Week3-Bloch’s Theorem

ECE 695-O Semiconductor Transport Theory

Fall 2018

Instructor: Byoung-Don Kong

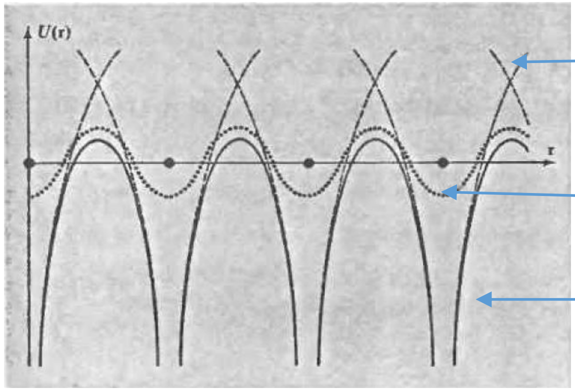
POSTECH POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY

Contents

- Bloch's Theorem
- Born-von Karman Boundary Conditions

The Periodic Potential

- The full Hamiltonian of the solid contains not only the one-electron potentials describing the interactions of the electrons with the massive atomic nuclei, but also pair potentials describing the electron-electron interactions.
- Thus, the problem of electrons in a solid is in principle a many-electron problem.
- In the independent electron approximation, these interactiosn are represented by an effective one-electron potential U(**r**).
- A typical crystalline potential might be expected to have the form of the figure shown below.



Potential of single isolated ions

Potential along the line between planes of ions

Potential along the line of ions

Bloch's Theorem

- We need to examine the general properties of Schrödinger Eq. for a single electron under periodic potential U(**r**).

$$H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right)\psi = \mathcal{E}\psi$$

- Bloch's Theorem
  - The eigenstates ψ of the one-electron Hamiltonian $H = -\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})$, where $U(\mathbf{r}) = U(\mathbf{r}+\mathbf{R})$ for all $\mathbf{R}$ 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:

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

    where

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

    for all $\mathbf{R}$ in the Bravais lattice.
  - Or equivalently,

Bloch's Theorem(2)

- The eigenfunction of a periodic Hamiltonian H can be chosen so that associated with each ψ is a wave vector $\mathbf{k}$ such that

$$\boxed{\psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})}$$

Periodic Boundary Condition

- In 3D, we can write down the periodicity such as

$$\begin{aligned}\psi(\mathbf{r}) &= \psi(\mathbf{r}+N_1\mathbf{a_1}) \\ &= \psi(\mathbf{r}+N_2\mathbf{a}_2) \\ &= \psi(\mathbf{r}+N_3\mathbf{a}_3)\end{aligned}$$

where N_i is integer.

Periodic Boundary Condition : Born-von Karman B.C.

- From Bloch's theorem,

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

where

$$\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$$

and $\mathbf{b}_i$ is reciprocal lattice vector.

$$e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot(\mathbf{r}+N_i\mathbf{a}_i)} \underbrace{u_{n\mathbf{k}}(\mathbf{r}+N_i\mathbf{a}_i)}_{= u_{n\mathbf{k}}(\mathbf{r})}$$

$$\Rightarrow e^{i\mathbf{k}\cdot N_i\mathbf{a}_i} = 1$$

.

Periodic Boundary Condition : Born-von Karman B.C.(2)

- Since

$$\mathbf{a}_i \cdot \mathbf{b}_i = 2\pi\delta_{ij} \quad ,$$

$$\mathbf{k} \cdot N_i\mathbf{a}_i = k_i\mathbf{b}_i \cdot N_i\mathbf{a}_i = 2\pi n_i \quad \cdot$$

$$\Rightarrow 2\pi k_i N_i = 2\pi n_i$$

$$\Rightarrow k_i = \frac{n_i}{N_i} \qquad n_i : \text{integer}$$

- Therefore the general form for allowed Bloch wave vectors is

$$\mathbf{k} = \frac{n_1}{N_1}\mathbf{b}_1 + \frac{n_2}{N_2}\mathbf{b}_2 + \frac{n_3}{N_3}\mathbf{b}_3 \ .$$

Bloch's Theorem(3)

- Proof:
  - Any function obeying periodic a boundary condition can be expanded in the set of all plane wave that satisfy that boundary condition.

$$\psi(\mathbf{r}) = \sum_{\mathbf{q}} c_q \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}$$

  - Since the crystal potential $U(\mathbf{r})$ is periodic in the lattice, its plane wave expansion contain plane waves with the periodicity of the lattice. These plane waves has wave vectors that are vectors of the reciprocal lattice.

$$U(\mathbf{r}) = \sum_{\mathbf{K}} U_{\mathbf{K}} \mathrm{e}^{\mathrm{i}\mathbf{K}\cdot\mathbf{r}}$$

Bloch's Theorem(4)

- The Fourier coefficients $U_{\mathbf{K}}$ are related to $U(\mathbf{r})$ by

$$U_{\mathbf{K}} = \frac{1}{v}\int_{cell} \mathrm{d}\mathbf{r}\, e^{\mathrm{i}\mathbf{K}\cdot\mathbf{r}} U(\mathbf{r}) \quad .$$

- Upon the Fourier transform, DC components give no influence to the results. Thus, we have freedom to choose additive constants to $U(\mathbf{r})$. We choose a constant that makes the spatial average U_0 of the potential over a primitive cell vanish.

$$U_0 = \frac{1}{v}\int_{cell} d\mathbf{r} U(\mathbf{r}) = 0$$

- Because the potential $U(\mathbf{r})$ is real, the Fourier coefficients satisfy

$$U_{-\mathbf{K}} = U_{\mathbf{K}}^{*} \quad .$$

- If we assume that the crystal has inversion symmetry ($U(\mathbf{r}) = U(-\mathbf{r})$ with a suitable choice of origin), $U_{\mathbf{K}}$ is real, and thus

$$U_{-\mathbf{K}} = U_{\mathbf{K}} = U_{\mathbf{K}}^{*} \quad .$$

Bloch's Theorem(5)

- We now apply the plane wave expansion to the Schödinger Eq..

$$\frac{p^2}{2m}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi = \sum_{\mathbf{q}} \frac{\hbar^2}{2m} q^2 c_{\mathbf{q}} e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}$$

- The potential energy term can be written as

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

$$= \sum_{\mathbf{K}\mathbf{q}} U_{\mathbf{K}} c_{\mathbf{q}} e^{i(\mathbf{K}+\mathbf{q})\cdot\mathbf{r}} = \sum_{\mathbf{K}\mathbf{q}'} U_{\mathbf{K}} c_{\mathbf{q}'-\mathbf{K}} e^{i\mathbf{q}'\cdot\mathbf{r}}$$

- Then, the Schödinger Eq. becomes,

$$\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \left\{ \left(\frac{\hbar^2}{2m} q^2 - \varepsilon \right) c_{\mathbf{q}} + \sum_{\mathbf{K}'} U_{\mathbf{K}'} c_{\mathbf{q}-\mathbf{K}'} \right\} = 0$$

POSTECH POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY

Bloch's Theorem(6)

- Since the plane waves satisfying the Born-Karman b.c. are an orthogonal set, the coefficient of each separate term in the above expression must vanish. Thus, for all allowed wave vectors **q**,

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

- It is convenient to write q in the form of **q=k-K**, where **K** is a reciprocal lattice vector chosen so that **k** lies in the first Brillouin zone.

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

- If we further simplify by change of variables **K'** → **K'-K**

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

Bloch's Theorem(6)

- This is simply a restatement of the original Schödinger Eq. in momentum space, simplified by the fact that the Fourier coefficient of the periodic potential ($U_{\mathbf{k}}$) is nonvanishing only when **k** is a vector of the reciprocal lattice.

$$\left(-\frac{\hbar^2}{2m}(\nabla^2+\mathcal{E})+U(\mathbf{r})\right)\psi=0 \quad \longrightarrow \quad \left(\frac{\hbar^2}{2m}(\mathbf{k}-\mathbf{K})^2-\mathcal{E}\right)c_{\mathbf{k}-\mathbf{K}}+\sum_{\mathbf{K}'}U_{\mathbf{K}'-\mathbf{K}}\,c_{\mathbf{k}-\mathbf{K}'}=0$$

- Thus, the original problem has separated into N independent problems: one for each allowed value of **k** in the first Brillouin zone.
- Each such problem has solutions that are superpositions of plane waves containing only the wave vector **k** and wave vector differing from **k** by a reciprocal lattice vectors.

Bloch's Theorem(7)

- Putting this information back to the plane wave expansion of wave function ψ,

$$\psi(\mathbf{r}) = \sum_{\mathbf{q}} c_q \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \quad \longrightarrow \quad \psi_{\mathbf{k}} = \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}}\, e^{i(\mathbf{k}-\mathbf{K})\cdot\mathbf{r}}$$

- Then, we can write this as

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}}\, e^{-i\mathbf{K}\cdot\mathbf{r}}$$

- and, the Bloch form with the periodic function u(r) is given by

$$u(\mathbf{r}) = \sum_{\mathbf{K}} c_{\mathbf{k}-\mathbf{K}}\, e^{-i\mathbf{K}\cdot\mathbf{r}} \quad \longleftarrow \quad \psi_{n\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

Bloch's Theorem(8)

- Implications of Bloch's Theorem
  - $\hbar\mathbf{k}$ is so-called crystal momentum.
  - The wave vector appearing in the Bloch's theorem can be confined to the FBZ.
  - For a give **k**, there are many solutions to the Schrödinger Eq. So, we need the band index n.
  - For a give n, the eigenstates and eigenvalues are periodic functions of k in the reciprocal lattice.

$$\psi_{n\mathbf{k}}(r) = \psi_{n\mathbf{k}+\mathbf{K}}(r)$$

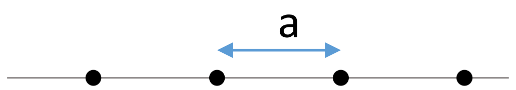
$$\mathcal{E}_{n\mathbf{k}} = \mathcal{E}_{n\mathbf{k}+\mathbf{K}}$$

Ex) A free electron in an empty lattice

- Let's say the lattice spacing is a.
  - Hamiltonian：

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}\right)$$

$$H(x) = H(x + na)$$



No potential(Coulomb Force) but just periodicity imposed.

  - From Bloch's theorem,

$$\psi = e^{ikx} u_k(x) \quad \text{where} \quad u_k(x) = u_k(x + na)$$

  - If we chose, for instance, $u_k(x)$=1 (constant function also satisfies this condition, although it is trivial)

$$\psi = e^{ikx}$$

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

$$\mathcal{E} = \frac{\hbar^2 k^2}{2m}$$

Ex) A free electron in an empty lattice

- In non-trivial case, $\psi = e^{i\left(k \pm \frac{2\pi}{a} n\right)x}$

$$= e^{ikx} \underbrace{e^{\pm i\frac{2\pi}{a}nx}}_{u = e^{i\frac{2\pi}{a}nx}}$$

$$u(x+ma) = e^{i\frac{2\pi}{a}nx} e^{i2\pi nm}$$

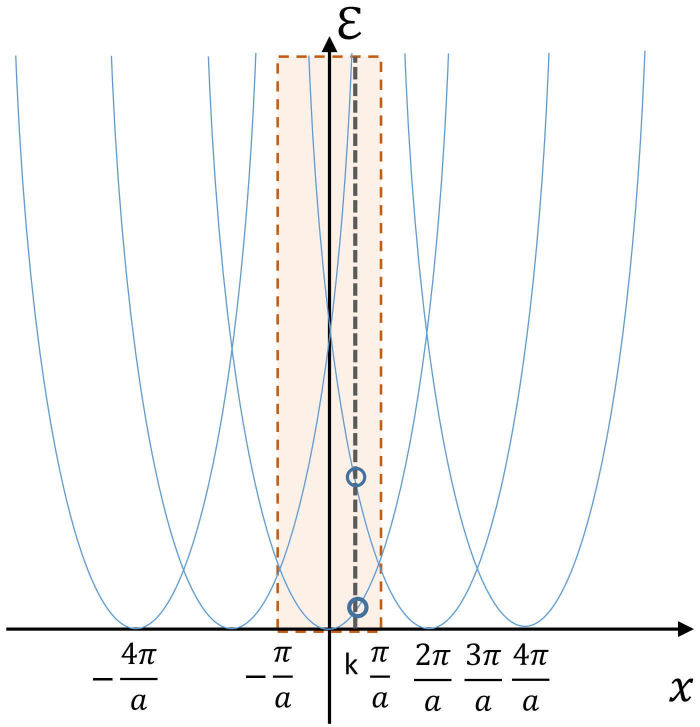
$$= u(x)$$

$$\mathcal{E} = \frac{\hbar^2\left(k \pm \frac{2\pi}{a} n\right)^2}{2m}$$

n=+1 → $\mathcal{E} = \frac{\hbar^2\left(k + \frac{2\pi}{a}\right)^2}{2m}$

n=0 → $\mathcal{E} = \frac{\hbar^2 k^2}{2m}$

n=-1 → $\mathcal{E} = \frac{\hbar^2\left(k - \frac{2\pi}{a}\right)^2}{2m}$



- 1st BZ is repeated.
- For fixed k, there are many solutions (so we need band indices)
- Band indices correspond to the nth BZ.