

Week6 - Electronic Bands in Real Crystals

ECE 695-O Semiconductor Transport Theory
Fall 2018
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Contents

- Hole concept review
- Energy bands in real crystals
- Density of States
- Carrier Density

Hole Concept

- Current from electron point of view:

$$I = -q \sum_{\mathbf{k}_e} \mathbf{v}_{\mathbf{k}_e}$$

{occupied}

- A completely occupied band contribute no current: $I = -q \sum_{\mathbf{k}_e} \mathbf{v}_{\mathbf{k}_e} = 0$
{All}
- We can separate the current into two parts:

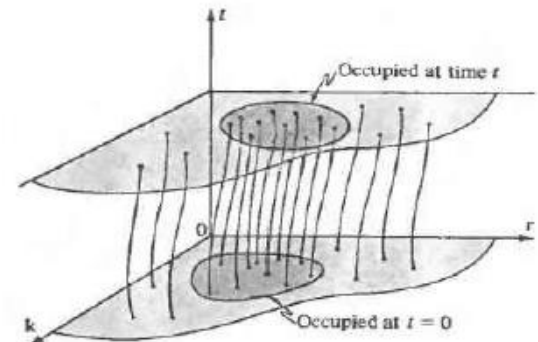
$$I = -q \sum_{\mathbf{k}_e} \mathbf{v}_{\mathbf{k}_e} = -q \sum_{\mathbf{k}_e} \mathbf{v}_{\mathbf{k}_e} - q \sum_{\mathbf{k}_e} \mathbf{v}_{\mathbf{k}_e} = 0$$

{All} {occupied} {empty}

- Then, the contribution from the occupied is

$$I = -q \sum_{\mathbf{k}_e} \mathbf{v}_{\mathbf{k}_e} = q \sum_{\mathbf{k}_e} \mathbf{v}_{\mathbf{k}_e}$$

{occupied} {empty}



Hole Concept(2)

- Equations of motion: $\mathbf{F}_{ext} = \hbar \frac{d\mathbf{k}}{dt} = -q\mathbf{E}$

\mathbf{E} : e-field

\mathcal{E} : energy

$$\mathbf{v} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}$$

- From electron point of view

$$I = +q \sum_{\substack{\mathbf{k}_e \\ \{empty\}}} \mathbf{v}_{\mathbf{k}_e}$$

$$\mathcal{E}_e = -\frac{\hbar^2 k^2}{2|m^*|}$$

$$\frac{d\mathbf{k}_e}{dt} = -\frac{q}{\hbar} \mathbf{E}$$

$$\mathbf{v}_{\mathbf{k}_e} = \frac{1}{\hbar} \nabla_{\mathbf{k}_e} \mathcal{E}_e(\mathbf{k}_e)$$

- From hole point of view

$$I = +q \sum_{\substack{\mathbf{k}_h \\ \{occupied\}}} \mathbf{v}_{\mathbf{k}_h}$$

$$\mathcal{E}_h = +\frac{\hbar^2 k^2}{2|m^*|}$$

$$\frac{d\mathbf{k}_h}{dt} = +\frac{q}{\hbar} \mathbf{E}$$

$$\mathbf{v}_{\mathbf{k}_h} = \frac{1}{\hbar} \nabla_{\mathbf{k}_h} \mathcal{E}_h(\mathbf{k}_h)$$

Hole Concept(3)

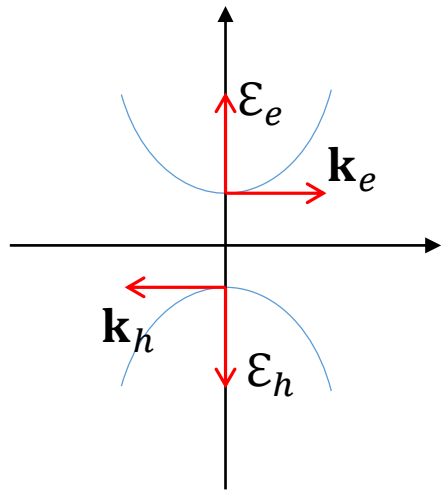
- These two pictures are equivalent only if

$$\mathbf{k}_e = -\mathbf{k}_h \text{ and } \mathcal{E}_h = -\mathcal{E}_e.$$

- Then,

$$\nabla_{\mathbf{k}_e} = -\nabla_{\mathbf{k}_h} \text{ and}$$

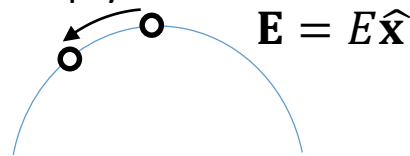
$$\mathbf{v}_{\mathbf{k}_e} = \mathbf{v}_{\mathbf{k}_h}.$$



Arrows are the increasing directions

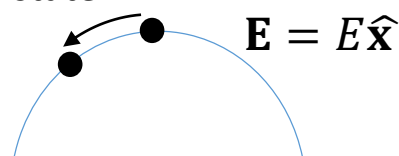
- Electron picture:

One empty state



- Hole picture:

One state



$$\frac{dk_x}{dt} = -\frac{q}{\hbar}E$$

\Rightarrow increase in negative direction

$$\frac{dk_x}{dt} = \frac{q}{\hbar}E$$

$$k_x = \frac{q}{\hbar}Et + k_x(t=0)$$

\Rightarrow increase in positive.
(the negative sign for momentum disappears)

Energy bands in real crystals

- Valence band of group IV and III-V semiconductors

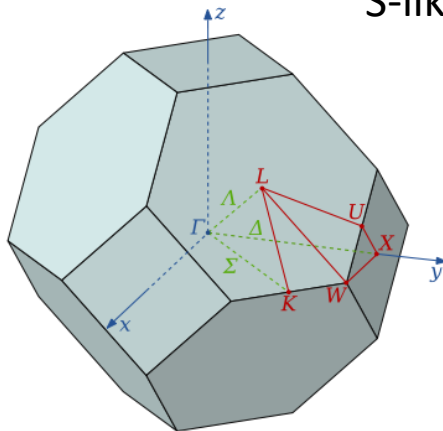
❖ Silicon

- 8 available electrons (two atoms in unit cell x 4 valence electrons per atom)
- 4 valence bands

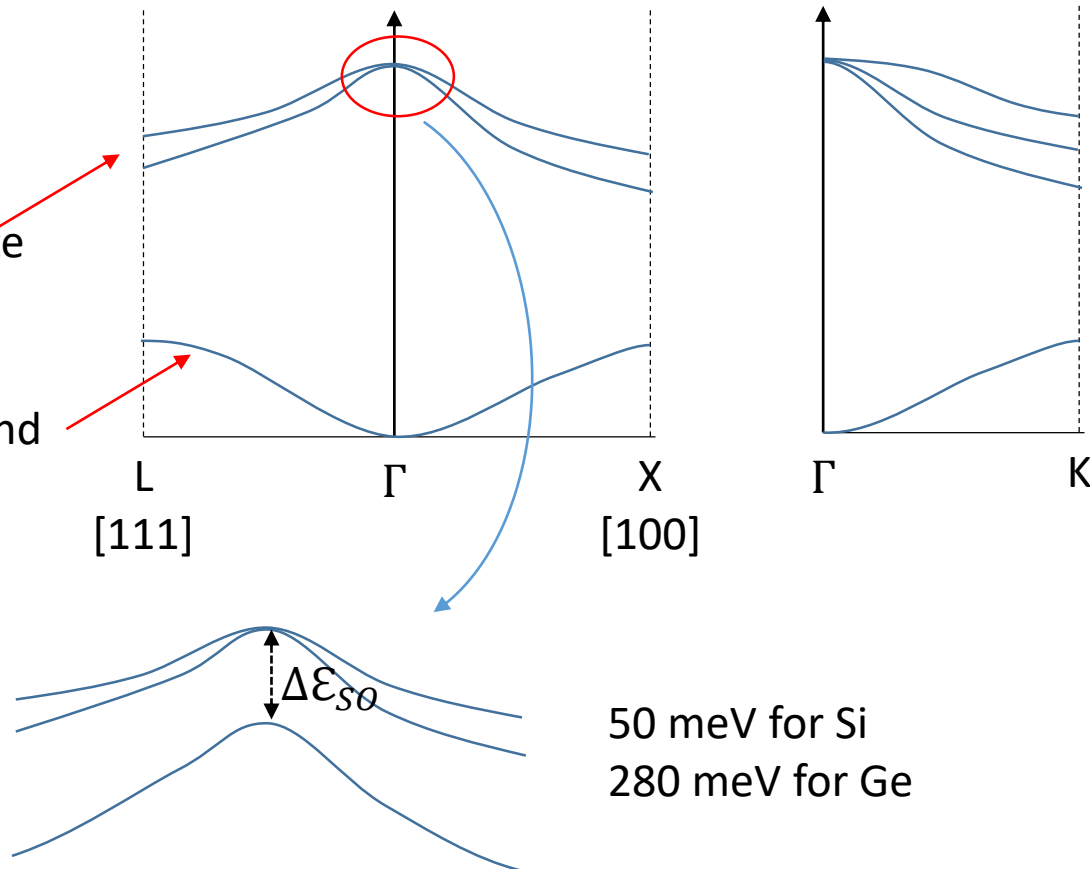
3 P-like bands:

1. double degenerate
2. Split off

S-like band



FBZ of FCC



50 meV for Si
280 meV for Ge

Energy bands in real crystals(2)

❖ Silicon (continues)

- Deep s-like state (core state) does not contribute to the current.
- If $\Delta\epsilon_{SO}$ is large, the lowest p-like band can also be ignored.
- Under parabolic energy band approximation,

$$\epsilon_{SO}(k) = \epsilon_{SO\ MAX} - \frac{\hbar^2 k^2}{2m_{SO}^*}$$

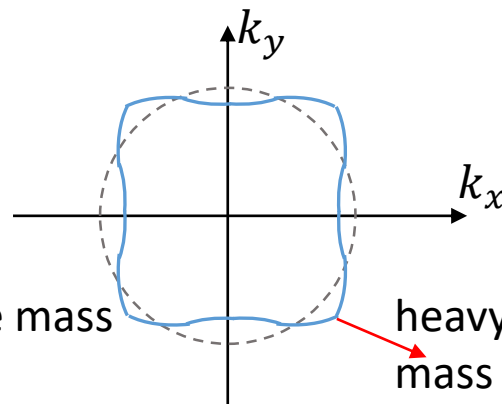
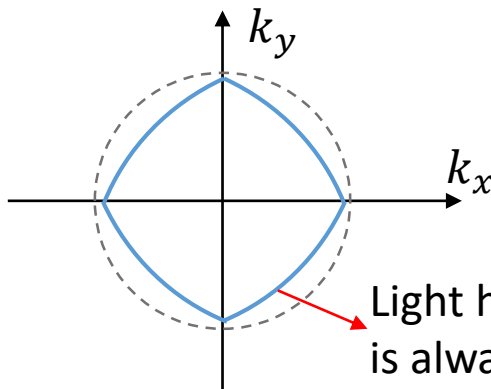
	A	B	C
Ge	13.1	8.3	12.5
Si	4.0	1.1	4.1

$$\epsilon_{lh\ or\ hh}(k) = -\frac{\hbar^2}{2m} \left\{ Ak^2 \pm \sqrt{B^2 k^4 + C^2 (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2)} \right\}$$

+: lh -: hh

*Dresselhaus Eq

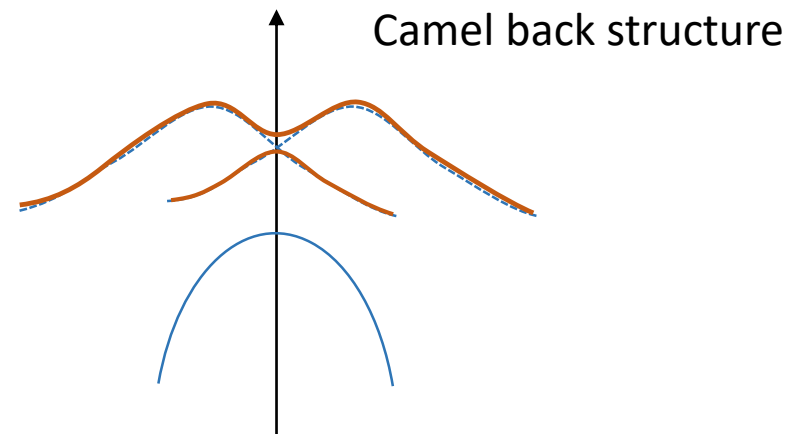
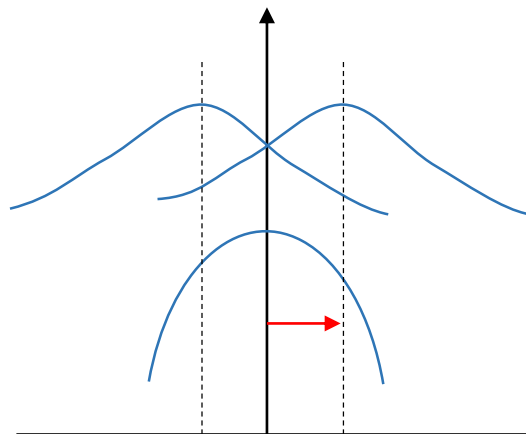
- Equivalent energy contour



Energy bands in real crystals(3)

❖ III-V

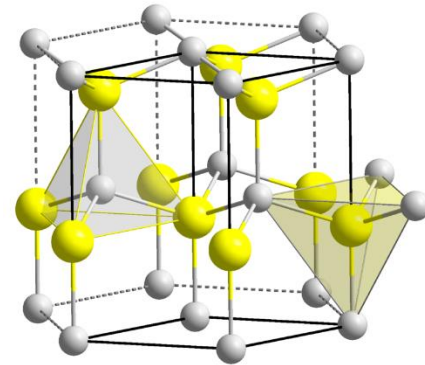
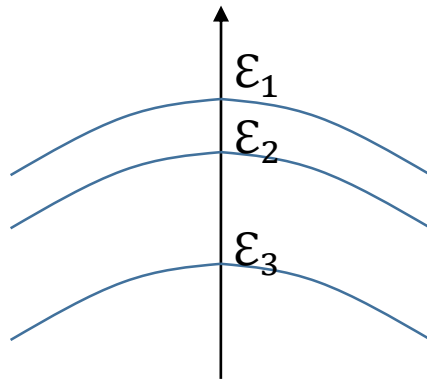
- III-V semiconductors are lack of the inversion symmetry with respect to basis.
- Si or Ge have inversion symmetry with respect to basis (the same species)
- III-V valence bands minima has similar to that of IV and they are treated like IV diamond crystal in many cases.
- However, the extreme points of balance bands are shifted due to this lack of inversion symmetry.



Dresselhaus effect

Energy bands in real crystals(4)

- ❖ Wurtzites (two interpenetrated hcps : GaN, CdS ...)
 - Wurtzites crystal valence bands usually has three distinctive bands.
 - Spin-orbit splitting (Rashba – effect) : $\epsilon_1 - \epsilon_2$
 - Hexagonal crystal field splitting: $\epsilon_1 - \epsilon_3$



- A, B, C bands (it is hard to distinguish by curvature like hh lh)

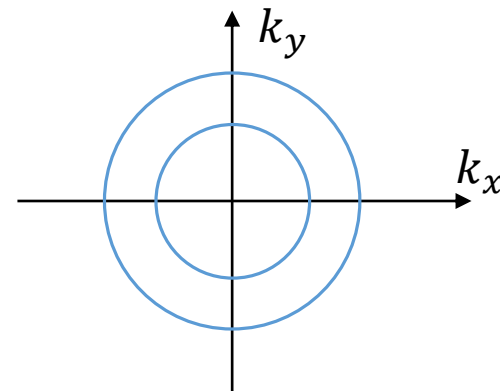
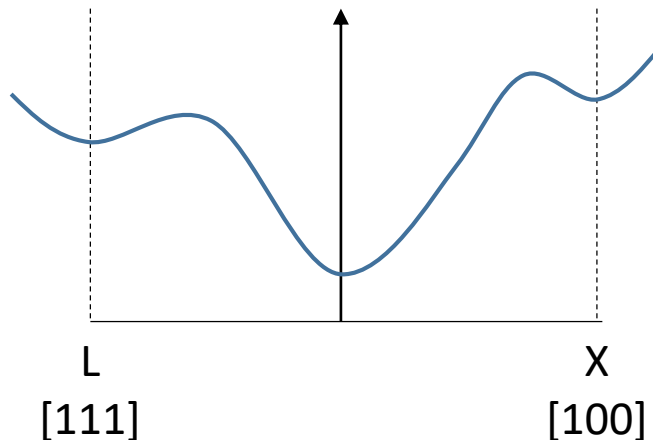
Energy bands in real crystals(5)

- Conduction bands

- i. Minimum at $k = 0$ (FBZ center)

- GaAs, InAs, InP
 - These are called direct gap semiconductors
 - The energy band is spherically symmetric near $k=0$:

$$\epsilon_c(k) = \epsilon_{c \min} + \frac{\hbar^2 k^2}{2m^*}$$

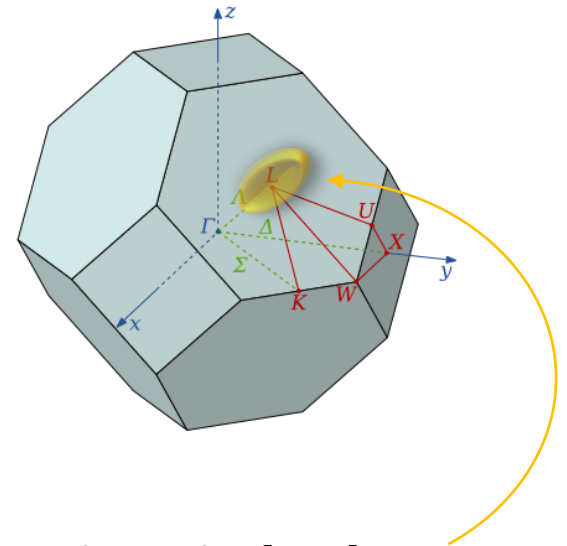
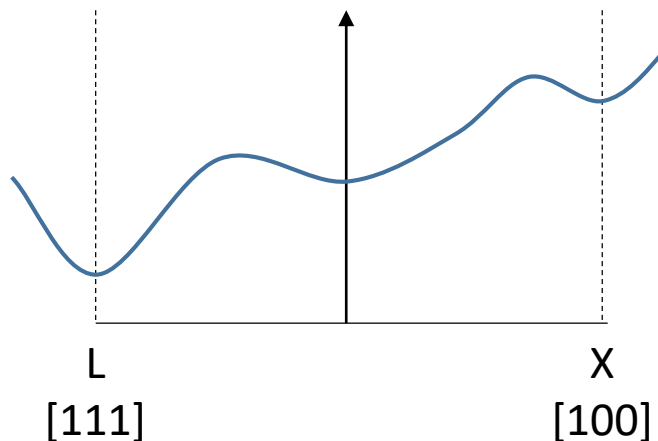


Energy bands in real crystals(6)

- Conduction bands

- ii. Minimum at L (FBZ edge along [111])

- Ge



- Constant energy surfaces are ellipsoids of revolution about the [111] axis.
- Near the minima, $k_0 \sim \frac{\pi}{a}(1,1,1)$,

$$\mathcal{E}_C = \mathcal{E}_{C \min} + \frac{\hbar^2}{2} \left(\frac{k_l^2}{m_l^*} + \frac{k_{t1}^2 + k_{t2}^2}{m_t^*} \right)$$

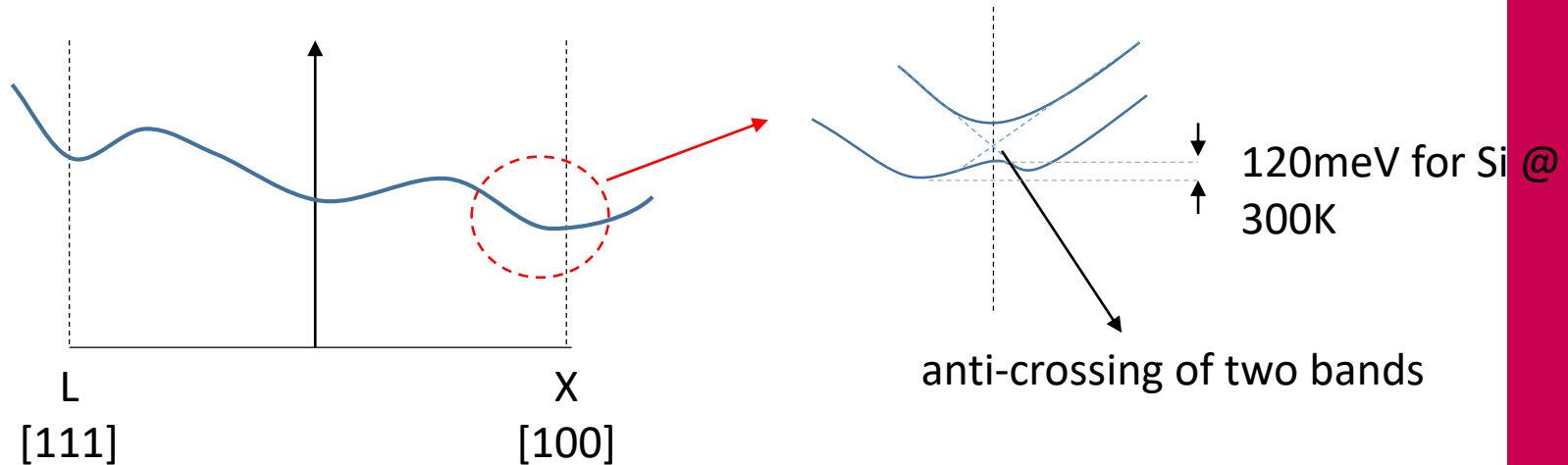
($k_l // [1,1,1]$ and $k_l \perp k_{t1} \perp k_{t2}$)

- 8 symmetry points => 4 equivalent minima since each point contributes half

Energy bands in real crystals(7)

iii. Minima along the [100] direction near BZ edge

- Si, GaP ,



$$\epsilon_c = \epsilon_{c \min} + \frac{\hbar^2}{2} \left(\frac{k_l^2}{m_l^*} + \frac{k_{t1}^2 + k_{t2}^2}{m_t^*} \right)$$

6 equivalent minima

Density of States

- The total number of electrons n is the sum of all the electrons at the minima (or holes at maxima):

$$n = \sum_i n_i$$

- $n_i = \sum_{\text{all } k \text{ in } i \text{ th min}} f(k)$ where $f(k)$ is a distribution function.
- For a very large crystal, all discrete k s get very close so we can treat them like a continuum: change the summation into integration.

- $n_i = \int_{FBZ} f(k) \frac{d^3k}{(2\pi)^3/V}$

- If we consider the spin degeneracy,

$$\Rightarrow \frac{2V}{(2\pi)^3} \int_{FBZ} f(k) d^3k$$

- per unit volume, $\Rightarrow \frac{2}{(2\pi)^3} \int_{FBZ} f(k) d^3k$

- To convert this into the integration with respect to energy like $\int f(\mathcal{E})g(\mathcal{E})d\mathcal{E}$ we need the concept of density of states, $g(\mathcal{E})$.

Density of States(2)

- $g_i(\mathcal{E})$: density of states per unit volume per unit energy for i th minimum.
- Total density of state is the sum of all bands minima:

$$g(\mathcal{E}) = \sum_i g_i(\mathcal{E}) .$$

- $g_i(\mathcal{E})d\mathcal{E} = \frac{2}{V} \times \left(\begin{array}{l} \text{the number of allowed states in the } i\text{th} \\ \text{minimum in the energy range from } \mathcal{E} \text{ to } \mathcal{E} + d\mathcal{E} \end{array} \right)$
$$= \frac{2}{V} \int_{\mathcal{E} \text{ to } \mathcal{E} + d\mathcal{E}} \text{volume between } \frac{d^3k}{(2\pi)^3/V}$$

$$= \frac{1}{4\pi^3} \int \text{the corr. volume in } k\text{-space } \frac{d^3k}{(2\pi)^3/V}$$

Density of States(3)

- Consider the equivalent energy surface like this.

$$g_i(\mathcal{E}) = \int_{S_i(\mathcal{E})} \frac{dS}{4\pi^3} \delta k(\mathbf{k})$$

where $\delta k(\mathbf{k})$ is the perpendicular distance between the surface $S_i(\mathcal{E})$ and $S_i(\mathcal{E} + d\mathcal{E})$

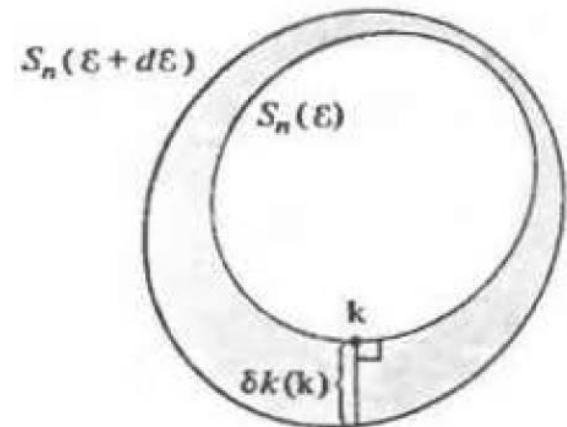
$$\mathcal{E} + d\mathcal{E} = \mathcal{E} + |\nabla \mathcal{E}_i(\mathbf{k})| \delta k(\mathbf{k})$$

and hence,

$$\delta k(\mathbf{k}) = \frac{d\mathcal{E}}{|\nabla \mathcal{E}_i(\mathbf{k})|}$$

Finally, we arrive

$$g_i(\mathcal{E}) = \int_{S_i(\mathcal{E})} \frac{dS}{4\pi^3} \frac{1}{|\nabla \mathcal{E}_i(\mathbf{k})|}$$



Density of States (4)

- EX) Simple spherical energy

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

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

$$g(\mathcal{E}) = \int_{\text{sphere}} \frac{dS}{4\pi^3} \frac{m^*}{\hbar^2 k} = 4\pi k^2 \frac{1}{4\pi^3} \frac{m^*}{\hbar^2 k} = \frac{m^*}{\pi^2 \hbar^2} k$$

$$g(\mathcal{E}) \propto \sqrt{\mathcal{E}}$$

2D case $g(\mathcal{E}) \propto \text{constant}$

1D case $g(\mathcal{E}) \propto 1/\sqrt{\mathcal{E}}$

Carrier Density

- Carrier density:

$$n_i = \frac{1}{4\pi^3} \int f(\mathbf{k}) d^3k$$

where $f(\mathbf{k})$ is the occupation probability.


- In equilibrium,

$$f(\mathbf{k}) = \frac{1}{1 + \exp\left(\frac{\mathcal{E}(\mathbf{k}) - \mathcal{E}_F}{k_B T}\right)}$$

and

$$\mathcal{E}(\mathbf{k}) = \mathcal{E}_C + \sum_{i=1}^3 \frac{\hbar^2 k_i^2}{2m_i^*}$$

We are dealing this case


$$\begin{pmatrix} m_{11}^* & 0 & 0 \\ 0 & m_{22}^* & 0 \\ 0 & 0 & m_{33}^* \end{pmatrix}$$

Carrier Density(2)

$$\Rightarrow n_i = \frac{1}{4\pi^3} \int f(\mathbf{k}) dk_1 dk_2 dk_3$$

• Let
$$z_1^2 = \frac{\hbar^2 k_1^2}{2k_B T m_1^*} \quad z_2^2 = \frac{\hbar^2 k_2^2}{2k_B T m_2^*} \quad z_3^2 = \frac{\hbar^2 k_3^2}{2k_B T m_3^*}$$

(<= This variable change to convert the ellipsoidal function into a spherical function.)

• Then,

$$dk_1 dk_2 dk_3 = \left(\frac{2k_B T}{\hbar^2} \right)^{3/2} (m_1^* m_2^* m_3^*)^{1/2} dz_1 dz_2 dz_3$$

$$\Rightarrow n_i = \frac{1}{4\pi^3} \left(\frac{2k_B T}{\hbar^2} \right)^{3/2} (m_1^* m_2^* m_3^*)^{1/2} \int \frac{dz_1 dz_2 dz_3}{1 + \exp \left(\frac{\epsilon_C - \epsilon_F}{k_B T} + z_1^2 + z_2^2 + z_3^2 \right)}$$

Carrier Density(3)

- Let

$$\eta_C \equiv \frac{\mathcal{E}_C - \mathcal{E}_F}{k_B T} \quad m_{Ci}^* = (m_1^* m_2^* m_3^*)^{1/3}$$

- And we assume z_i from $-\infty$ to ∞ .
- Let $E = z_1^2 + z_2^2 + z_3^2 = z^2$

$$\Rightarrow n_i = \frac{1}{4\pi^3} \left(\frac{2k_B T m_{Ci}^*}{\hbar^2} \right)^{3/2} \int_{-\infty}^{\infty} \frac{dz_1 dz_2 dz_3}{1 + \exp(-\eta_C + E)}$$

(this means there is no angular dependence)

- Then, we can write $n_i = N_{Ci} F_{1/2}(\eta_C)$

where $N_{Ci} = 2 \left(\frac{2\pi k_B T m_{Ci}^*}{\hbar^2} \right)^{3/2}$ is the effective density of states and

$$F_{1/2}(\eta_C) = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{E^{1/2} dE}{1 + \exp(E - \eta_C)}$$