Electronic properties of solids - Electrons, holes and density of states

Lecture 16

CHM 637
Chemistry & Physics of Materials

Varadharajan Srinivasan
Dept. Of Chemistry
IISER Bhopal

Lecture Plan

- Electrons, holes and density of states in semiconductors

Band structures

Density of states : $g(\mathcal{E})$

$g(\mathcal{E})\,d\mathcal{E}$ is the no. of electronic states lying between $\mathcal{E}$ and $\mathcal{E} + d\mathcal{E}$ per unit volume of crystal

Total electronic energy of a solid per unit volume:

$$\overline{E} = 2 \sum_n \int_{B.Z} \frac{d^3k}{(2\pi)^3} \, \overbrace{\varepsilon_n(\vec{k}) \, \underbrace{f(\varepsilon_n(\vec{k}))}_{\substack{\text{occupation funct} \\ \Theta(\varepsilon_n(\vec{k}) - \varepsilon_F)}}}^{p(\varepsilon)}$$

$$= \int_{\varepsilon_{min}}^{\varepsilon_{max}} d\varepsilon \, f(\varepsilon) \, \varepsilon \times \overbrace{\left(2 \sum_n \int \frac{d^3k}{(2\pi)^3} \, \delta(\varepsilon - \varepsilon_n(\vec{k})) \right)}^{g(\varepsilon)}$$

$$g(\varepsilon) \equiv \overset{\text{spin}}{2} \sum_{n} \int_{B.Z.} \frac{d^3k}{(2\pi)^3}\, \delta(\varepsilon - \varepsilon_n(\vec{k}))$$

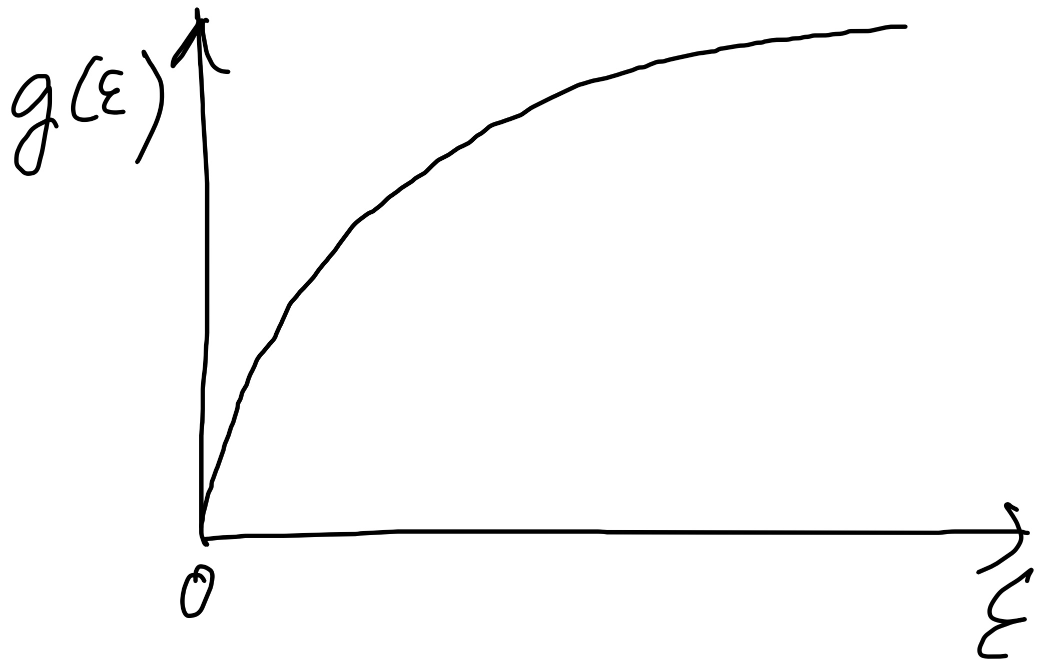
→ Density of states

E.g. 3-d free e^- gas:

$$\varepsilon(\vec{k}) = \hbar^2 k^2 / 2m$$

$$g(\varepsilon) = 2 \int \frac{d^3k}{(2\pi)^3}\, \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) = \frac{4\pi \times 2}{(2\pi)^3} \int k^2 dk\, \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right)$$

$$= \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{\varepsilon} \quad , \quad \varepsilon > 0$$



e.g. TB model in 1-d w/ 1-band

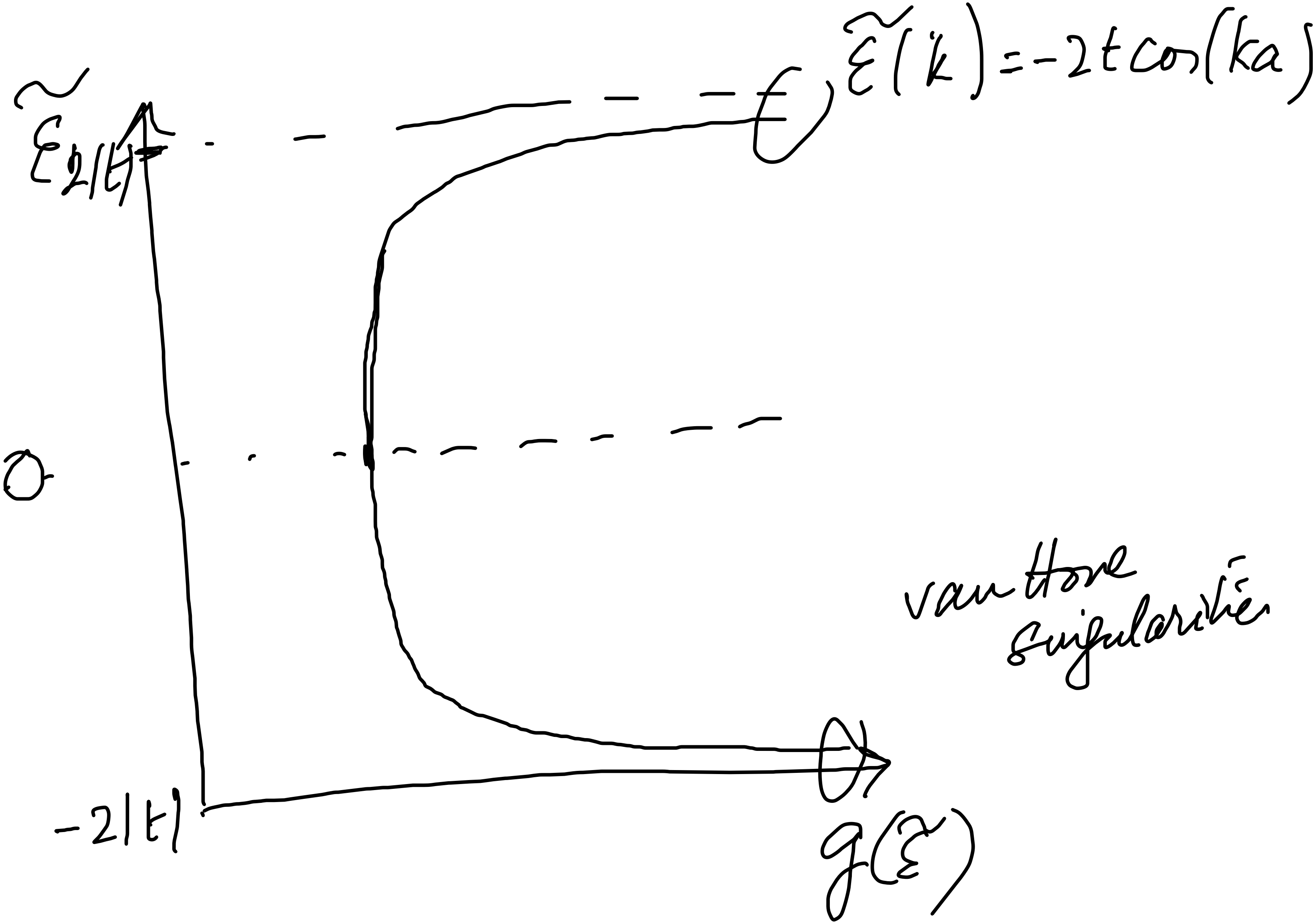
$$\mathcal{E}(\vec{k}) = \mathcal{E}_0 - 2|t|\cos(ka)$$

$$\tilde{\mathcal{E}}(\vec{k}) = \mathcal{E}(\vec{k}) - \mathcal{E}_0 = -2|t|\cos(ka).$$

$$\int \frac{dk}{2\pi}\,\delta\big(E - \tilde{\mathcal{E}}(k)\big) = \frac{1}{2\pi}\int \left|\frac{dk}{d\tilde{\mathcal{E}}}\right| \delta(E - \tilde{\mathcal{E}})\,d\tilde{\mathcal{E}}$$

$$\left|\frac{dk}{d\tilde{\mathcal{E}}}\right| \to \frac{1}{a}\frac{1}{\sqrt{4t^2 - \tilde{\mathcal{E}}^2}}$$

$$\boxed{g(\mathcal{E}) = \frac{1}{\pi a}\frac{1}{\sqrt{4t^2 - \tilde{\mathcal{E}}^2}}}$$

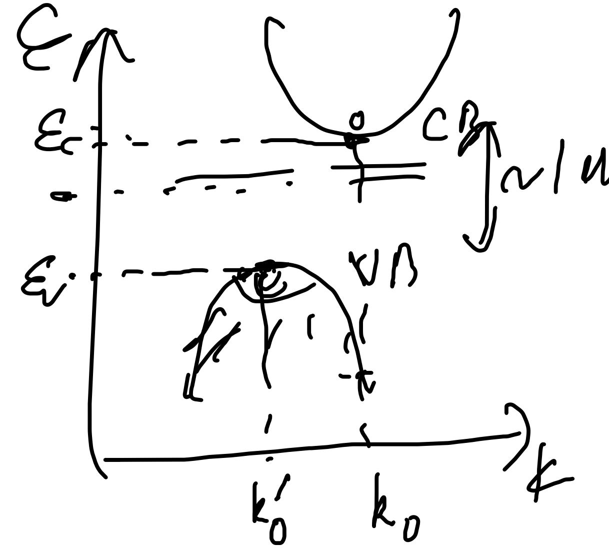


$\tilde{\varepsilon}(k) = -2t\cos(ka)$
$\tilde{\varepsilon}$
$2|t|$
0
$-2|t|$
van Hove singularities
$g(\tilde{\varepsilon})$

$$\hbar \frac{d\vec{k}}{dt} = -e\left(\vec{E} + \vec{v}_n \times \vec{B}\right)$$

$$\Rightarrow \vec{v}_n = \frac{1}{\hbar} \nabla_{\vec{k}} \mathcal{E}_n(\vec{k})$$

Semi-classical eqns of motion



$$\mathcal{E}_n(\vec{k} + \vec{G}) = \mathcal{E}_n(\vec{k})$$

CBM

$$\mathcal{E}_n(\vec{k}) \simeq \mathcal{E}_c + \frac{1}{2}\sum_i \sum_j (k_i - k_0) \left.\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_i \partial k_j}\right|_{\vec{k}_0} (k_j - k_0)$$

$$= \mathcal{E}_c + \frac{\hbar^2}{2}\sum_i \sum_j (k_i - k_0)\left(\frac{1}{\overleftrightarrow{m}_e^*}\right)_{ij}(k_j - k_0) + O(k^3)$$

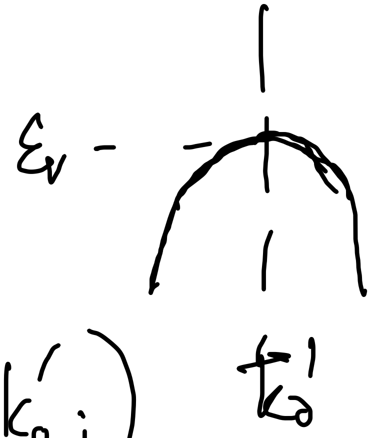
$$\left(\frac{1}{\overleftrightarrow{m}_e^*}\right)_{ij} = \frac{1}{\hbar^2}\left(\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_i \, \partial k_j}\right)_{\vec{k}_0}$$

effective mass tensor. $\rightarrow$ m_1, m_2, m_3

$$\boxed{\overleftrightarrow{m}_e^* \cdot \frac{d\vec{v}_n}{dt} = -e\left(\vec{E} + \vec{v}_n \times \vec{B}\right)}$$

VBM:

$$\mathcal{E}_n(\vec{k}) = \mathcal{E}_v + \frac{1}{2}\sum_{i,j}(k_i - k'_{0,i}) \left.\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_i \partial k_j}\right|_{\vec{k}_0'} (k_j - k'_{0,j})$$



$$\equiv \mathcal{E}_v - \frac{\hbar^2}{2}\sum_{i,j}(k_i - k'_{0,i})\left(\frac{1}{\overleftrightarrow{m}^*_h}\right)_{ij}(k_j - k'_{0,j})$$

where $$\left(\frac{1}{\overleftrightarrow{m}^*_h}\right)_{i,j} = -\frac{1}{\hbar^2}\left(\frac{\partial^2 \mathcal{E}_{nk}(\vec{k})}{\partial k_i \partial k_j}\right)_{\vec{k}_0'}$$

$$\overleftrightarrow{m}_h^* \cdot \frac{d\vec{v}_n}{dt} = (+e)\left(\vec{E} + \vec{v}_n \times \vec{B}\right) \to \text{holes}$$

$$\vec{m}_e^* \cdot \frac{d\vec{v}_n}{dt} = \underline{-e}\left(\vec{E} + \vec{v}_n \times \vec{B}\right) \to \text{electrons}$$

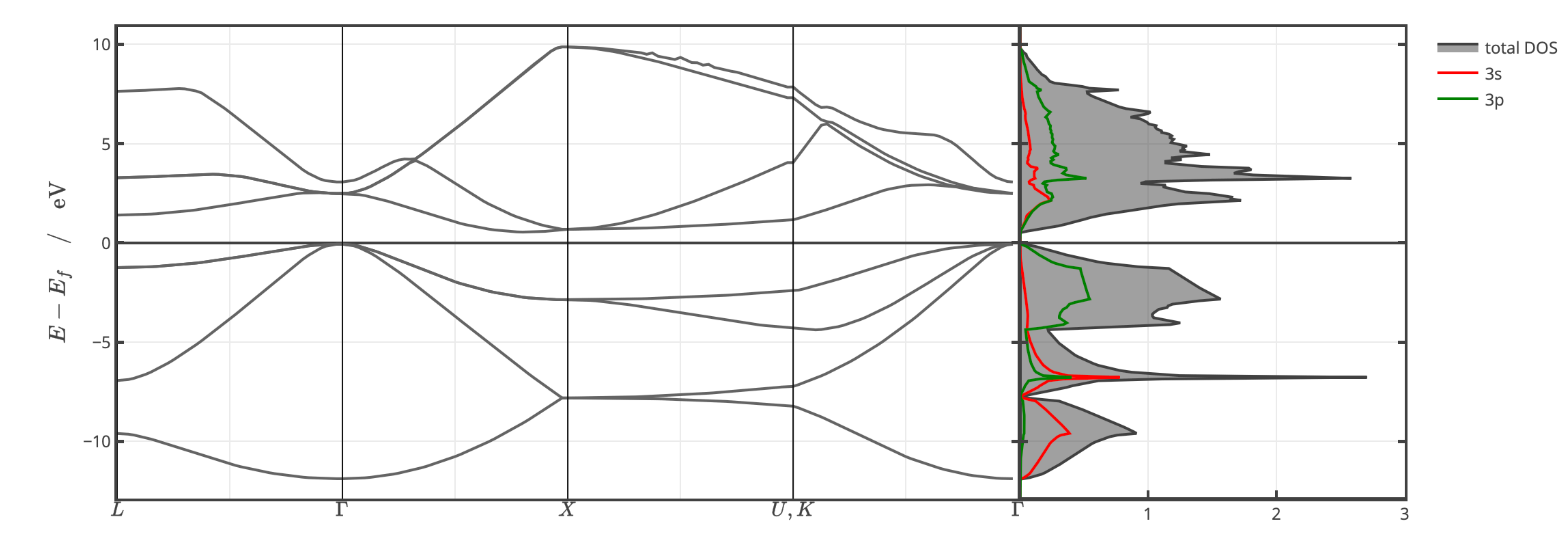
$$\overleftrightarrow{m}_e^* \cdot \left(\frac{d\vec{v}_e}{dt} + \frac{1}{\overleftrightarrow{\tau}_e} \cdot \vec{v}_e\right) = -e\left(\vec{E} + \vec{v}_e \times \vec{B}\right)$$

$$\overleftrightarrow{m}_h^* \cdot \left(\frac{d\vec{v}_h}{dt} + \frac{1}{\overleftrightarrow{\tau}_h} \cdot \vec{v}_h\right) = +e\left(\vec{E} + \vec{v}_h \times \vec{B}\right)$$

$$\boxed{\overleftrightarrow{\sigma} = e^2 \left(\underbrace{n_h \overleftrightarrow{\tau}_h \cdot \frac{1}{\overleftrightarrow{m}_h^*}} + n_e \overleftrightarrow{\tau}_e \cdot \frac{1}{\overleftrightarrow{m}_e^*} \right)}$$

$$\vec{J} = \underbrace{\overleftrightarrow{\sigma}} \cdot \vec{E}$$

Density of states



Source: https://plotly.com/python/v3/ipython-notebooks/density-of-states/