LECTURE #23

CONSEQUENCES OF THE BAND THEORY OF SOLIDS:

WE HAVE SHOWN THAT THE E-K DIAGRAM FOR A CRYSTAL WITHIN A PARTICULAR BAND IS VERY SIMILAR TO THAT OF A FREE ELECTRON.

THEREFORE, WE WILL USE THE FREE PARTICLE SOLUTION OF THE SCHRÖDINGER EQUATION AS A STARTING POINT FOR THE THEORY OF ELECTRICAL CONDUCTION IN SOLIDS.

RECALL: FREE PARTICLES TRAVEL AS WAVE PACKETS WITH A GROUP VELOCITY:

$$V_g = \frac{\partial \omega}{\partial K} = \frac{1}{\hbar}\frac{\partial E}{\partial K} \quad (\text{SINCE } E = \hbar\omega).$$

HOWEVER, WE KNOW FROM ELECTROSTATICS THAT A FREE ELECTRON ACCELERATED BY AN ELECTRIC FIELD ($\mathcal{E}$) OBEYS CLASSICAL NEWTONIAN MECHANICS:

$$\underset{\substack{\uparrow \\ \text{CHANGE} \\ \text{IN ENERGY}}}{dE} = \underbrace{e\,\mathcal{E}}_{\text{FORCE}}\ \underbrace{v_g\, dt}_{\text{CHANGE IN DISTANCE}}$$

COMBINING THE QUANTUM MECHANICAL AND CLASSICAL RESULTS LEADS TO A SEMI-CLASSICAL MODEL:

$$dE = e\mathcal{E}\frac{1}{\hbar}\frac{\partial E}{\partial k}dt \Rightarrow \frac{\partial k}{\partial E}\cdot\frac{dE}{dt} = \frac{1}{\hbar}e\mathcal{E} \Rightarrow \underline{\frac{dk}{dt} = \frac{e\mathcal{E}}{\hbar}}$$

BUT $v_g = \dfrac{1}{\hbar}\dfrac{\partial E}{\partial k}$

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$$\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\frac{\partial E}{\partial k} = \frac{1}{\hbar}\frac{\partial^2 E}{\partial k^2}\frac{dk}{dt} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}e\mathcal{E}$$

$$\therefore\ e\mathcal{E} = \hbar^2\left(\frac{\partial^2 E}{\partial k^2}\right)^{-1}\frac{dv_g}{dt}$$

CLASSICALLY, $F = ma \Rightarrow e\mathcal{E} = m\dfrac{dv_g}{dt}$

THESE TWO EQUATIONS ARE CONSISTENT IF WE DEFINE AN <u>EFFECTIVE MASS</u>:

$$\boxed{m^* = \hbar^2\left(\frac{\partial^2 E}{\partial k^2}\right)^{-1}}$$

<u>NOTE</u>: FOR A FREE ELECTRON, $E = \dfrac{\hbar^2 k^2}{2m}$

$$\therefore\ \frac{\partial E}{\partial k} = \frac{\hbar^2 k}{m},\quad \frac{\partial^2 E}{\partial k^2} = \frac{\hbar^2}{m} \Rightarrow m^* = \hbar^2\left(\frac{m}{\hbar^2}\right) = m$$

(AS EXPECTED)

HOWEVER, IN A SOLID, THE E-K DIAGRAM DEVIATES FROM THE FREE ELECTRON MODEL

$\boxed{\text{SEE FIGURE 7.12}}$

NOTE: (1) EFFECTIVE MASS VARIES AS A FUNCTION OF K

(2) NEAR THE TOP OF THE BAND, THE EFFECTIVE MASS IS NEGATIVE.

(3) V_g AND m^* ARE PERIODIC IN K.

CONSIDER CURRENT FLOW FOR FREE ELECTRONS IN 1-D:

$$I = e v_g \frac{N}{L} = e v_g n$$

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$$\frac{dI}{dt} = e \frac{dv_g}{dt} n = \frac{e^2 \mathcal{E}}{m} n \quad \text{SINCE} \quad \frac{dv_g}{dt} = \frac{e\mathcal{E}}{m}$$

HOWEVER, IN A CRYSTAL,

$$n = \int_0^\infty f(E)\, g(E)\, dE = \int_{-\infty}^{\infty} f(k)\, g(k)\, dk$$

IN 1-D, WHAT IS $g(E)$?

$$N = \frac{K/2}{\pi/2L} = \frac{Lk}{\pi} \Rightarrow n = \frac{k}{\pi}$$

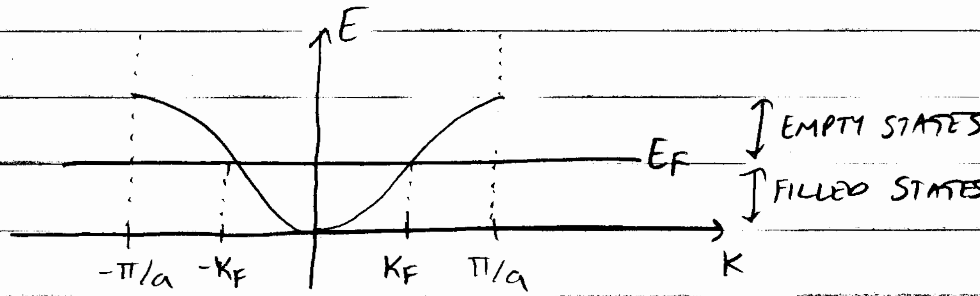
$$\therefore g(k) = \frac{dn}{dk} = \frac{1}{\pi}$$

$$\therefore \frac{dI}{dt} = e \int_{-\infty}^{\infty} \frac{dv_g}{dt} f(k)\, g(k)\, dk$$

$$= \frac{e^2 \mathcal{E}}{\pi} \int_{-\infty}^{\infty} \frac{f(k)}{m^*}\, dk$$

$$= \frac{e^2 \mathcal{E}}{\pi \hbar^2} \int_{-\infty}^{\infty} \frac{\partial^2 E}{\partial k^2} f(k)\, dk$$

AT $T = 0K$, $f(E) = \begin{cases} 1, & E < E_F \\ 0, & E > E_F \end{cases}$



$$\therefore \frac{dI}{dt} = \frac{e^2 \mathcal{E}}{\pi \hbar^2} \int_{-K_F}^{K_F} \frac{\partial^2 E}{\partial k^2} dk = \frac{2e^2 \mathcal{E}}{\pi \hbar^2} \left(\frac{\partial E}{\partial k} \right) \Big|_{K=K_F}$$

COMPARE THIS EQUATION TO FREE ELECTRONS:

$$\frac{dI}{dt} = \frac{e^2 \mathcal{E}}{m} n$$

THESE TWO EQUATIONS ARE CONSISTENT IF WE DEFINE AN EFFECTIVE NUMBER OF ELECTRONS THAT CONTRIBUTE TO CONDUCTION IN A CRYSTAL:

$$n_{eff} = \frac{2m}{\pi \hbar^2} \left(\frac{\partial E}{\partial k} \right) \Big|_{K=K_F}$$

NOTE: (1) WHEN E_F IS IN THE MIDDLE OF A BAND, $(\partial E / \partial k)|_{k=K_F}$ IS MAXIMIZED, WHICH IMPLIES n_{eff} IS MAXIMIZED
$\Rightarrow$ HIGH CONDUCTIVITY FROM HALF-FILLED BANDS

(2) WHEN E_F IS IN THE BANDGAP, THE BAND IS COMPLETELY FILLED

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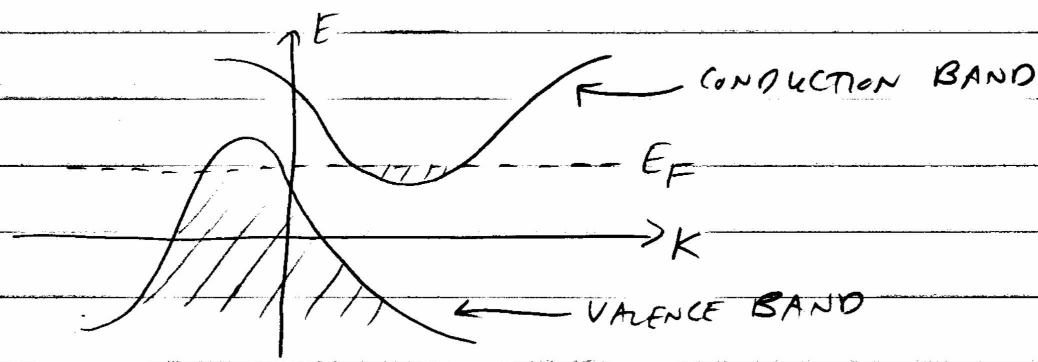
$$\left.\frac{\partial E}{\partial k}\right|_{k=k_F} = 0 \quad (\text{i.e., } n_{eff} = 0)$$

$$\Downarrow$$

NO CONDUCTIVITY FROM FILLED BANDS

$\therefore$ THE ALIGNMENT OF THE FERMI LEVEL W.R.T. THE BANDSTRUCTURE DICTATES IF A MATERIAL WILL BE AN INSULATOR OR CONDUCTOR AT $T=0\,K$.

CONSIDER THE FOLLOWING CASE AT $T=0\,K$:



A MATERIAL WITH OVERLAPPING BANDS AT E_F IS KNOWN AS A SEMIMETAL.

IN THIS CASE, THE CONDUCTION BAND IS NEARLY EMPTY, AND CHARGE TRANSPORT BEHAVES NORMALLY WITH A CLEARLY DEFINED POSITIVE EFFECTIVE MASS FOR THE ELECTRONS.

HOWEVER, THE VALENCE BAND IS NEARLY FULL. HOW DO WE DESCRIBE CHARGE TRANSPORT IN THIS CASE?

ASSUME THAT THERE ARE i FILLED STATES.

$$\therefore \frac{dI}{dt} = \sum_i \frac{e^2 \mathcal{E}}{m_i^*}, \quad m_i^* = \hbar^2 \left(\frac{\partial^2 E}{\partial k^2} \right)^{-1} \Bigg|_{k=k_i}$$

SINCE THE VALENCE BAND IS NEARLY FULL, THIS SUM IS DIFFICULT TO CALCULATE SINCE m_i^* WILL VARY SIGNIFICANTLY AS A FUNCTION OF k.

HOWEVER, CONSIDER THE j EMPTY STATES IN THE VALENCE BAND. IN PARTICULAR, IF THE BAND WERE COMPLETELY FULL, $\frac{dI}{dt} = 0$

$$\therefore e^2 \mathcal{E} \left(\sum_i \frac{1}{m_i^*} + \sum_j \frac{1}{m_j^*} \right) = 0$$

$$\Rightarrow \sum_i \frac{1}{m_i^*} = - \sum_j \frac{1}{m_j^*}$$

$$\therefore \frac{dI}{dt} = -e^2 \mathcal{E} \sum_j \frac{1}{m_j^*}$$

SINCE THE EFFECTIVE MASS IS NEGATIVE NEAR THE TOP OF THE BAND,

$$\frac{dI}{dt} = e^2 \mathcal{E} \sum_j \frac{1}{|m_j^*|}$$

$\therefore$ IT IS EQUIVALENT TO CONSIDER MISSING ELECTRONS NEAR THE TOP OF A BAND AS POSITIVE CHARGE CARRIERS WITH POSITIVE EFFECTIVE MASS $\Rightarrow$ $\boxed{\text{HOLES}}$

$\therefore$ IN SEMIMETALS, THERE ARE TWO CHARGE CARRIERS:

(1) ELECTRONS FROM THE PARTIALLY FILLED CONDUCTION BAND

(2) HOLES FROM THE PARTIALLY EMPTY VALENCE BAND.

SO FAR, WE HAVE ONLY CONSIDERED ELECTRICAL PROPERTIES AT $T=0K$.

WHAT HAPPENS AT FINITE TEMPERATURES?

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THE FERMI-DIRAC DISTRIBUTION IS BROADENED.

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MATERIALS WITH NARROW BAND GAPS AT THE FERMI LEVEL WILL HAVE PARTIALLY FILLED AND PARTIALLY EMPTY BANDS AT FINITE TEMPERATURES $\Rightarrow$ $\boxed{\text{SEMICONDUCTORS}}$

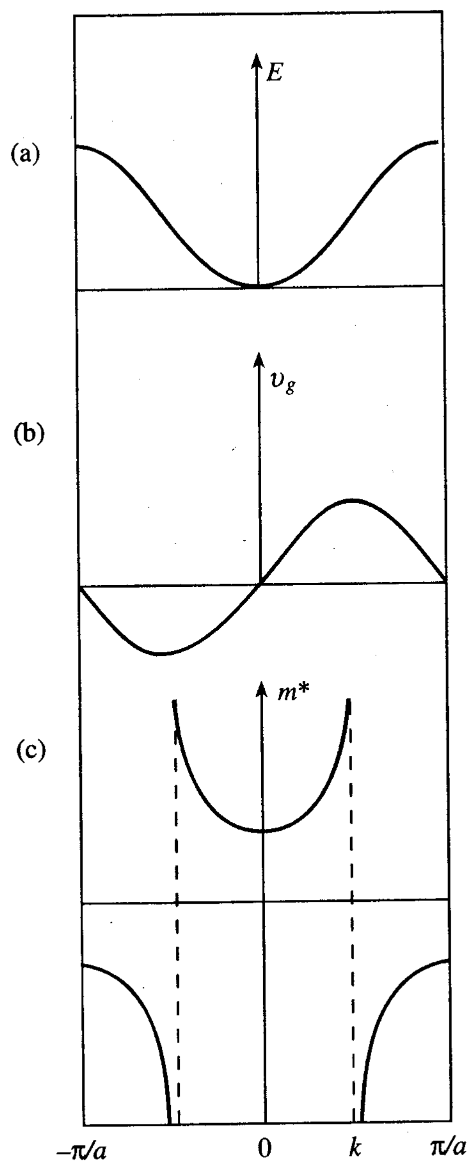

Fig. 7.12
Energy, group velocity, and effective mass as a function of k.