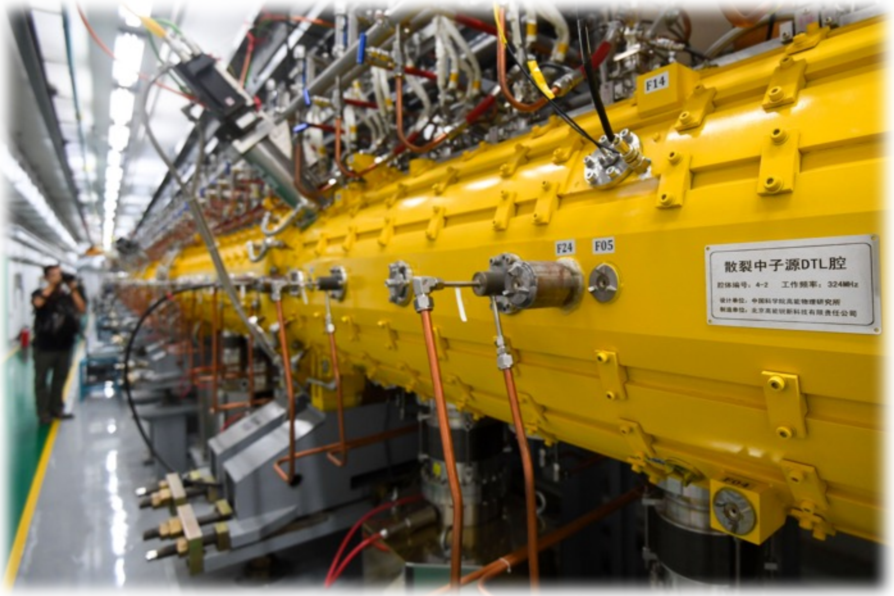
$$E = \frac{p^2}{2M} \approx 0.02\sim0.04\ eV$$

$$\lambda = \frac{\hbar}{p} \approx 2\sim3\ \text{Å}$$

Chapter 3.2: Phonons (声子)

➢ Phonons (声子)

❖ Experimental probe of phonon dispersion:



China Spallation Neutron Source (CSNS 中国散裂中子源, 广东东莞, 2018年8月23日正式投入运行)

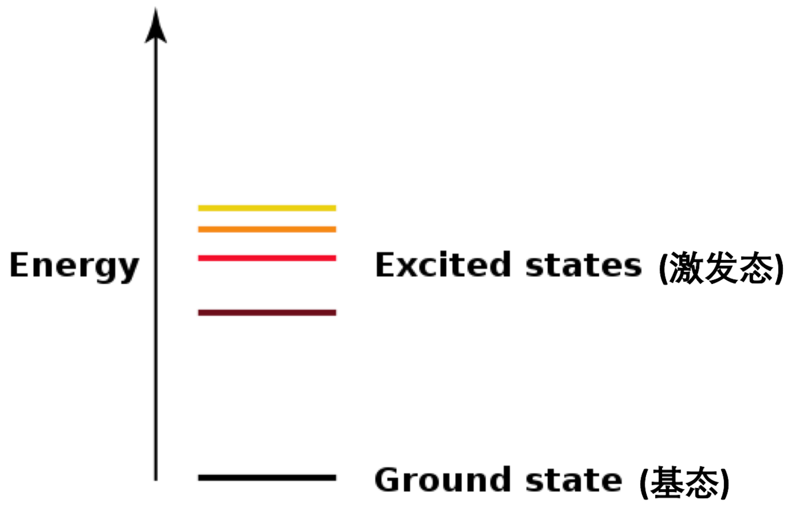
Quasi-particles (准粒子)

➢ Quasi-particles (准粒子)

- ❖ Quasi-particles, also called **elementary excitations** (元激发), are the **quanta of the low-lying excited states (低能激发态的量子)** of a solid- or condensed-state system.

- ❖ Quasi-particles can be either **single excitations** (单激发) or **collective excitations** (集体激发).

- ❖ Quasi-particles have a **definite energy**, and sometimes a **definite quasi-momentum**.



Chapter 3.2: Phonons (声子)

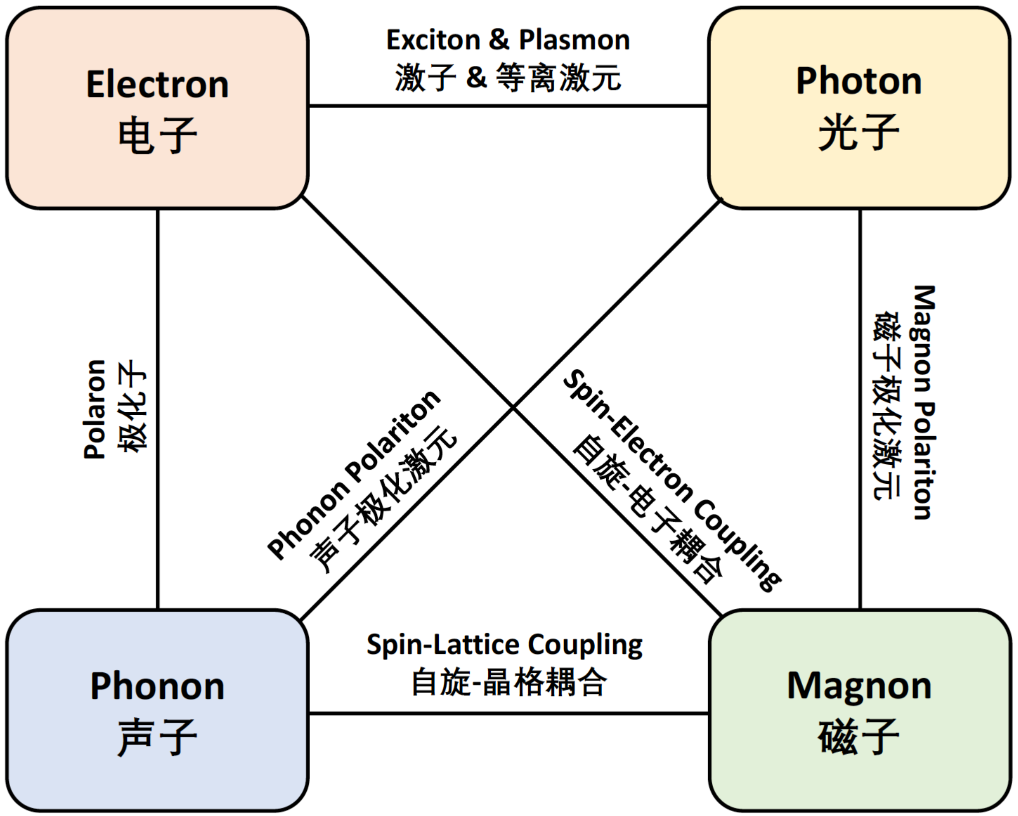
➢ Quasi-particles (准粒子)

❖ Some important quasi-particles in solids:

Quasiparticle	Field	Type
Electron/Hole Quasiparticle 电子/空穴准粒子	Free Electron + Coulomb Interactions 自由电子 + 库伦相互作用	Fermion 费米子
Phonon 声子	Lattice Wave 格波	Boson 玻色子
Polaron 极化子	Electron/Hole + Phonon “Cloud” (Lattice Distortion) 电子/空穴 + 声子“云” (晶格畸变)	Fermion 费米子
Exciton 激子	Electron + Hole 电子 + 空穴	Boson 玻色子
Plasmon 等离激元	Collective Electron Wave 集体电子波	Boson 玻色子
Magnon 磁子	Spin Wave 自旋波	Boson 玻色子
Polariton 极化激元	Photon + Phonon/Exciton/Plasmon/Magnon 光子 + 声子/激子/等离激元/磁子	Boson 玻色子

- **Quasi-particles (准粒子)**

  - Interactions between particles and/or quasiparticles (粒子或准粒子之间的相互作用):



➢ Quasi-particles (准粒子)

❖ Electron/Hole Quasiparticle (电子/空穴准粒子):

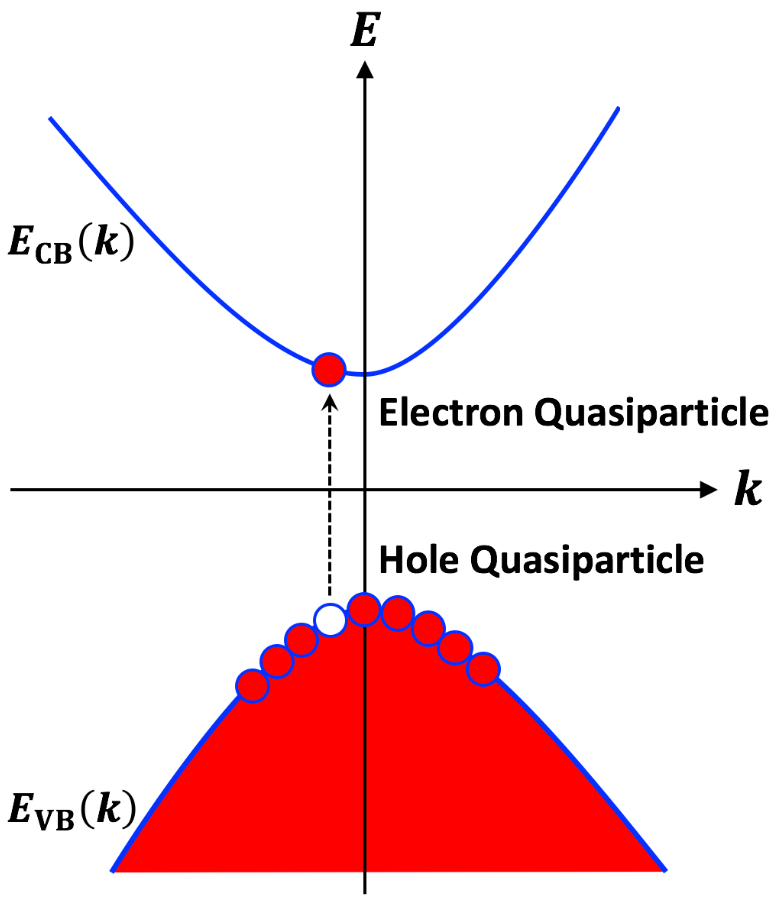
- Electron/hole quasiparticles are charged quasiparticles travelling in solids.

- The **effective mass** (**有效质量**) of an electron/hole is determined by its energy dispersion $E(k)$:

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}$$

$$\boxed{m^* \neq m_0}$$

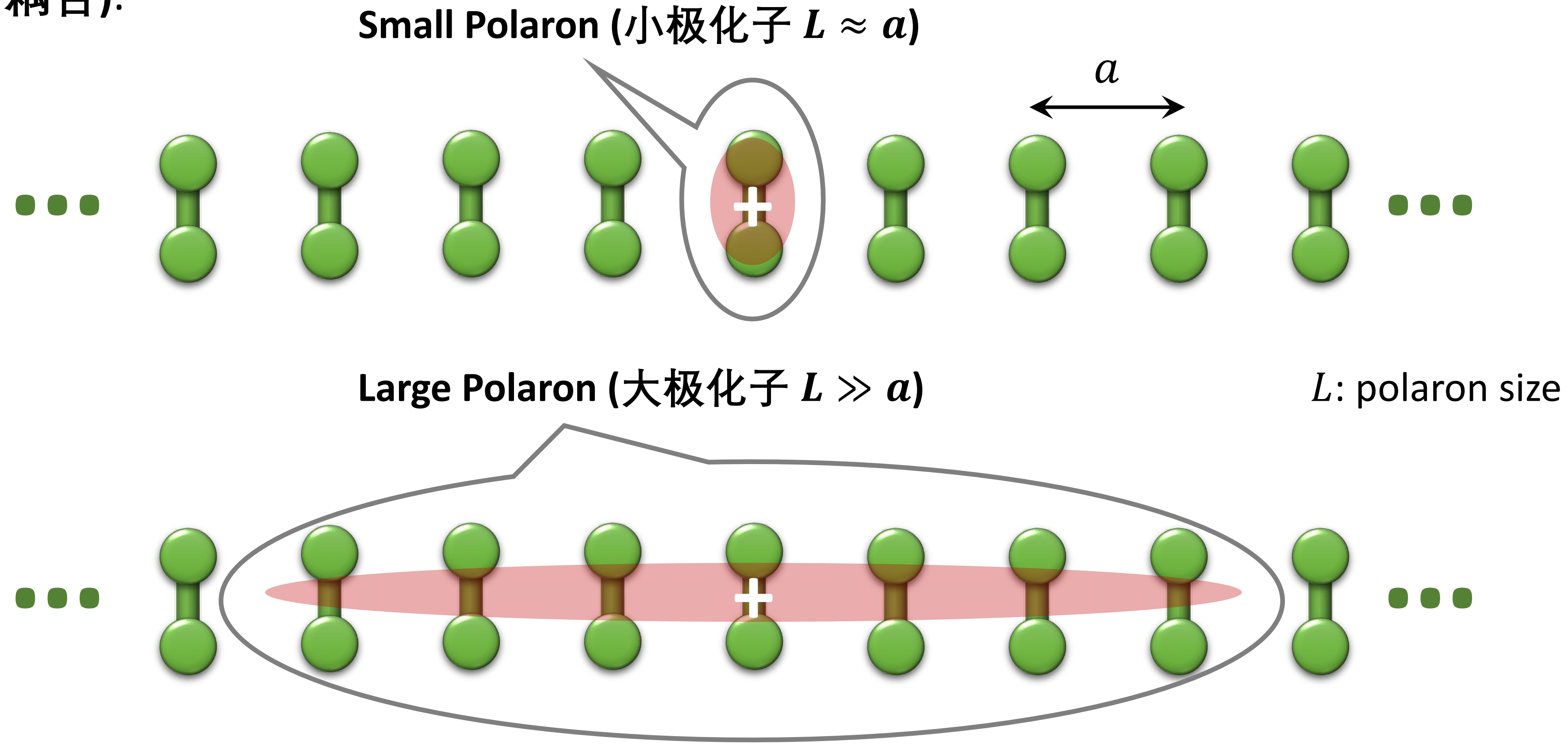
m_0 denotes the mass of free electron.



➢ Quasi-particles (准粒子)

❖ Polaron (极化子):

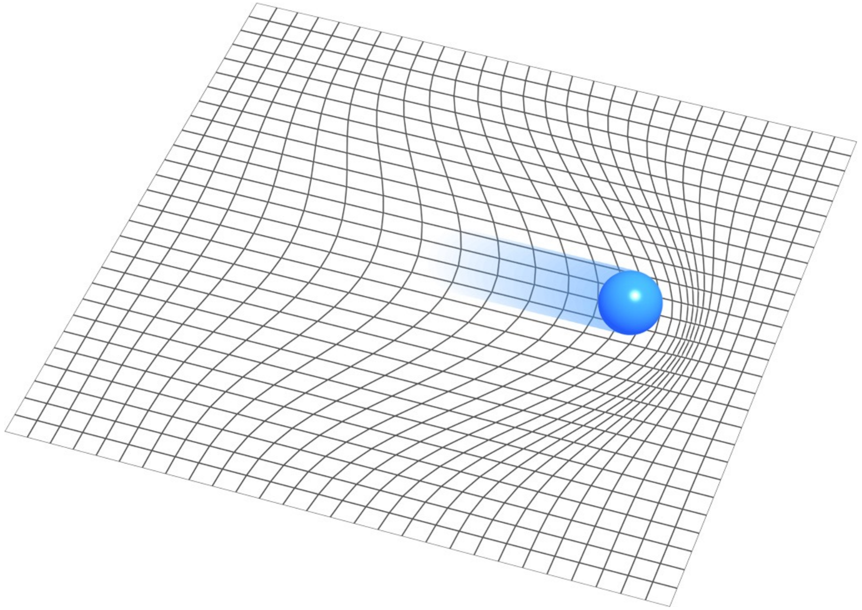
- A polaron is an electron/hole surrounded by phonon cloud as a result of **electron-phonon coupling** **(电子声子耦合)**.

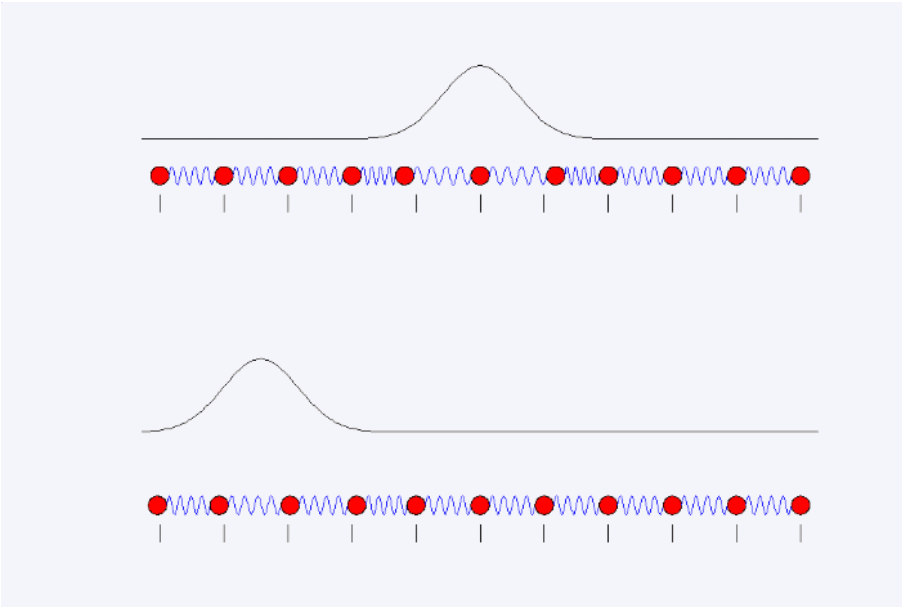


➢ Quasi-particles (准粒子)

❖ Polaron (极化子):

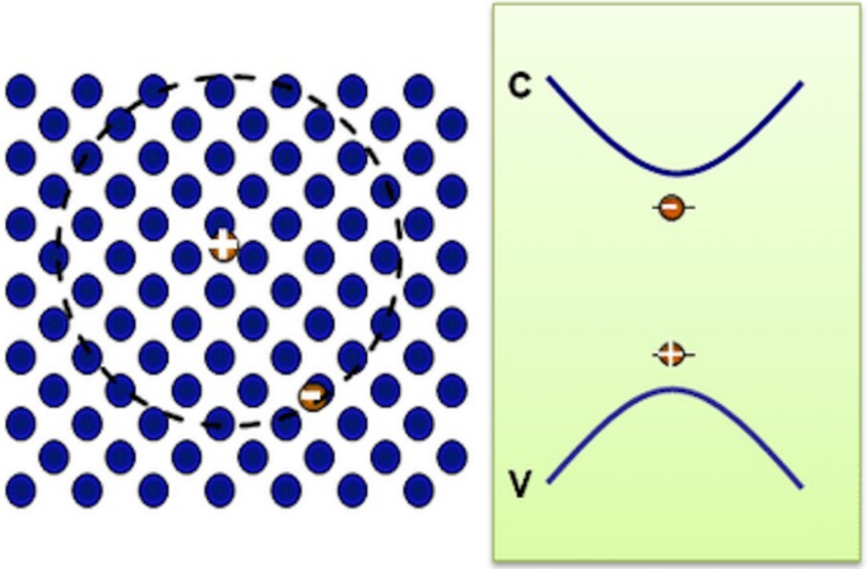
- A polaron is a **self-trapped state** (自陷态) of an electron/hole. Dynamically, the electron/hole and the induced lattice distortion move as a whole.



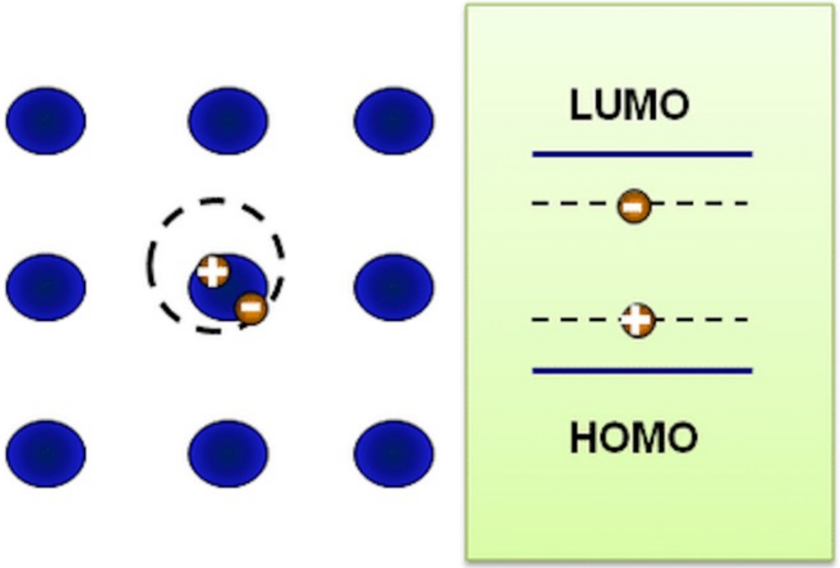


- **Quasi-particles (准粒子)**
  - **Exciton (激子):**
    - An exciton is an **electron-hole pair (电子-空穴对) combined by Coulomb attraction**.

Wannier-Mott Exciton (瓦尼尔-莫特激子)



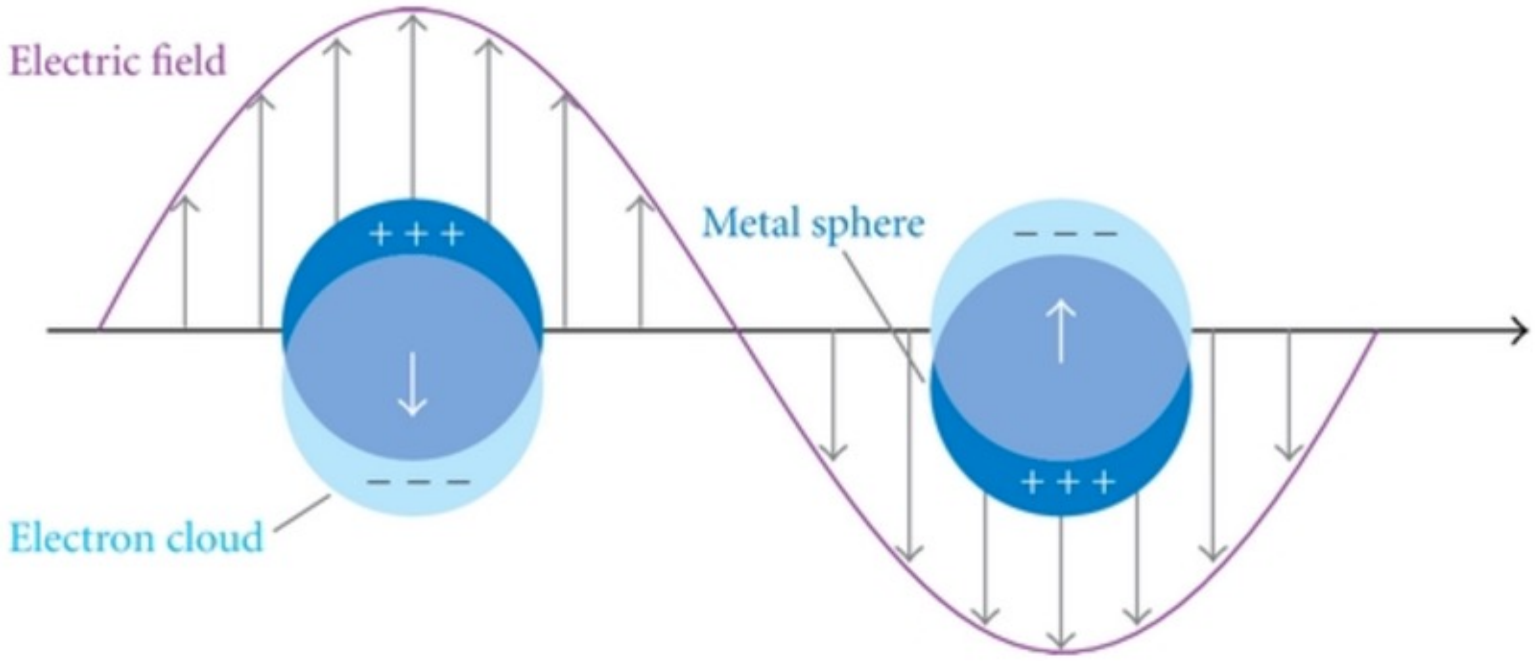
Frenkel Exciton (弗伦克尔激子)



- **Quasi-particles (准粒子)**

  - **Plasmon (等离激元):**

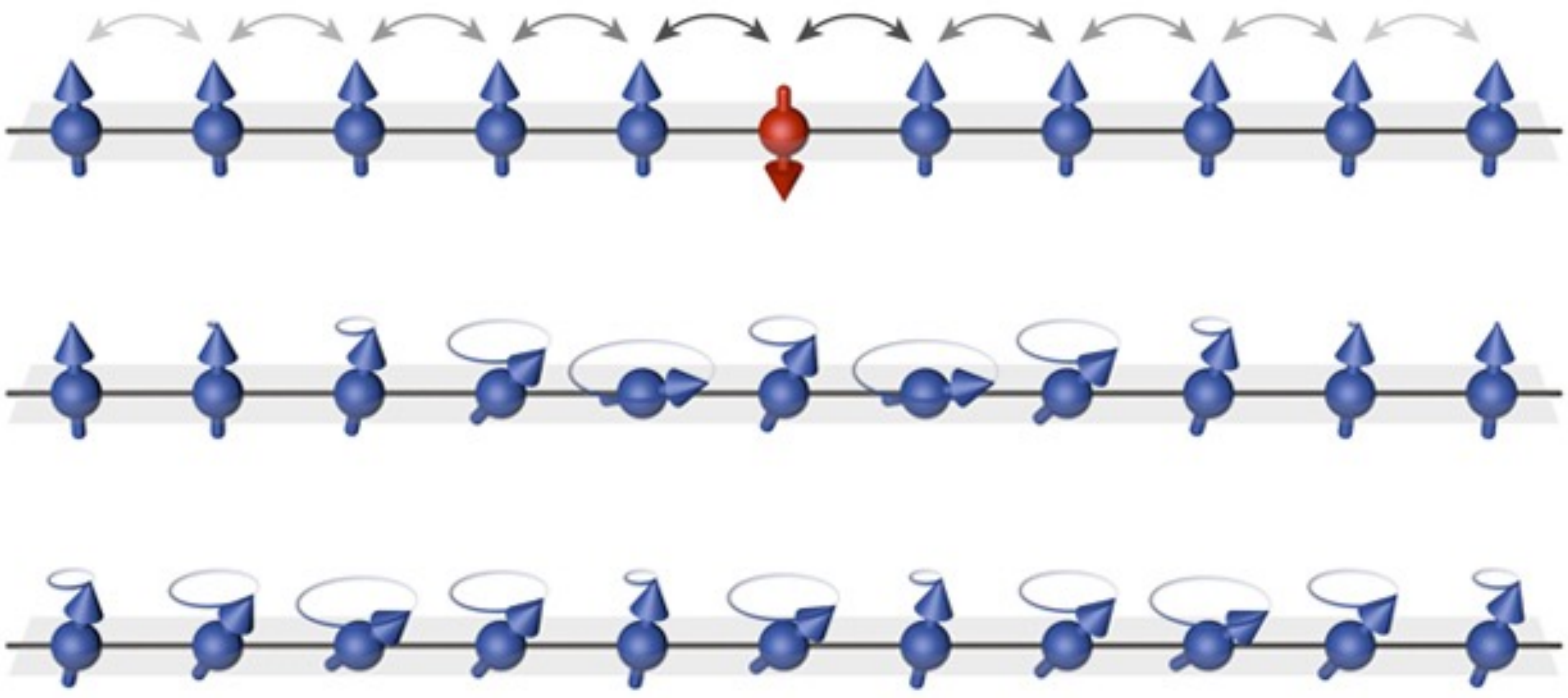
    - A plasmon is a **quantum of plasma oscillation (等离子体振荡量子)**.



➢ Quasi-particles (准粒子)

❖ Magnon (磁子):

- A magnon is a **quantum of spin wave** (自旋波量子).



➢ Quasi-particles (准粒子)

❖ Polariton (极化激元):

- In general, polaritons are quasiparticles resulting from strong coupling of electromagnetic waves (photons) with an **electric or magnetic dipole-carrying excitation**, such as:

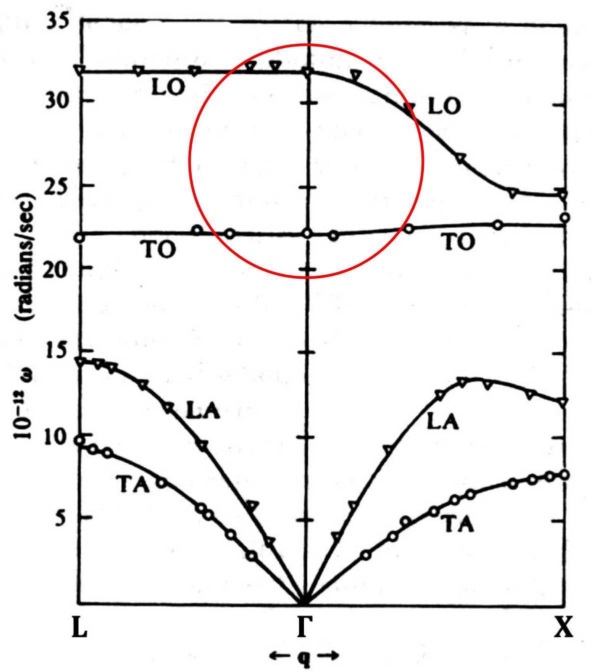
1) phonon-polariton (photon + optical phonon 声子极化激元)
2) exciton-polariton (photon + exciton 激子极化激元)
3) plasmon-polariton (photon + plasmon 等离极化激元)
4) magnon-polariton (photon + magnon 磁子极化激元)

Chapter 3.2: Phonons (声子)

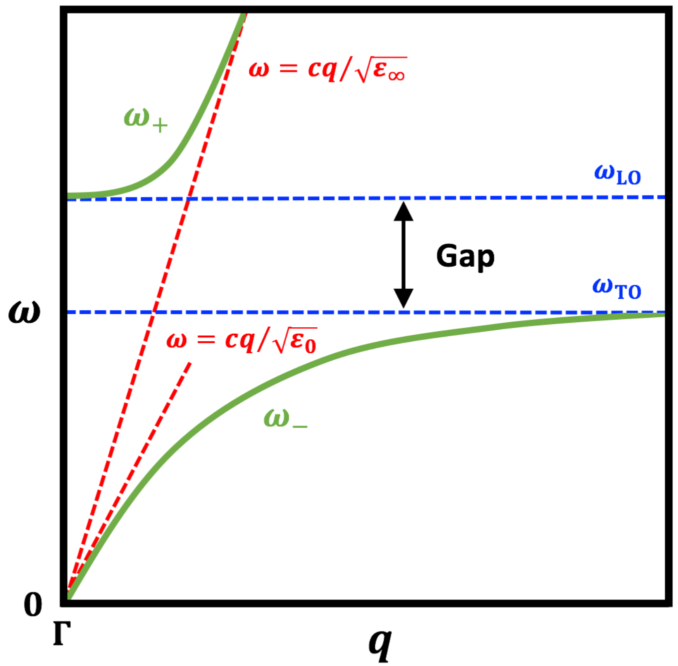
➢ Quasi-particles (准粒子)

❖ Phonon-Polariton (声子极化激元):

- Phonon-polaritons result from strong coupling of **infrared electromagnetic waves (红外电磁波)** with **optical phonons in ionic crystals (离子晶体的光学声子)**.



Phonon Spectrum of NaCl Crystal



Dispersion Relation of Phonon-Polariton

➢ Quasi-particles (准粒子)

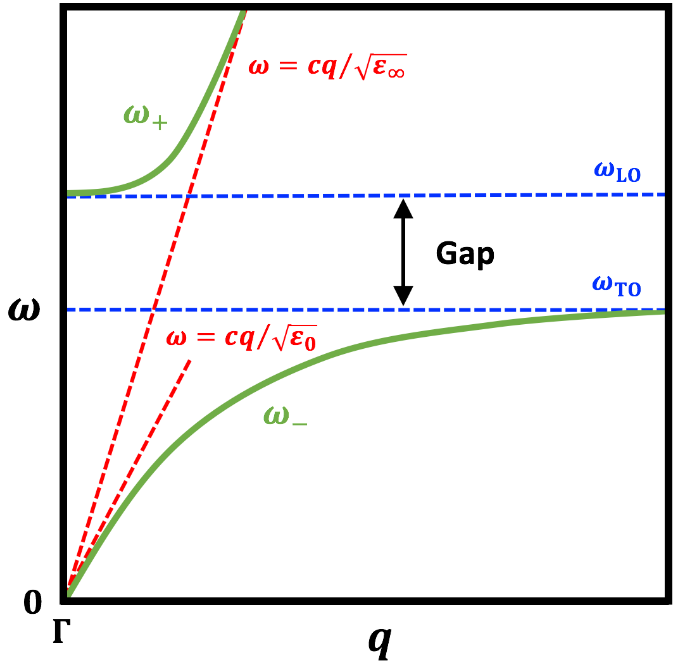
❖ Phonon-Polariton (声子极化激元):

- Phonon-polaritons result from strong coupling of **infrared electromagnetic waves (红外电磁波)** with **optical phonons in ionic crystals (离子晶体的光学声子)**.

Lyddane-Sachs-Teller (LST) relation:

$$\frac{\omega_{\mathrm{LO}}^2}{\omega_{\mathrm{TO}}^2} = \frac{\varepsilon_0}{\varepsilon_\infty}$$

Electromagnetic waves with $\omega_{\mathrm{TO}} < \omega < \omega_{\mathrm{LO}}$ cannot travel in the ionic crystals!



Dispersion Relation of Phonon-Polariton

Chapter 3.2: Phonons (声子)

➢ **Quasi-particles (准粒子)**

❖ **Phonon-Polariton (声子极化激元):**

黄昆
(1919-2005)
著名物理学家
中国固体物理和半导体物理奠基人之一
"声子极化激元"概念的提出者 (1951年)

年轻时的黄昆

与夫人李爱扶 (Avril Rhys)

合作导师Max Born

M. Born and **K. Huang**, *Dynamical Theory of Crystal Lattices* (Oxford, 1954).

Summary (总结)

➢ Summary (总结)

❖ **Normal Coordinates**

❖ **Phonon:**

A quantum of lattice vibrations.

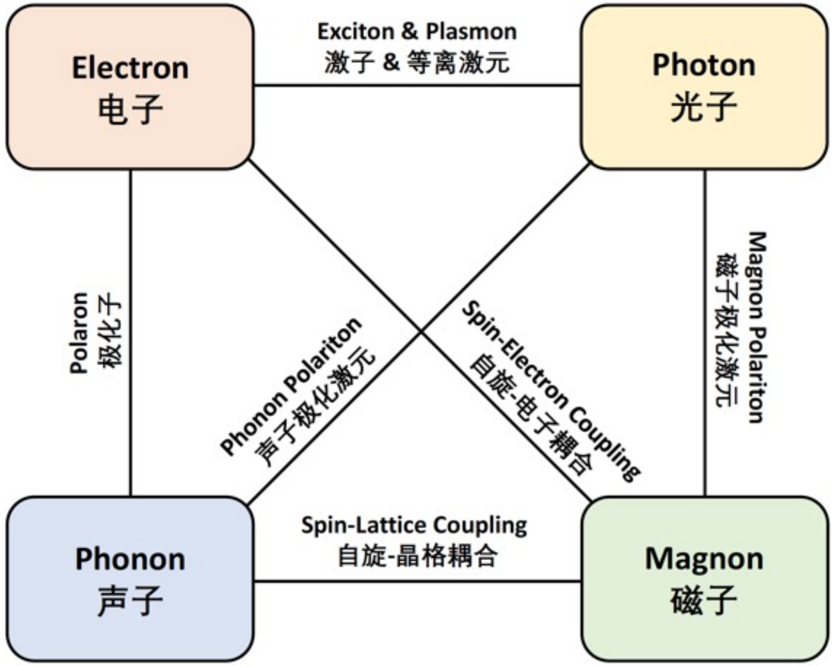
❖ **Quasi-particles:**

1) Electron/hole quasiparticles

2) Polaron

3) Exciton 4) Plasmon

5) Magnon 6) Polariton



Chapter 3.2: 课后作业

考虑一维量子谐振子 $\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2$,

令 $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$ 和 $\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$

证明:

1) $[\hat{a}, \hat{a}^+] = 1$

2) $[\hat{a}^+\hat{a}, \hat{a}^+] = \hat{a}^+$

3) $[\hat{a}^+\hat{a}, \hat{a}] = -\hat{a}$

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

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