Band Theory and Electronic Properties of Solids

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Lecture No. 06

Electron Levels in a Periodic Potential Part 2
(Ashcroft Chapter 08)

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Electron Levels in a Periodic Potential

Introduction

- ✓ Introduction
- ✓ THE BORN - VON KARMAN BOUNDARY CONDITION
- ✓ Density of Levels (states)
- ✓ SECOND PROOF OF BLOCH's THEOREM

Electron Levels in a Periodic Potential

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:

$$\left.\begin{aligned}\psi(x+L,y,z)&=\psi x,y,z)\\ \psi(x,y+L,z)&=\psi x,y,z)\\ \psi x,y,z+L)&=\psi(x,y,z)\end{aligned}\right\} \qquad (2.4)$$

- The generalized periodic boundary becomes:

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

- 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.

THE BORN - VON KARMAN BOUNDARY CONDITION

❑Applying Bloch's theorem to the boundary condition (8.22):

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

With :

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

and

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

$$N_i \mathrm{k.a_i}=2\pi m_i$$

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

How to get eq. (8.27)?

$$\therefore \bar{K}\cdot\bar{a}_i = \frac{2\pi m_i}{N_i} \quad \text{---} \quad (1)$$

$$\because \bar{b}_i\cdot\bar{a}_j = 2\pi\delta_{ij} \quad - \quad (2)$$

$$\therefore \bar{K} = x_1\bar{b}_1 + x_2\bar{b}_2 + x_3\bar{b}_3 \quad - \quad (3)$$

$$\therefore x_i = \frac{m_i}{N_i} \quad \text{---} \quad (4)$$

$$\therefore \bar{K} = \sum_{i=1}^{3} x_i b_i = \sum_{i=1}^{3} \frac{m_i}{N_i} b_i$$

$$\therefore \bar{K} = \sum_{i=1}^{3} \frac{m_i}{N_i}\bar{b}_i \quad \text{---} \quad (5)$$

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 $\boldsymbol{b}_i/N_i$:

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

- 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.

Comparing $\vec{k}$ in Free Electron model and $\vec{k}$ in Bloch's Theorem?

① in FEM: $H = \frac{p^2}{2m}$

$\Rightarrow \quad \vec{p} = \hbar \vec{k}$

$\Rightarrow \vec{k}$ α to electron's actual momentum

② in Bloch Th. $H = \frac{p^2}{2m} + V(\vec{r})$

with $V(\vec{r} + \vec{R}) = V(\vec{r})$

$\Rightarrow$ total momentum is not "conserved"

since we now have "crystal momentum"

$\Rightarrow \vec{p} \neq \hbar k$ But $\vec{p} = \hbar(\vec{k} + \vec{G})$

$\therefore \vec{p}$ is associated with wave function not the electron momentum.

GENERAL REMARKS ABOUT BLOCH'S THEOREM

$\Rightarrow$ $\vec{p}\psi \equiv \frac{\hbar}{i}\vec{\nabla}\psi$ will not give a momentum Eigenstates.

GENERAL REMARKS ABOUT BLOCH'S THEOREM

How to get (8.30) ?

Question: Prove that $\vec{p}$ does not have momentum eigenstates:

$$\because \psi_{nk}(\bar{r}) = e^{i\bar{k}\cdot\bar{r}} u_{nk}(\bar{r}) \quad \text{---} (1)$$

we need to workout: $\frac{\hbar}{i}\bar{\nabla}\psi_{nk}(\bar{r})$ -- (2)

$$\therefore \bar{\nabla}\psi_{nk}(\bar{r}) = \bar{\nabla}\left(e^{i\bar{k}\cdot\bar{r}} u_{nk}(\bar{r})\right)$$

$$= e^{i\bar{k}\cdot\bar{r}} \bar{\nabla} u_{nk}(\bar{r}) + u_{nk}(\bar{r}) \bar{\nabla} e^{i\bar{k}\cdot\bar{r}} \quad (3)$$

$$= e^{i\bar{k}\cdot\bar{r}} \bar{\nabla} u_{nk}(\bar{r}) + u_{nk}(\bar{r})(i\cdot\bar{k}) e^{(i\bar{k}\cdot\bar{r})} \quad (4)$$

$$= e^{i\bar{k}\cdot\bar{r}} \left[\bar{\nabla} u_{nk}(\bar{r}) + i\bar{k} u_{nk}(\bar{r}) \right] \quad (5)$$

$\times \frac{\hbar}{i}$: $\Rightarrow$

$$\frac{\hbar}{i} \bar{\nabla} \psi_{nk}(\bar{r}) = e^{i\bar{k}\cdot\bar{r}} \frac{\hbar}{i} \nabla u_{nk}(\bar{r}) + \frac{\hbar}{i} \cdot i\bar{k}\, e^{i\bar{k}\cdot\bar{r}} u_{nk}(\bar{r}) \quad --- (6)$$

$$\Rightarrow \frac{\hbar}{i}\bar{\nabla}\psi_{nk}(\bar{r}) = e^{i\bar{k}\cdot\bar{r}}\frac{\hbar}{i}\bar{\nabla}u_{nk}(\bar{r}) + \hbar k\, \underbrace{e^{i\bar{k}\cdot\bar{r}}u_{nk}(\bar{r})}_{\psi_{nk}(\bar{r})}$$

$$\therefore = \hbar\bar{k}\psi_{nk}(\bar{r}) + e^{i\bar{k}\cdot\bar{r}}\frac{\hbar}{i}\bar{\nabla}u_{nk}(\bar{r}) \quad (7)$$

(1) (2)

(1) $\propto k \equiv$ crystal momentum

(2) has $\bar{\nabla}u_{nk}(\bar{r})$ accounting for the periodic part of the wavefunction.

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.

GENERAL REMARKS ABOUT BLOCH'S THEOREM

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**

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

First Brillouin Zone (FBZ): The FBZ is the smallest region in reciprocal space that contains all unique wave vectors **k** necessary to describe the electronic states in a crystal. Any wave vector **k'** outside the FBZ can be mapped back into the FBZ by adding or subtracting a reciprocal lattice vector **K**. ➔ **reduced Brillouin Zone**

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:

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

- 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:

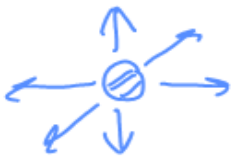
$$\mathrm{v}_n(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k}) \qquad (3.36)$$

- 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)

Density of states

We shall start from normal modes in crystals:



all directions

Vibrations of atoms are quantized

E for one oscillator: $(n+\frac{1}{2})\hbar\omega$

We need to find:

1. Energy of a normal mode
2. density of normal modes at a freq. ω.

In other words; we need to find Density of states $D(\omega)$

Now:

Consider the freq. Range $\omega \rightarrow \omega + d\omega$

$\therefore D(\omega)\,d\omega$ = No. of modes in the Range $\omega \rightarrow \omega + d\omega$

Similarly:

$D(k)$ = No. of states in the Range $k \rightarrow k + dk$

Density of Levels (states)

density of states $= \begin{cases} D(\omega) & \omega \text{ space} \\ D(k) & k \text{ space} \end{cases}$

No. of states in the range $\omega + d\omega = D(\omega)\,d\omega$

$=$ " " " " " " $k + dk = D(k)\,dk$

$\therefore D(\omega) = D(k)\,\frac{dk}{d\omega}$ - - - (1)

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

$\therefore D(\omega) = \frac{D(k)}{v_g}$ - - - - (2)

∴ we shall search for $D(k) = ?$

to do that; we relay on the

Periodicity of the crystal:

Electron Levels in a Periodic Potential

Density of Levels (states)

From chapter 5 in Kittel:

this is a 1-D chain of atoms

$\Rightarrow$ total length $l = Na$

$\therefore$ Boundary Conditions $\Rightarrow$

$$e^{ika} = e^{ika(N+1)} \quad \text{---} (3)$$

$$\Rightarrow e^{ikNa} = 1 \quad \text{---} (4)$$

$$\therefore kNa = 2n\pi \quad \text{---} (5) \qquad n = 0, \pm 1, \pm 2, \ldots$$

$$\therefore k = \frac{2n\pi}{Na} = \frac{2n\pi}{l} \quad \text{---} (6)$$

Electron Levels in a Periodic Potential

Density of Levels (states)

taking $n = 1 \Rightarrow k = \frac{2\pi}{a}$ $(N = 1)$

this defines length of FBZ

∴ We have 1 k value for the Range: $\frac{2\pi}{L}$

$\Rightarrow$ density $= \frac{1}{\frac{2\pi}{L}} = \left(\frac{L}{2\pi}\right)$ 1-D

$= \frac{L^3}{8\pi^3}$ 3-D (7)

$\equiv$ No. of k-values in this Range.

$\therefore D(k) = \left(\frac{L}{2\pi}\right)$ 1-D

$= \frac{L^3}{8\pi^3} = \frac{V}{8\pi^3}$ 3-D (8)

Density of Levels (states)

To check:

$$\int_{-\frac{\pi}{a}}^{\pi/a} D(k)\,dk = \frac{L}{2\pi}\cdot\int_{-\pi/a}^{+\pi/a} dk$$

$$= \frac{L}{2\pi}\left(\frac{\pi}{a}+\frac{\pi}{a}\right) = \frac{L}{\cancel{2\pi}}\,\frac{\cancel{2}\pi}{a} = \frac{L}{a} = N \quad \#$$

In 3-D:

every $\left(\frac{2\pi}{L}\right)^3$ has one k Point

$\Rightarrow$ Density of states in k-space

$$= \frac{1}{\left(\frac{2\pi}{L}\right)^3} = \frac{L^3}{8\pi^3}$$

$$\therefore D(k) = \frac{L^3}{8\pi^3} \quad \text{or} \left(\frac{V}{8\pi^3}\right)$$

then $\Rightarrow$ lecture

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 $D(\omega)$, 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 ω and $\omega + d\omega$ is a right cylinder of base dS_ω and altitude $dK_\perp$ so that

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

Density of Levels (states)

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

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

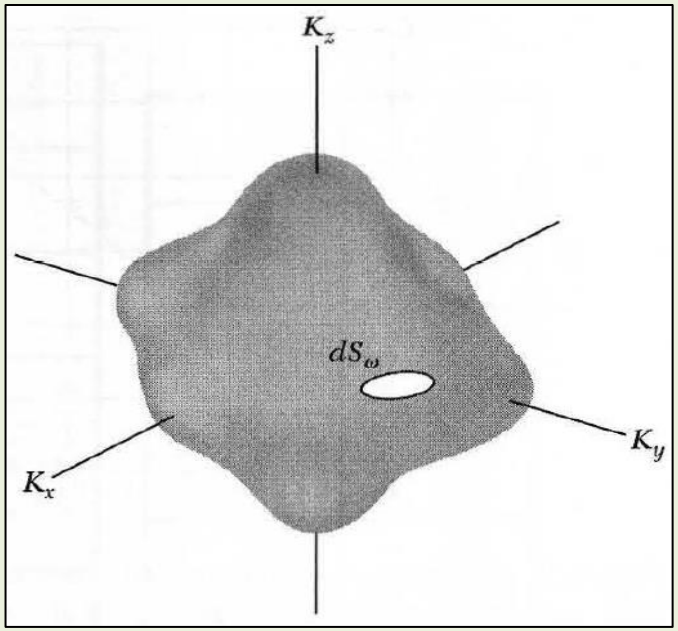
is the difference in frequency between the two surfaces connected by $dk_\perp$. Thus the element of the volume is

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

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

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:

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

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

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

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

$$\Rightarrow g(\varepsilon) = \frac{1}{4\pi^3} \int \frac{dS}{|\nabla_k \varepsilon|} \qquad (8.44)$$

- we multiplied by 2/V : 2 for the allowed spin states. V to normalize to a unit volume V

SECOND PROOF OF BLOCH's THEOREM

- We can alway expand any function obeying the Born- von Karman 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 $U_{\mathbf{K}}$ is real and thus:

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

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

(8.45) in (8.50) 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):

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

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

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

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

$$\therefore (8.55)\Rightarrow$$

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

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

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

- 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