Band Theory and Electronic Properties of Solids

Phys 674

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Lecture No. 05

Electron Levels in a Periodic Potential (Ashcroft Chapter 08)

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Introduction

- ✓ Introduction
- ✓ The Periodic Potential
- ✓ Bloch’s Theorem
- ✓ Proof of Bloch’s Theorem
- ✓ The Born - von Karman Boundary Conditions
- ✓ General Remarks about Bloch’s Theorem
- ✓ Density of Levels (states)
- ✓ SECOND PROOF OF BLOCH’s THEOREM

Drude model: no Potential at al

Sommerfeld model: free electron $U = 0$

Now: The reality is that we have to Consider the ionic Potential.

$\therefore \quad H\psi = E\psi$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi \longrightarrow \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right]\psi$$

Why periodic Potential is Important?

1. Bragg reflections are due to this Pot.
2. Band structure of solids is due to this Pot.
3. Band Gap " " " " "
4. Insulator & semiconductors cannot be explained without periodic Pot.
5. We need to correct problems of Sommerfeld that considers electron with fixed mass.

P. P. $\Rightarrow m_e$ is effective (not constant)

Electron Levels in a Periodic Potential

Introduction

- Ions in a perfect crystal are arranged in a regular periodic array. Hence:

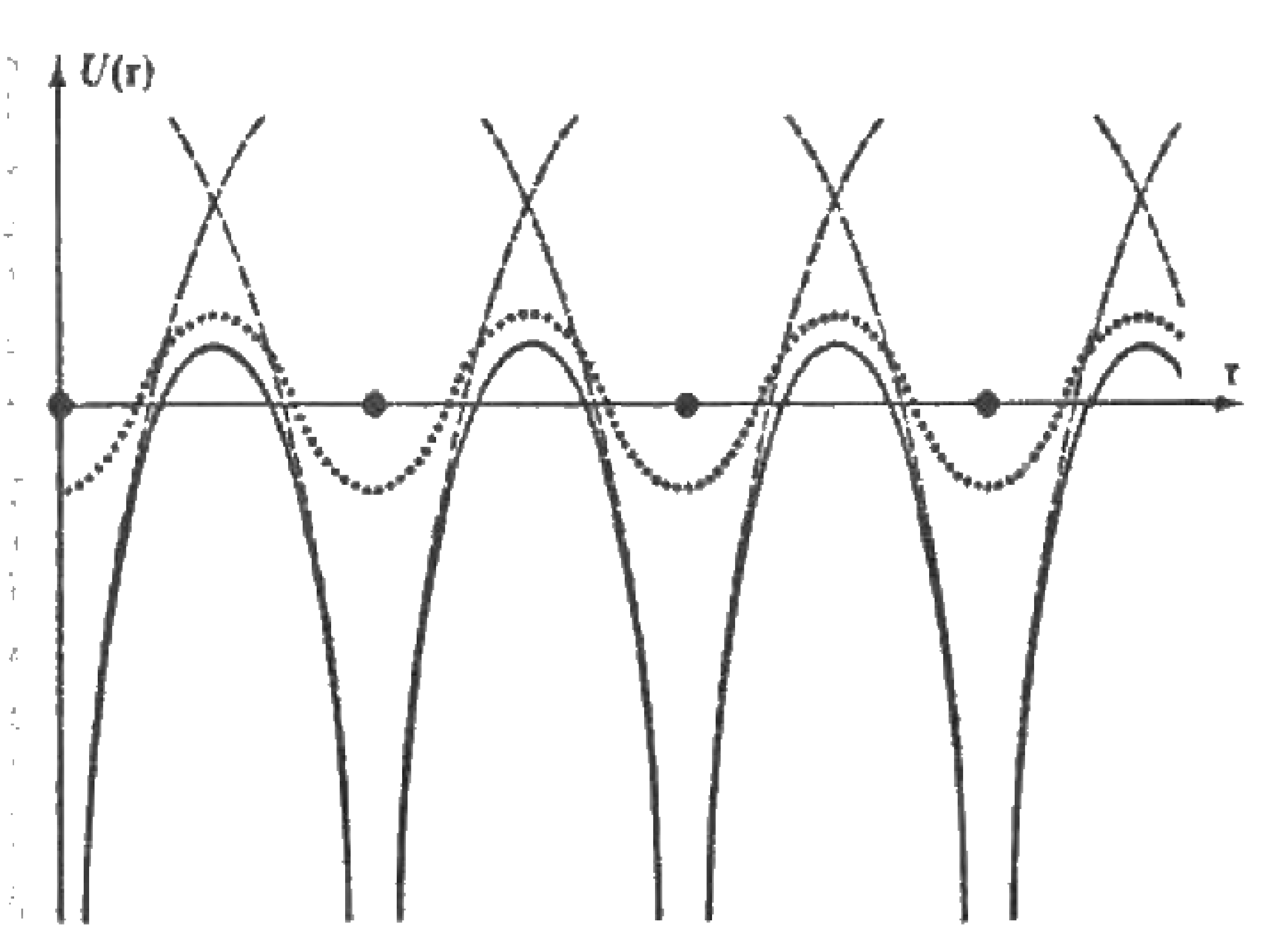
$$U(\mathbf{r}+\mathbf{R}) = U(\mathbf{r}) \qquad (8.1)$$

- Since the scale of periodicity of the potential *U* is the size of a typical de Broglie wavelength of an electron in the Sommerfeld free electron model, it is essential to use quantum mechanics in accounting for the effect of periodicity on electronic motion
- The solution to the problem must add this potential to the Shrodinger Equaittion:

$$H\psi = \left[-\frac{\hbar^2\nabla^2}{2m} + U(\boldsymbol{r})\right]\psi = \varepsilon\,\psi \qquad (8.2)$$

THE PERIODIC POTENTIAL

- If a crystal follows the equation (8.1) then potential is periodic



A typical crystalline periodic potential, plotted along a line of ions and along a line midway between a plane of ions. (Closed circles are the equilibrium ion sites; the solid curves give the potential along the line of ions; the dotted curves give the potential along a line between planes of ions; the dashed curves give the potential or single isolated ions.)

Electron Levels in a Periodic Potential

BLOCH'S THEOREM

- Bloch's theorem is a **foundational principle in solid-state physics**, named after the Swiss physicist ***Felix Bloch***, who formulated the theorem in 1928.
- The theorem addresses the behavior of electrons in a periodic potential, which is a typical scenario in crystalline solids.
- Bloch's theorem has profound implications for understanding the electronic properties of materials and forms the basis for the band theory of solids.

- **Felix Bloch (1905–1983):** Bloch introduced his theorem in his doctoral thesis while working under ***Werner Heisenberg***. His work was essential in the development of quantum mechanics and its application to condensed matter physics.
- **Quantum Mechanics Revolution:** Bloch's theorem was formulated during the early years of quantum mechanics, a period of significant advancement in understanding atomic and subatomic phenomena. It applied the principles of quantum mechanics to the periodic potential experienced by electrons in a crystal lattice.

Electron Levels in a Periodic Potential
BLOCH'S THEOREM

Main Points of Bloch's Theorem

1.Periodic Potential: Bloch's theorem applies to particles (typically electrons) moving in a periodic potential, such as that found in the crystal lattice of a solid. The periodicity of the potential is a direct consequence of the regular, repeating arrangement of atoms in a crystal.

2.Wave Function Formulation: The theorem states that the ***wave functions*** (ψ) of electrons in a periodic potential can be expressed as a product of two terms: a **plane wave** exp(i**k**·**r**) and a **function** u(**r**) that has the same periodicity as the crystal lattice. Mathematically, this is represented as:

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

- Here, **k** is the wave vector associated with the electron, **r** is the position vector, and $\mathbf{u}_k(\mathbf{r})$ is a function that is periodic with the lattice.

Electron Levels in a Periodic Potential

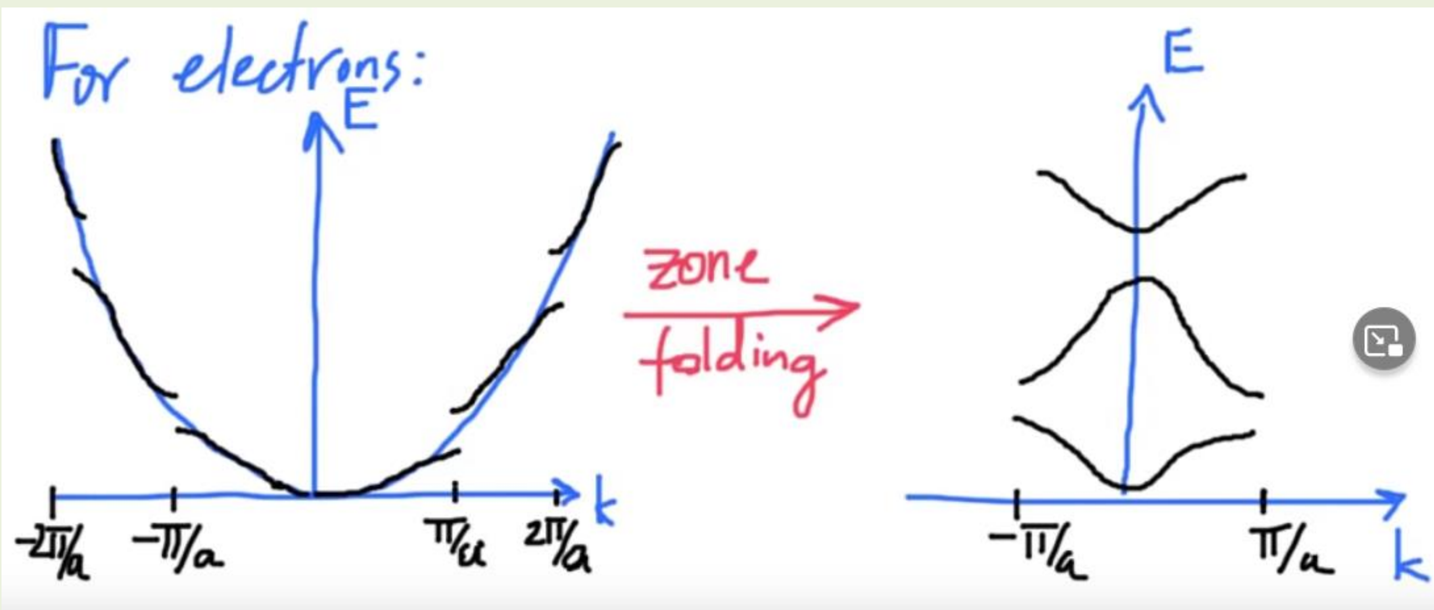
BLOCH'S THEOREM

- **Implications for Electron Dynamics**: This formulation implies that electrons in a crystal do not behave as if they are free but are instead influenced by the periodic potential in a way that can be precisely described. The presence of the periodic potential leads to the formation of energy bands and band gaps, which are critical for understanding the electrical, thermal, and optical properties of materials.
- **Energy Bands and Band Gaps**: Bloch's theorem underpins the band theory of solids, explaining why electrons in a solid have discrete energy levels (bands) and why there are forbidden energy ranges (band gaps) where no electron states can exist. This explains the distinction between conductors, semiconductors, and insulators based on their electronic band structures.
- **Brillouin Zones**: The theorem also leads to the concept of Brillouin zones in the reciprocal lattice, which are key to understanding electron dynamics, including the behavior of electrons under external fields, and phenomena such as electron diffraction and the formation of Fermi surfaces in metals.

- Blue line when using no periodic potential V=0

$$V(r) \to 0 \Rightarrow \psi(r) = e^{ik\cdot r}; \quad E = \frac{\hbar^2 k^2}{2m}$$

- Black lines when it is turned on



Proof of BLOCH'S THEOREM

- Block Theorm is a consequence of the periodic potential that electrons encounter
- Why? Due to symettry of the system

Bloch's theorem: If $V(r)$ is periodic,

$$\psi_k(r) = e^{ik.r}\, u_k(r)$$

not necessarily periodic! But, $|\psi|^2$ has to be periodic

phase factor

periodic part of wave function

labels solutions (also a point in reciprocal space)

Electron Levels in a Periodic Potential

BLOCH'S THEOREM

❑The eigenstates ψ of the one-electron Hamiltonian

$$H = -\frac{\hbar^2 \nabla^2}{2m} + U(\boldsymbol{r}),$$

where $U(\boldsymbol{r}+\boldsymbol{R}) = U(\boldsymbol{r})$, for all $\boldsymbol{R}$ in a Bravais lattice, can be chosen to have the form of a plane wave times a function with the periodicity of the Bravais lattice :

$$\psi_{nk}(\mathbf{r}) = u_{nk}(\mathbf{r})\,\mathrm{e}^{i\mathbf{k.r}} \qquad (8.2)$$

wehre:

$$u_{nk}(\mathbf{r}+\mathbf{R}) = u_{nk}(\mathbf{r}) \qquad (8.3)$$

$$\rightarrow$$

$$\psi_{nk}(\mathbf{r}+\mathbf{R}) = \psi_{nk}(\mathbf{r})\,\mathrm{e}^{i\mathbf{k.R}} \qquad (8.4)$$

or simply:

$$\psi(\mathbf{r}+\mathbf{R}) = \psi(\mathbf{r})\,\mathrm{e}^{i\mathbf{k.R}} \qquad (8.5)$$

❑ Either (8.2) or (8.5) can be used to express *Bloch's theorem*

Bloch's Theorem can be derived in different ways

We need to show that:

$$\psi(r) = e^{i\bar{k}\cdot\bar{r}} u_k(r) \quad \text{---} \quad (1)$$

where $u_k(r) = u_k(\bar{r}+\bar{R})$ --- (2)

$\bar{R}$ is a translation vector in k-space

∵ the potential is periodic:

$$\Rightarrow \quad V(\bar{r}+\bar{R}) = V(\bar{r}) \quad \text{---} \quad (3)$$

Consider: T_R : Translation operator.

$$\Rightarrow \quad T_R\,\psi(r) = \psi(\bar{r}+\bar{R}) \quad \text{---} \quad (4)$$

$$\because \quad [H, T_R] = 0 \quad \text{------} \quad (5)$$

H commutes with T_R due to the fact that V is periodic

⑤ $\Rightarrow$ Eigenfunctions of H can be also used with T_R.

$\therefore$ $T_R \psi(r) = C_R \psi(\bar{r})$ --- ⑥

↳ phase factor

$\therefore$ applying two successive T_R:

$T_{R_1} T_{R_2} \psi(r) = C_{R_1} C_{R_2} \psi(\bar{r})$ -- ⑦

since Bravais lattice is: "Abelian Group"

Because the operation are commutative.

$\therefore (7) \Rightarrow \quad C_{R_1+R_2} = C_{R_1} C_{R_2}$ ------ (8)

the only solution is:

$$C_R = e^{i\bar{k}\cdot\bar{R}} \quad \text{------ (9)}$$

(4), (6) and (9) $\Rightarrow$

$$\psi(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot\bar{R}} \psi(\bar{r}) \quad \text{--- (10)}$$

let $u_k(\bar{r}) = e^{-i\bar{k}\cdot\bar{r}} \psi(\bar{r})$ ---- (11)

$(10) \times e^{-i\bar{k}\cdot(\bar{r}+\bar{R})}$

$$\Rightarrow e^{-i\bar{k}\cdot(\bar{r}+\bar{R})} \psi(\bar{r}+\bar{R}) = e^{-i\bar{k}\cdot(\bar{r}+\cancel{\bar{R}})} \cancel{e^{i\bar{k}\cdot\bar{R}}} \psi(\bar{r}) \quad \text{- (12)}$$

$$(11) \Rightarrow \underbrace{e^{-i\bar{k}(\bar{r}+\bar{R})} \psi(\bar{r}+\bar{R})}_{u_k(\bar{r}+\bar{R})} = \underbrace{e^{-i\bar{k}\cdot\bar{r}} \psi(\bar{r})}_{u_k(\bar{r})} \quad (13)$$

$\therefore$ (7) $\Rightarrow \quad C_{R_1+R_2} = C_{R_1} C_{R_2}$ ------ (8)

the only solution is:

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(4), (6) and (9) $\Rightarrow$

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let $u_k(\bar{r}) = e^{-i\bar{k}\cdot\bar{r}}\,\psi(\bar{r})$ ---- (11)

(10) $\times\ e^{-i\bar{k}\cdot(\bar{r}+\bar{R})}$

$$\Rightarrow e^{-i\bar{k}\cdot(\bar{r}+\bar{R})}\,\psi(\bar{r}+\bar{R}) = e^{-i\bar{k}\cdot(\bar{r}+\cancel{\bar{R}})}\,\cancel{e^{i\bar{k}\cdot\bar{R}}}\,\psi(\bar{r}) \text{ - (12)}$$

(11) $\Rightarrow$

$$\underbrace{e^{-i\bar{k}(\bar{r}+\bar{R})}\,\psi(\bar{r}+\bar{R})}_{u_k(\bar{r}+\bar{R})} = \underbrace{e^{-i\bar{k}\cdot\bar{r}}\,\psi(\bar{r})}_{u_k(\bar{r})} \quad (13)$$

BLOCH'S THEOREM

$\therefore \; u_k(\bar{r}+\bar{R}) = u_k(\bar{r})$ --- (14)

$\therefore$ No matter what $\psi(\bar{r})$ we have [does not have to be periodic.]

$$\Rightarrow \quad \psi_k(\bar{r}) = e^{i\bar{k}\cdot\bar{r}} u_k(\bar{r}) \quad \#$$

$\psi_k(\bar{r})$ is Called: "modulated plane wave"

Proof of BLOCH'S THEOREM

- For each Bravais lattice vector **R**. we define a translation operator T_R which, when operating on any function f(**r**), shifts the argument by **R**:

$$T_{\mathbf{R}} f(\mathbf{r}) = f(\mathbf{r}+\mathbf{R}) \qquad (8.6)$$

Since the Hamiltonian is periodic,we have

$$T_{\mathbf{R}} H\psi = H(\mathbf{r}+\mathbf{R})\psi(\mathbf{r}+\mathbf{R}) = H(\mathbf{r})\psi(\mathbf{r}+\mathbf{R}) = HT_{\mathbf{R}}\psi \qquad (8.7)$$

$$\therefore T_{\mathbf{R}} H = HT_{\mathbf{R}} \qquad (8.8)$$

In addition, the result of applying two successive translations does not depend on the order in which they are applied, since for any $\mathrm{T}\psi(\mathrm{r})$:

$$T_{\mathbf{R}} T_{\mathbf{R}'}\psi = T_{\mathbf{R}'} T_{\mathbf{R}}\psi = \psi(\mathbf{r}+\mathbf{R}+\mathbf{R}') \qquad (8.9)$$

Therefore

$$T_{\mathbf{R}} T_{\mathbf{R}'} = T_{\mathbf{R}'} T_{\mathbf{R}} = T_{\mathbf{R}+\mathbf{R}'} \qquad (8.10)$$

Proof of BLOCH'S THEOREM

- Equations (8.8) and (8.10) assert that the T_R for all Bravais lattice vectors **R** and the Hamiltonian H form a set of commuting operators. It follows from a fundamental theorem of quantum mechanics that the eigenstates of H can therefore be chosen to be simultaneous eigenstates of all the T_R :

$$H\psi = \varepsilon\psi \tag{8.11}$$

$$T_{\mathbf{R}}\psi = c(\mathbf{R})\psi \tag{8.12}$$

- The eigenvalues c(**R**) of the translation operator are related because of the condition (8.10), for on the one hand:

$$T_{\mathbf{R}}T_{\mathbf{R}'}\psi = c(\mathbf{R})T_{\mathbf{R}'}\psi = c(\mathbf{R})c(\mathbf{R}')\psi \tag{8.13}$$

$$(8.10) \rightarrow$$

$$T_{\mathbf{R}}T_{\mathbf{R}'}\psi = c(\mathbf{R}+\mathbf{R}')\psi \tag{8.14}$$

$\therefore$ eigenvalues must atisfy:

$$c(\mathbf{R}+\mathbf{R}') = c(\mathbf{R})c(\mathbf{R}') \tag{8.15}$$

Proof of BLOCH'S THEOREM

- Now let $\boldsymbol{a}_i$, be three primitive vectors for the Bravais lattice. We can always write the c($\boldsymbol{a}_i$) in the form:

$$c(\mathbf{a}_i) = e^{2\pi i x_i} \qquad (8.16)$$

- It then follows by successive applications of (8.15) that **R** is a general Bravais lattice vector given by:

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \qquad (8.17)$$

$$\rightarrow$$

$$\mathrm{c(R)} = c(\mathbf{a}_1)^{n_1} + c(\mathbf{a}_2)^{n_2} + c(\mathbf{a}_3)^{n_3} \qquad (8.18)$$

$$\rightarrow$$

$$c(\mathbf{R}) = e^{i\mathbf{k.R}} \qquad (8.19)$$

with :

$$\mathbf{k} = x_1\mathbf{b}_1 + x_2\mathbf{b}_2 + x_3\mathbf{b}_3 \qquad (8.20)$$

- where orthogonally condition was applied: $\boldsymbol{b}_i.\boldsymbol{a}_i = 2\pi\delta_{ij}$

Electron Levels in a Periodic Potential

Proof of BLOCH'S THEOREM

- Summarizing, we have shown that we can choose the eigenstates ψ of *H* so that for every Bravais lattice vector **R:**

$$T_{\mathbf{R}}\psi = \psi(\mathbf{r}+\mathbf{R}) = c(\mathbf{R})\psi = e^{i\mathbf{k}.\mathbf{R}}\psi(\mathbf{r}) \qquad (8.21)$$

- This is precisely ***Bloch's theorem***, in the form (8.5)
- Hence, we have proven the Bloch's theorem using the translation vector property of the Bravais lattice in its reciprocal form

THE BORN - VON KARMAN BOUNDARY CONDITION

- By imposing an appropriate boundary condition on the wave functions we can demonstrate that the wavevector **k** must be real, and arrive at a condition restricting the allowed values or **k**.
- The condition generally chosen is the natural generalization of the condition used in the Sommerfeld theory of free electrons in a cubical box.
- As in that case, we introduce the volume containing the electrons into the theory through a Born-von Karman boundary condition or macroscopic periodicity.
- We will not use a cubic box now, instead we deal directly with the primitive cell of the underlying Bravais lattice.

this boundary condition treats a finite crystal as if it were infinite by assuming that the crystal repeats itself periodically in all directions

THE BORN - VON KARMAN BOUNDARY CONDITION

- We will generalize the periodic boundary condition (2.4) in lecture No. 2:

$$\psi(\mathbf{r}+N_i\mathbf{a}_i)=\psi(\mathbf{r}) \qquad (8.22)$$

- where the $\mathbf{a}_i$ are three primitive vectors and N_i are all integers of order $N^{1/3}$,where $N = N_1N_2N_3$ is the total number of primitive cells in the crystal.
- Applying Bloch's theorem to the boundary condition (8.22):

$$\psi_{nk}(\mathbf{r}+N_i\mathbf{a}_i)=\psi_{nk}(\mathbf{r})\,\mathrm{e}^{iN_i\mathbf{k}.\mathbf{a}_i} \qquad (8.23)$$

With :

$$\mathrm{e}^{iN_i\mathbf{k}.\mathbf{a}_i}=1 \qquad (8.24)$$

and

$$\mathrm{e}^{2\pi iN_i x_i}=1 \qquad (8.25)$$

$$\Rightarrow x_i=\frac{m_i}{N_i} \qquad m_i=\text{integer} \qquad (8.26)$$

THE BORN - VON KARMAN BOUNDARY CONDITION

- Therefore the general form for allowed Bloch wave vectors is:

$$\mathbf{k} = \sum_{i=1}^{3} \frac{m_i}{N_i} \mathbf{b}_i \qquad (8.27)$$

- It follows that the volume $\Delta\mathbf{k}$ of k-space per allowed value of $\mathbf{k}$ is just the volume of the little parallelepiped with edges $\boldsymbol{b}_i/N_i$:

$$\Delta\mathbf{k} = \frac{\mathbf{b}_1}{N_1} \cdot \left(\frac{\mathbf{b}_2}{N_2} \times \frac{\mathbf{b}_3}{N_3} \right) = \frac{1}{N} \mathbf{b}_1 \cdot \left(\mathbf{b}_2 \times \mathbf{b}_3 \right) \qquad (8.28)$$

- since $\boldsymbol{b}_1 . (\boldsymbol{b}_2 \times \boldsymbol{b}_3)$ is the volume of primitive cell, Eq. (8.28) says that *the number of allowed wavevector in a primitive cell of the reciprocal lattice is equal to the number of sites in the crystal.*
- *Since volume of primitive cell is:* $(2\pi)^3 N/V$ we have: (in agreement with (2.10) in lecture 2 for free electron gas)

$$\Delta\mathbf{k} = \frac{(2\pi)^3}{V} \qquad (8.29)$$

GENERAL REMARKS ABOUT BLOCH'S THEOREM

1-

- Bloch' theorem introduces a wave vector **k**, which turns, out to play the same role in the periodic potential that the Free electron wave vector **k** plays in the Sommerfeld theory.
- Note, however that although *the free electron wave vector* is simply **p**/ħ**,** where **p** is the momentum of the electron. In the Bloch case **k** is not proportional to the electronic momentum.
- This is clear on general grounds, since the Hamiltonian does not have complete translational invariance in the presence of a non-constant potential.
- Therefore its eigenstate will not be simultaneous eigenstates of the momentum operator.
- This conclusion is confirmed by the fact that the momentum operator **p** = (ħ/i)∇**,** when acting on ψ will not give a momentum eigenstate.

GENERAL REMARKS ABOUT BLOCH'S THEOREM

- To show that the momentum operator **p,** when acting on ψ will not give a momentum eigenstate.

$$\frac{\hbar}{i}\nabla\psi_{n\mathbf{k}} = \frac{\hbar}{i}\left(\nabla u_{n\mathbf{k}}(\mathbf{r})\,\mathrm{e}^{i\mathbf{k}.\mathbf{r}}\right)$$

$$= \hbar\mathbf{k}\,\psi_{n\mathbf{k}} + \mathrm{e}^{i\mathbf{k}.\mathbf{r}}\frac{\hbar}{i}\nabla u_{n\mathbf{k}}(\mathbf{r}) \qquad (8.30)$$

- Hence, ψ_{nk} is not a momentum eigenstate.

2- The wave vector **k** appearing in Bloch's theorem can always be confined to the first Brillouin zone (or to any other conventional primitive cell of the reciprocal lattice. It is because any **k**' not in the FBZ can be written as:

$$\mathbf{k}' = \mathbf{k} + \mathbf{K} \qquad (8.31)$$

- **K** is also a reciprocal lattice vector and **k** is in the FBZ.
- Since $e^{iK.R} = 1$ for any **K**, then if (8.5) holds for **k'**, it will hold for **k**

GENERAL REMARKS ABOUT BLOCH'S THEOREM

3-

- The index ,n appears in Bloch's theorem because for given **k** there are many solutions to the Schrödinger equation.
- Let us look for all solutions to the Schrodinger equation that have the Bloch form:

$$\psi_{nk}(\mathbf{r}) = u_{nk}(\mathbf{r})\,\mathrm{e}^{i\mathbf{k.r}} \qquad (8.32)$$

- where **k** is fixed and *u* has the periodicity of the Bravais lattice.
- Substituting this into the Schrodinger equation, we find that *u* is determined by the eigenvalue problem.

$$H_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{r}) = \left[\frac{\hbar^2}{2m}\left(\frac{1}{i}\nabla + \mathbf{k}\right) + U(\mathbf{r})\right]u_{\mathbf{k}}(\mathbf{r}) = \varepsilon_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{r}) \qquad (8.33)$$

with:

$$u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) \qquad (8.34)$$

GENERAL REMARKS ABOUT BLOCH'S THEOREM

- Because of the periodic boundary condition we can regard (8.33) as a Hermitian eigenvalue problem restricted to a ingle primitive cell of the crystal. Because the eigenvalue problem is set is fixed in a finite volume, we can find an infinite family of solutions with *discretely* spaced eigenvalue.

4-

- Although the full set or level can be described with **k** restricted to a single primitive cell, it is often useful to allow **k** to range through all of **k**-space.
- we can assign the indices n to the levels in such a way that *for given n, the eigenstates and eigenvalues are periodic functions of* **k** *in the reciprocal lattice:*

$$\left.\begin{aligned} \psi_{n,\mathbf{k}+\mathbf{K}}(\mathbf{r}) &= \psi_{n,\mathbf{k}}(\mathbf{r}) \\ \varepsilon_{n,\mathbf{k}+\mathbf{K}} &= \varepsilon_{n,\mathbf{k}} \end{aligned}\right\} \qquad (8.35)$$

GENERAL REMARKS ABOUT BLOCH'S THEOREM

5-

- It can be shown that ,an electron in a level specified by band index *n* and wave vector **k** has a non-vanishing mean velocity, given by:

$$\mathrm{v}_n(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k}) \qquad (3.36)$$

- It says that there are stationary levels for an electron in a periodic potential in which, in spite of the interaction of the electron with the fixed lattice of ions, it moves forever without any degradation of its mean velocity

Density of Levels (states)

- In this section we shall find out an expression of general form of density of states (levels):
- We want to find a general expression for *D(ω),* the number of states per unit frequency range. The number of allowed values of **K** for which the frequency is between ω and $\omega + d\omega$ is:

$$D(\omega)d\omega = \left(\frac{L}{2\pi}\right)^3 \int_{shell} d^3K \qquad (8.37)$$

- The real problem is to evaluate the volume of this shell. We let *dS.* Denote an element of area. The element of volume between the constant frequency surfaces wand ω + $d\omega$ is a right cylinder of base dS_ω and altitude $dK_\perp$ so that

$$\int_{shell} d^3K = \int dS_\omega dK_\perp \qquad (8.38)$$

Electron Levels in a Periodic Potential

Density of Levels (states)

- The gradient of ω, which is ∇K_{ω}, is also normal to the surface ω constant, and the quantity

$$|\nabla_k \omega| dk_{\perp} = d\omega$$

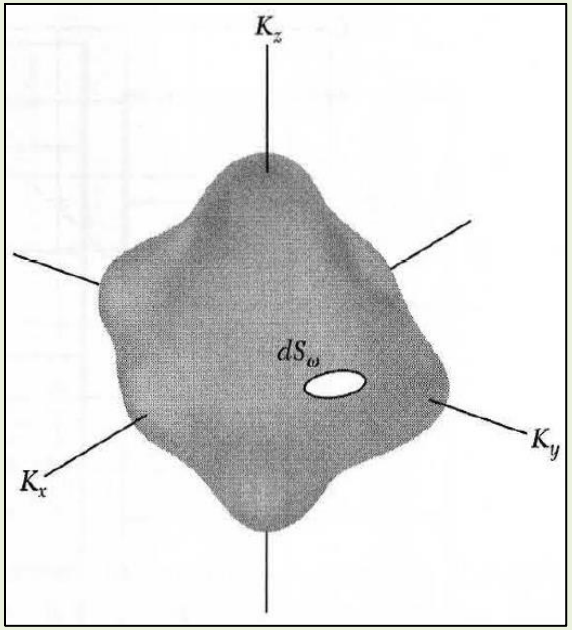
is the difference in frequency between the two surfaces connected by $dK_{\perp}$. Thus the element of the volume is

$$dS_{\omega} dK_{\perp} = dS_{\omega} \frac{d\omega}{|\nabla_k \omega|} = dS_{\omega} \frac{d\omega}{v_g} \qquad (3.39)$$

$$\because D(\omega) d\omega = \left(\frac{L}{2\pi}\right)^3 \int_{shell} d^3K \qquad (3.40)$$

with

$$\int_{shell} d^3K = \int dS_{\omega} dK_{\perp} \qquad (3.41)$$



Density of Levels (states)

- We divide both sides by $d\omega$ and write V = L[3] for the volume of the crystal: the result for the density of states is:

$$D(\omega)d\omega = \left(\frac{L}{2\pi}\right)^3 \int dS_\omega \frac{d\omega}{v_g} \qquad (8.42)$$

$$D(\omega) = \frac{V^3}{(2\pi)^3} \int \frac{dS_\omega}{v_g} \qquad (8.43)$$

$$\because v_g = |\nabla_k \omega|$$

$$\therefore D(\omega) = \frac{V^3}{(2\pi)^3} \int \frac{dS_\omega}{|\nabla_k \omega|} \qquad (8.44)$$

SECOND PROOF OF BLOCH's THEOREM

- We can alway expand any function obeying the Born- von Kaiman boundary condition (8.22).
- Therefore we have wave vectors of the form (8.27):

$$\psi(\mathbf{r}) = \sum_{\mathbf{q}} c_{\mathbf{q}} e^{i\mathbf{q}.\mathbf{r}} \qquad (8.45)$$

- Because U(**r**) is periodic in the lattice, its plane wave expansion will only contain plane waves with the periodicity of the lattice and hence with wave vectors that are of the reciprocal lattice.

$$U(\mathbf{r}) = \sum_{\mathbf{K}} U_{\mathbf{K}}\, e^{i\mathbf{K}.\mathbf{r}} \qquad (8.46)$$

With :

$$U_{\mathbf{K}} = \frac{1}{v}\int_{cell} d\mathbf{r}\, U(r)\, e^{-i\mathbf{K}.\mathbf{r}} \qquad (8.47)$$

- Where $U_{\mathbf{K}}$ is the Fourier coefficients

SECOND PROOF OF BLOCH's THEOREM

- Since $U(\mathbf{r})$ is real, then:

$$U_{-\mathbf{K}} = U_{\mathbf{K}}^{*} \tag{8.48}$$

- If we assume that the crystal has inversion symmetry so that, for a suitable choice of origin $U(\mathbf{r}) = U(-\mathbf{r})$ then (8.46) implies that U_K is real and thus:

$$U_{-\mathbf{K}} = U_{\mathbf{K}} = U_{\mathbf{K}}^{*} \tag{8.49}$$

$$\because H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right)\psi = \varepsilon\psi \tag{8.50}$$

(3.45) in (3.50) for kinetic energy term:

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \frac{\hbar^2}{2m}\sum_{\mathbf{q}} \mathrm{q}^2 \mathrm{c}_{\mathbf{q}} \mathrm{e}^{i\mathbf{q}.\mathbf{r}} \tag{8.51}$$

SECOND PROOF OF BLOCH's THEOREM

- For the potential energy term (8.45) & (8.46) in (8.50):

$$U(\mathbf{r})\psi = \left(\sum_{\mathbf{K}} U_{\mathbf{K}}\, e^{i\mathbf{K}.\mathbf{r}}\right)\left(\sum_{\mathbf{q}} c_{\mathbf{q}} e^{i\mathbf{q}.\mathbf{r}}\right) = \sum_{\mathbf{K},\mathbf{q}} U_{\mathbf{K}}\, c_{\mathbf{q}} e^{i(\mathbf{K}+\mathbf{q}).\mathbf{r}}$$

$$\text{let } \mathbf{q}'=\mathbf{K}+\mathbf{q}$$

$$\therefore U(\mathbf{r})\psi = \sum_{\mathbf{K},\mathbf{q}'} U_{\mathbf{K}}\, c_{\mathbf{q}'-\mathbf{K}} e^{i\mathbf{q}'.\mathbf{r}} \qquad (8.52)$$

- Now, (8.51) & (8.52) back in (8.50):

$$\left[\frac{\hbar^2}{2m}\sum_{\mathbf{q}} q^2 c_{\mathbf{q}} e^{i\mathbf{q}.\mathbf{r}} + \sum_{\mathbf{K},\mathbf{q}'} U_{\mathbf{K}}\, c_{\mathbf{q}'-\mathbf{K}} e^{i\mathbf{q}'.\mathbf{r}}\right]\psi = \varepsilon\psi = \varepsilon \sum_{\mathbf{q}} c_{\mathbf{q}} e^{i\mathbf{q}.\mathbf{r}} \qquad (8.53)$$

$$\therefore \sum_{\mathbf{q}} \left[\left(\frac{\hbar^2}{2m} q^2 - \varepsilon\right) c_{\mathbf{q}} + \sum_{\mathbf{K}'} U_{\mathbf{K}'}\, c_{\mathbf{q}-\mathbf{K}'}\right] e^{i\mathbf{q}.\mathbf{r}} = 0 \qquad (8.54)$$

- Since the plane waves satisfying the BVK boundary condition are an orthogonal set, the coefficient of each term in (8.54) must vanish, and therefore for all allowed wave vectors **q**

SECOND PROOF OF BLOCH's THEOREM

❑Hence, we have

$$\left(\frac{\hbar^2}{2m}\mathrm{q}^2-\varepsilon\right)\mathrm{c}_{\mathbf{q}}+\sum_{\mathbf{K}'}U_{\mathbf{K}'}\,\mathrm{c}_{\mathbf{q}-\mathbf{K}'}=0 \qquad (8.55)$$

❑Let: **q = k – K** where **K** is selected such that **k** lies in the FBZ

$\therefore (8.55) \Rightarrow$

$$\left(\frac{\hbar^2}{2m}(\mathbf{k}-\mathbf{K})^2-\varepsilon\right)\mathrm{c}_{\mathbf{k}-\mathbf{K}}+\sum_{\mathbf{K}'}U_{\mathbf{K}'}\,\mathrm{c}_{\mathbf{k}-\mathbf{K}-\mathbf{K}'}=0 \qquad (8.56)$$

then back to: $\mathbf{K}'\rightarrow\mathbf{K}'\text{-}\mathbf{K}$

$$\left(\frac{\hbar^2}{2m}(\mathbf{k}-\mathbf{K})^2-\varepsilon\right)\mathrm{c}_{\mathbf{k}-\mathbf{K}}+\sum_{\mathbf{K}'}U_{\mathbf{K}'-\mathbf{K}}\,\mathrm{c}_{\mathbf{k}-\mathbf{K}'}=0 \qquad (8.57)$$

❑This equation is same as Schrodinger equation but in momentum space. **K**'s in this equation are all reciprocal lattice vectors

SECOND PROOF OF BLOCH's THEOREM

- Now, back to Eq. (8.45):

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}} e^{i(\mathbf{k}-\mathbf{K}).\mathbf{r}} \qquad (8.57)$$

$$= e^{i\mathbf{k}.\mathbf{r}} \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}'} e^{-i\mathbf{K}.\mathbf{r}} \qquad (8.58)$$

this is same as Block theorm with:

$$u(r) = \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}'} e^{-i\mathbf{K}.\mathbf{r}} \qquad (8.59)$$

- Hence, we have used a different rout than before to prove same theorem.

Thanks