Handout 13

Properties of Electrons in Energy Bands

In this lecture you will learn:

- Properties of Bloch functions
- Average momentum and velocity of electrons in energy bands
- Energy band dispersion near band extrema
- Effective mass tensor
- Crystal momentum

Bloch Functions: A Review

1) The quantum states of an electron in a crystal are given by Bloch functions that obey the Schrodinger equation:

$$\hat{H}\,\psi_{n,\vec{k}}(\vec{r}) = E_n(\vec{k})\,\psi_{n,\vec{k}}(\vec{r})$$

where the wavevector $\vec{k}$ is confined to the FBZ and "n" is the band index

2) Under a lattice translation, Bloch functions obey the relation:

$$\psi_{n,\vec{k}}(\vec{r}+\vec{R}) = e^{i\,\vec{k}\,.\,\vec{R}}\,\psi_{n,\vec{k}}(\vec{r})$$

3) Bloch functions can be written as the product of a plane wave times a lattice periodic function:

$$\psi_{n,\vec{k}}(\vec{r}) = \frac{e^{i\,\vec{k}\,.\,\vec{r}}}{\sqrt{V}}\,u_{n,\vec{k}}(\vec{r})$$

4) Bloch function of wavevector $\vec{k}$ can be written as a superposition of plane waves with wavevectors that differ from $\vec{k}$ by reciprocal lattice vectors:

$$\psi_{n,\vec{k}}(\vec{r}) = \sum_j c_{n,\vec{k}}(\vec{G}_j)\sqrt{\frac{1}{V}}\,e^{i\,(\vec{k}+\vec{G}_j)\,.\,\vec{r}}$$

Bloch Functions: Orthogonality and Completeness

Orthogonality:

Bloch functions are eigenstates of a Hermitian operator and therefore must be orthogonal. In "*d*" dimensions:

$$\int d^d\vec{r}\ \ \psi^*_{n,\vec{k}}(\vec{r})\,\psi_{m,\vec{k}'}(\vec{r}) = \delta_{\vec{k},\vec{k}'}\ \ \delta_{n,m}$$

$$= \frac{(2\pi)^d}{V}\,\delta^d\left(\vec{k}-\vec{k}'\right)\ \delta_{n,m}$$

Both expression valid depending upon context

Completeness:

Bloch functions for ALL wavevectors in the FBZ and for ALL energy band satisfy the following completeness relation in "*d*" dimensions:

$$\sum_n \sum_{\vec{k}\,\text{in FBZ}} \psi_{n,\vec{k}}(\vec{r})\,\psi^*_{n,\vec{k}}(\vec{r}') = \sum_n V \int_{\text{FBZ}} \frac{d^d\vec{k}}{(2\pi)^d}\ \psi_{n,\vec{k}}(\vec{r})\,\psi^*_{n,\vec{k}}(\vec{r}') = \delta^d(\vec{r}-\vec{r}')$$

Another Schrodinger-like Equation for Bloch Functions

The periodic part of a Bloch function satisfies a Schrodinger-like equation:

$$\hat{H}\,\psi_{n,\vec{k}}(\vec{r}) = E_n(\vec{k})\,\psi_{n,\vec{k}}(\vec{r})$$

$$\Rightarrow \left(\frac{\hat{\vec{P}}^2}{2m} + V(\hat{\vec{r}})\right)\psi_{n,\vec{k}}(\vec{r}) = E_n(\vec{k})\,\psi_{n,\vec{k}}(\vec{r})$$

$$\Rightarrow\ e^{i\vec{k}\cdot\vec{r}}\left(\frac{\left(\hat{\vec{P}}+\hbar\vec{k}\right)^2}{2m} + V(\hat{\vec{r}})\right)u_{n,\vec{k}}(\vec{r}) = E_n(\vec{k})\ e^{i\vec{k}\cdot\vec{r}}\,u_{n,\vec{k}}(\vec{r})$$

$$\Rightarrow \left(\frac{\left(\hat{\vec{P}}+\hbar\vec{k}\right)^2}{2m} + V(\hat{\vec{r}})\right)u_{n,\vec{k}}(\vec{r}) = E_n(\vec{k})\,u_{n,\vec{k}}(\vec{r})$$

Result:

$$\Rightarrow \left(\frac{\hat{\vec{P}}^2}{2m} + \frac{\hat{\vec{P}}}{m}\cdot\hbar\vec{k} + \frac{\hbar^2k^2}{2m} + V(\hat{\vec{r}})\right)u_{n,\vec{k}}(\vec{r}) = E_n(\vec{k})\,u_{n,\vec{k}}(\vec{r})$$

Where the following two relations have been used:

$$\hat{\vec{P}}\ e^{i\vec{k}\cdot\vec{r}}\ f(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\left(\hat{\vec{P}}+\hbar\vec{k}\right)f(\vec{r})$$

$$\hat{\vec{P}}^2\ e^{i\vec{k}\cdot\vec{r}}\ f(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\left(\hat{\vec{P}}+\hbar\vec{k}\right)^2 f(\vec{r})$$

Bloch Functions and Electron Momentum

• For an electron with wavefunction given by a plane wave:

$$\phi_{\vec{k}}(\vec{r}) = \sqrt{\frac{1}{V}}\, e^{i\,\vec{k}\,.\,\vec{r}}$$

the quantity $\hbar\vec{k}$ is the momentum of the electron

• A plane wave is an eigenfunction of the momentum operator with eigenvalue $\hbar\vec{k}$:

$$\hat{\vec{P}}\,\phi_{\vec{k}}(\vec{r}) = \frac{\hbar}{i}\nabla\,\phi_{\vec{k}}(\vec{r}) = \hbar\vec{k}\,\phi_{\vec{k}}(\vec{r})$$

• A Bloch function is a superposition of plane waves of different wavevectors:

$$\psi_{n,\vec{k}}(\vec{r}) = \sum_j c_{n,\vec{k}}\left(\vec{G}_j\right)\sqrt{\frac{1}{V}}\, e^{i\left(\vec{k}+\vec{G}_j\right).\vec{r}}$$

So clearly it is not an eigenfunction of the momentum operator (i.e. it has no well defined momentum). So what exactly is the significance of the wavevector $\vec{k}$ that labels a Bloch function?

• As you will see, even the average momentum of an electron in a Bloch state is NOT given by $\hbar\vec{k}$:

$$\left\langle \psi_{n,\vec{k}} \middle| \hat{\vec{P}} \middle| \psi_{n,\vec{k}} \right\rangle = \int d^d\vec{r}\;\; \psi^*_{n,\vec{k}}(\vec{r})\,\frac{\hbar}{i}\nabla\,\psi_{n,\vec{k}}(\vec{r}) \neq \hbar\vec{k}$$

Average Momentum and Velocity of Bloch States

We need to find the average momentum and average velocity of an electron in a Bloch state:

$$\left\langle \psi_{n,\vec{k}} \middle| \hat{\vec{P}} \middle| \psi_{n,\vec{k}} \right\rangle = ? \qquad \vec{v}_n\left(\vec{k}\right) = \left\langle \psi_{n,\vec{k}} \middle| \frac{\hat{\vec{P}}}{m} \middle| \psi_{n,\vec{k}} \right\rangle = ?$$

Start from a very different point:

Suppose we have solved the Schrodinger-like equation for a particular wavevector $\vec{k}$:

$$\left(\frac{\hat{\vec{P}}^2}{2m} + \frac{\hat{\vec{P}}}{m}.\,\hbar\vec{k} + \frac{\hbar^2k^2}{2m} + V\left(\hat{\vec{r}}\right)\right) u_{n,\vec{k}}(\vec{r}) = E_n\left(\vec{k}\right) u_{n,\vec{k}}(\vec{r})$$

The "Hamiltonian" is:

$$\hat{H}_{\vec{k}} = \frac{\hat{\vec{P}}^2}{2m} + \frac{\hat{\vec{P}}}{m}.\,\hbar\vec{k} + \frac{\hbar^2k^2}{2m} + V\left(\hat{\vec{r}}\right)$$

Suppose now we want to solve it again for a neighboring wavevector $\vec{k}+\Delta\vec{k}$:

$$\left(\frac{\hat{\vec{P}}^2}{2m} + \frac{\hat{\vec{P}}}{m}.\,\hbar\left(\vec{k}+\Delta\vec{k}\right) + \frac{\hbar^2\left(\vec{k}+\Delta\vec{k}\right)^2}{2m} + V\left(\hat{\vec{r}}\right)\right) u_{n,\vec{k}+\Delta\vec{k}}(\vec{r}) = E_n\left(\vec{k}+\Delta\vec{k}\right) u_{n,\vec{k}+\Delta\vec{k}}(\vec{r})$$

Average Momentum and Velocity of Bloch States

The new "Hamiltonian" is:

$$\hat{H}_{\vec{k}+\Delta\vec{k}} = \frac{\hat{\vec{P}}^2}{2m} + \frac{\hat{\vec{P}}}{m}.\hbar\left(\vec{k}+\Delta\vec{k}\right) + \frac{\hbar^2\left(\vec{k}+\Delta\vec{k}\right)^2}{2m} + V\left(\hat{\vec{r}}\right)$$

$$= \hat{H}_{\vec{k}} + \underbrace{\frac{\hat{\vec{P}}}{m}.\hbar\Delta\vec{k} + \frac{\hbar^2\left(2\vec{k}.\Delta\vec{k}+\Delta k^2\right)}{2m}}_{\text{Treat this part as a perturbation to the old "Hamiltonian"}} = \hat{H}_{\vec{k}} + \Delta\hat{H}_{\vec{k}}$$

Using concepts from time-independent perturbation theory, the first order correction to the energy eigenvalue would be:

$$E_n\left(\vec{k}+\Delta\vec{k}\right) - E_n\left(\vec{k}\right) \approx \left\langle u_{n,\vec{k}} \middle| \Delta\hat{H}_{\vec{k}} \middle| u_{n,\vec{k}} \right\rangle$$

As written, the above expression is approximate but becomes exact in the limit $\Delta\vec{k} \to 0$

$$\lim \Delta\vec{k} \to 0: \quad E_n\left(\vec{k}+\Delta\vec{k}\right) - E_n\left(\vec{k}\right) = \left\langle u_{n,\vec{k}} \middle| \Delta\hat{H}_{\vec{k}} \middle| u_{n,\vec{k}} \right\rangle$$

$$\Rightarrow \quad \Delta\vec{k}.\nabla_{\vec{k}} E_n\left(\vec{k}\right) = \left\langle u_{n,\vec{k}} \middle| \frac{\hat{\vec{P}}}{m}.\hbar\Delta\vec{k} + \frac{\hbar\vec{k}}{m}.\hbar\Delta\vec{k} \middle| u_{n,\vec{k}} \right\rangle$$

$$\Rightarrow \quad \frac{1}{\hbar}\nabla_{\vec{k}} E_n\left(\vec{k}\right) = \left\langle u_{n,\vec{k}} \middle| \frac{\left(\hat{\vec{P}}+\hbar\vec{k}\right)}{m} \middle| u_{n,\vec{k}} \right\rangle$$

Average Momentum and Velocity of Bloch States

(Contd…)

$$\frac{1}{\hbar}\nabla_{\vec{k}} E_n\left(\vec{k}\right) = \left\langle u_{n,\vec{k}} \middle| \frac{\left(\hat{\vec{P}}+\hbar\vec{k}\right)}{m} \middle| u_{n,\vec{k}} \right\rangle = \int d^d\vec{r}\ \ u^*_{n,\vec{k}}\left(\vec{r}\right) \frac{\left(\hat{\vec{P}}+\hbar\vec{k}\right)}{m} u_{n,\vec{k}}\left(\vec{r}\right)$$

$$\Rightarrow \frac{1}{\hbar}\nabla_{\vec{k}} E_n\left(\vec{k}\right) = \int d^d\vec{r}\ \ e^{-i\vec{k}.\vec{r}} e^{i\vec{k}.\vec{r}}\ \ u^*_{n,\vec{k}}\left(\vec{r}\right) \frac{\left(\hat{\vec{P}}+\hbar\vec{k}\right)}{m} u_{n,\vec{k}}\left(\vec{r}\right)$$

$$\Rightarrow \frac{1}{\hbar}\nabla_{\vec{k}} E_n\left(\vec{k}\right) = \int d^d\vec{r}\ \ e^{-i\vec{k}.\vec{r}}\ u^*_{n,\vec{k}}\left(\vec{r}\right) \frac{\hat{\vec{P}}}{m} e^{i\vec{k}.\vec{r}}\ u_{n,\vec{k}}\left(\vec{r}\right)$$

$$\Rightarrow \frac{1}{\hbar}\nabla_{\vec{k}} E_n\left(\vec{k}\right) = \int d^d\vec{r}\ \ \psi^*_{n,\vec{k}}\left(\vec{r}\right) \frac{\hat{\vec{P}}}{m}\ \psi_{n,\vec{k}}\left(\vec{r}\right)$$

$$\Rightarrow \frac{1}{\hbar}\nabla_{\vec{k}} E_n\left(\vec{k}\right) = \left\langle \psi_{n,\vec{k}} \middle| \frac{\hat{\vec{P}}}{m} \middle| \psi_{n,\vec{k}} \right\rangle$$

⇒ The average momentum of an electron in a Bloch state is:

$$\left\langle \psi_{n,\vec{k}} \middle| \hat{\vec{P}} \middle| \psi_{n,\vec{k}} \right\rangle = \frac{m}{\hbar}\nabla_{\vec{k}} E_n\left(\vec{k}\right)$$

⇒ The average velocity of an electron in a Bloch state is:

$$\vec{v}_n\left(\vec{k}\right) = \left\langle \psi_{n,\vec{k}} \middle| \frac{\hat{\vec{P}}}{m} \middle| \psi_{n,\vec{k}} \right\rangle = \frac{1}{\hbar}\nabla_{\vec{k}} E_n\left(\vec{k}\right)$$

Average Momentum and Velocity of Bloch States: 1D Example

The average velocity of an electron in a Bloch state is given by:

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}}\, E_n(\vec{k})$$

Recall from E&M theory (ECE303) that the group velocity of a electric field wavepacket made of plane waves:

$$\vec{E}(\vec{r},t) = \hat{x}\int_{k_o-\Delta k}^{k_o+\Delta k}\frac{dk}{2\pi}\,A(k)\,e^{i\,k\,x}\,e^{-i\,\omega(k)\,t}$$

is given by:

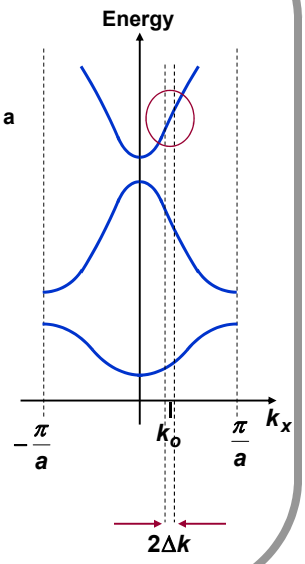
$$v_g(k_o) = \left.\frac{d\omega(k)}{dk}\right|_{k=k_o}$$

Similarly, the "group velocity" of an electron wavepacket made up of Bloch states from the *n*-th band:

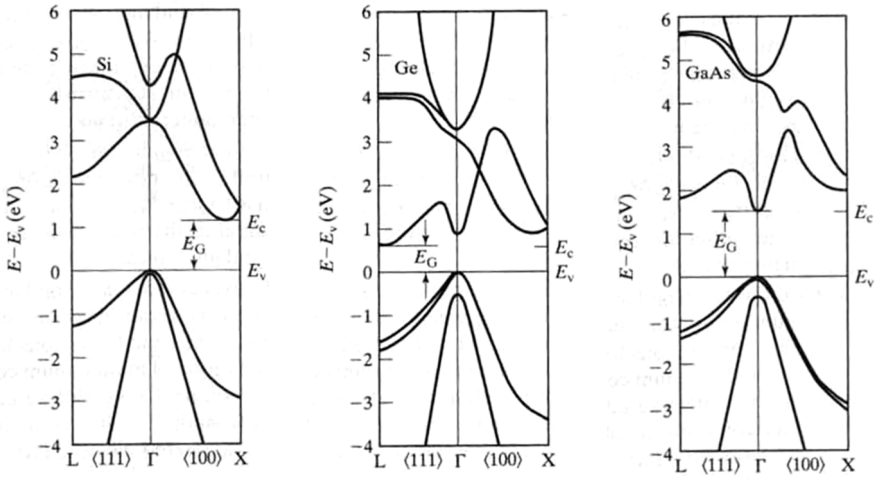
$$\psi(x,t) = \int_{k_o-\Delta k}^{k_o+\Delta k}\frac{dk}{2\pi}\,A(k)\quad \psi_{n,k}(x)\,e^{-i\frac{E_n(k)}{\hbar}t}$$

would be given by:

$$v_n(k_o) = \left.\frac{1}{\hbar}\frac{dE_n(k)}{dk}\right|_{k=k_o}$$



Energy Bands of Si, Ge, and GaAs for Reference



Energy Band Dispersion Near Band Extrema

Most of the times, it is useful to approximate the energy band dispersion near the band extrema (e.g. at bottom of the conduction band or at the top of the valence band)

Suppose the *n*-th band has an extrema at $\vec{k} = \vec{k}_o$. Therefore:

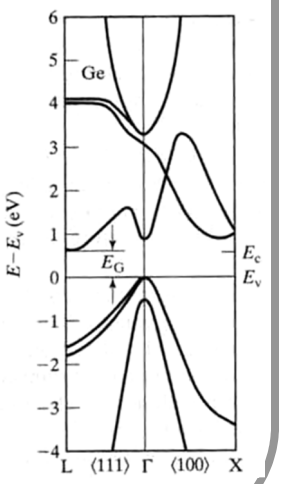
$$\nabla_{\vec{k}} E_n(\vec{k})\Big|_{\vec{k}=\vec{k}_o} = 0$$

$$\Rightarrow \left.\frac{dE_n(\vec{k})}{dk_x}\right|_{\vec{k}=\vec{k}_o} = \left.\frac{dE_n(\vec{k})}{dk_y}\right|_{\vec{k}=\vec{k}_o} = \left.\frac{dE_n(\vec{k})}{dk_z}\right|_{\vec{k}=\vec{k}_o} = 0$$

Now for $\vec{k}$ near $\vec{k}_o$ one can Taylor expand the energy dispersion relation:

$$E_n(\vec{k}) = E_n(\vec{k}_o) + \sum_{j=x,y,z} (\vec{k}-\vec{k}_o)_j \underbrace{\frac{dE_n(\vec{k})}{dk_j}}_{0} + \frac{1}{2}\sum_{\substack{r=x,y,z \\ j=x,y,z}} (\vec{k}-\vec{k}_o)_r \frac{d^2E_n(\vec{k})}{dk_r dk_j}(\vec{k}-\vec{k}_o)_j + ...$$

$$E_n(\vec{k}) = E_n(\vec{k}_o) + \frac{1}{2}\sum_{\substack{r=x,y,z \\ j=x,y,z}} (\vec{k}-\vec{k}_o)_r \frac{d^2E_n(\vec{k})}{dk_r dk_j}(\vec{k}-\vec{k}_o)_j + ...$$



Effective Mass Tensor

$$E_n(\vec{k}) = E_n(\vec{k}_o) + \frac{1}{2}\sum_{\substack{r=x,y,z \\ j=x,y,z}} (\vec{k}-\vec{k}_o)_r \left.\frac{d^2E_n(\vec{k})}{dk_r dk_j}\right|_{\vec{k}=\vec{k}_o} (\vec{k}-\vec{k}_o)_j + ...$$

$$E_n(\vec{k}) = E_n(\vec{k}_o) + \frac{\hbar^2}{2}\sum_{\substack{r=x,y,z \\ j=x,y,z}} (\vec{k}-\vec{k}_o)_r M_{rj}^{-1} (\vec{k}-\vec{k}_o)_j + ...$$

Parabolic approximation

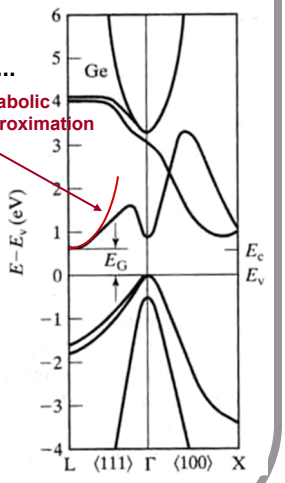
Where the elements of the matrix M^{-1} are defined as:

$$M_{rj}^{-1} = \frac{1}{\hbar^2}\left.\frac{d^2E_n(\vec{k})}{dk_r dk_j}\right|_{\vec{k}=\vec{k}_o}$$

M **is called the "effective mass" tensor.** M^{-1} **is the "inverse effective mass" tensor**

Note that M^{-1} **is symmetric:** $M_{rj}^{-1} = M_{jr}^{-1}$

And so ***M*** **is also symmetric:** $M_{rj} = M_{jr}$



Effective Mass Tensor and Electron Average Velocity

The energy band dispersion near a band extremum (e.g. at bottom of the conduction band or at the top of the valence band) can be written as:

$$E_n(\vec{k}) = E_n(\vec{k}_o) + \frac{\hbar^2}{2} \sum_{\substack{r=x,y,z \\ j=x,y,z}} (\vec{k}-\vec{k}_o)_r \, M^{-1}_{rj} \, (\vec{k}-\vec{k}_o)_j + ...$$

Or: $$E_n(\vec{k}) = E_n(\vec{k}_o) + \frac{\hbar^2}{2} \begin{bmatrix} k_x - k_{ox} & k_y - k_{oy} & k_z - k_{oz} \end{bmatrix} M^{-1} \begin{bmatrix} k_x - k_{ox} \\ k_y - k_{oy} \\ k_z - k_{oz} \end{bmatrix}$$

Or: $$E_n(\vec{k}) = E_n(\vec{k}_o) + \frac{\hbar^2}{2} (\vec{k}-\vec{k}_o)^T \, . \, M^{-1} \, . \, (\vec{k}-\vec{k}_o)$$

Equivalent ways of writing the same thing

Since the average velocity of an electron in a Bloch state is given by:

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar} \nabla_{\vec{k}} E_n(\vec{k})$$

Near a band extremum, we have:

$$\vec{v}_n(\vec{k}) = M^{-1} \, . \, \hbar (\vec{k}-\vec{k}_o) \qquad \text{Or :} \quad \vec{v}_n(\vec{k}) = M^{-1} \begin{bmatrix} \hbar (k_x - k_{ox}) \\ \hbar (k_y - k_{oy}) \\ \hbar (k_z - k_{oz}) \end{bmatrix}$$

Example: Conduction Band of GaAs

Consider the conduction band of GaAs near the band bottom at the Γ-point:

$$\vec{k}_o = 0 \qquad E_c(\vec{k}_o = 0) = E_c$$

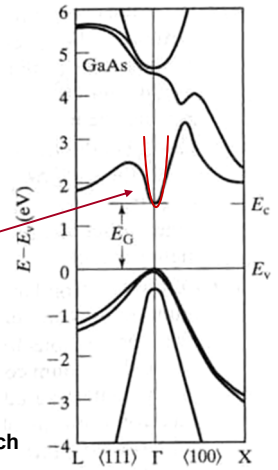
$$M^{-1} = \begin{bmatrix} 1/m_e & 0 & 0 \\ 0 & 1/m_e & 0 \\ 0 & 0 & 1/m_e \end{bmatrix}$$

Isotropic!

This implies the energy dispersion relation is:

$$E_c(\vec{k}) = E_c + \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2 m_e} = E_c + \frac{\hbar^2 k^2}{2 m_e}$$

Parabolic approximation



The dispersion looks like that of a free-electron with a mass equal to "m_e" instead of m. In GaAs, $m_e = .067\, m$

The average momentum and velocity of an electron in a Bloch state near the conduction band bottom is given by:

$$\langle \psi_{c,\vec{k}} | \hat{\vec{P}} | \psi_{c,\vec{k}} \rangle = \frac{m}{\hbar} \nabla_{\vec{k}} E_c(\vec{k}) = \left(\frac{m}{m_e} \right) \hbar \vec{k} \qquad \vec{v}_c(\vec{k}) = \frac{1}{\hbar} \nabla_{\vec{k}} E_c(\vec{k}) = \frac{\hbar \vec{k}}{m_e}$$

Example: Valence Band of GaAs – Heavy Hole Band

Consider the top most valence band (hh-band) of GaAs near the band maximum at the Γ-point:

$$\vec{k}_o = 0 \qquad E_{hh}(\vec{k}_o = 0) = E_v$$

$$M^{-1} = \begin{bmatrix} -1/m_{hh} & 0 & 0 \\ 0 & -1/m_{hh} & 0 \\ 0 & 0 & -1/m_{hh} \end{bmatrix}$$

Isotropic!

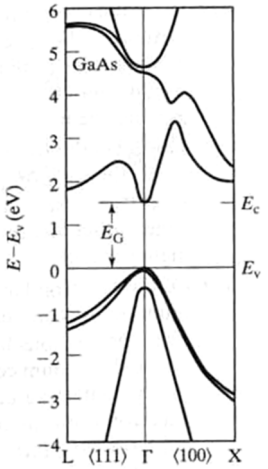
This implies:

$$E_{hh}(\vec{k}) = E_v - \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m_{hh}} = E_v - \frac{\hbar^2 k^2}{2m_{hh}}$$

The dispersion looks like that of a free-electron with a mass equal to "$-m_{hh}$" instead of m. In GaAs, $m_{hh} = .5\ m$

The average velocity of an electron in a Bloch state near the valence band maximum is given by:

$$\vec{v}_{hh}(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}} E_{hh}(\vec{k}) = -\frac{\hbar \vec{k}}{m_{hh}}$$



Example: Valence Band of GaAs – Light Hole Band

Now consider the top most valence band (ℓh-band) of GaAs near the band maximum at the Γ-point:

$$\vec{k}_o = 0 \qquad E_{\ell h}(\vec{k}_o = 0) = E_v$$

$$M^{-1} = \begin{bmatrix} -1/m_{\ell h} & 0 & 0 \\ 0 & -1/m_{\ell h} & 0 \\ 0 & 0 & -1/m_{\ell h} \end{bmatrix}$$

Isotropic!

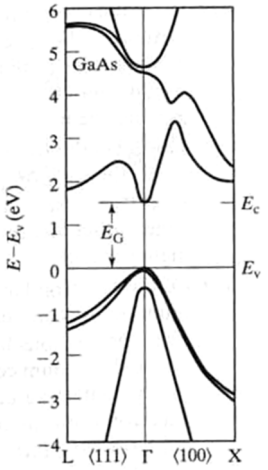
This implies:

$$E_{hh}(\vec{k}) = E_v - \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m_{\ell h}} = E_v - \frac{\hbar^2 k^2}{2m_{\ell h}}$$

The dispersion looks like that of a free-electron with a mass equal to "$-m_{\ell h}$" instead of m. In GaAs, $m_{\ell h} = .076\ m$

The average velocity of an electron in a Bloch state near the valence band maximum is given by:

$$\vec{v}_{\ell h}(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}} E_{\ell h}(\vec{k}) = -\frac{\hbar \vec{k}}{m_{\ell h}}$$



Example: Conduction Band of Silicon - I

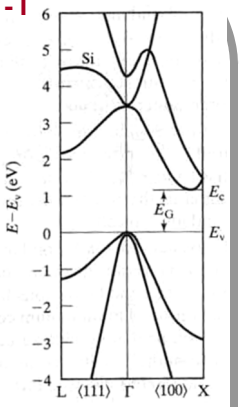
In Silicon there are six conduction band minima that occur along the six Γ-X directions. For the one that occurs along the Γ-X(2π/a,0,0) direction:

$$\vec{k}_o = 0.85\left(\frac{2\pi}{a},0,0\right) \qquad E_c(\vec{k}_o) = E_c$$

$$M^{-1} = \begin{bmatrix} 1/m_\ell & 0 & 0 \\ 0 & 1/m_t & 0 \\ 0 & 0 & 1/m_t \end{bmatrix}$$

Not isotropic!

$m_\ell = 0.92\ m$
$m_t = 0.19\ m$



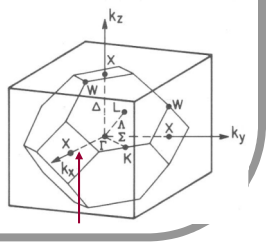
This implies:

$$E_c(\vec{k}) = E_c + \frac{\hbar^2(k_x - k_{ox})^2}{2m_\ell} + \frac{\hbar^2(k_y - k_{oy})^2}{2m_t} + \frac{\hbar^2(k_z - k_{oz})^2}{2m_t}$$

The average velocity of an electron in a Bloch state near the conduction band bottom is given by:

$$\vec{v}_c(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}} E_c(\vec{k})$$

$$= \frac{\hbar(k_x - k_{ox})}{m_\ell} + \frac{\hbar(k_y - k_{oy})}{m_t} + \frac{\hbar(k_z - k_{oz})}{m_t}$$



Example: Conduction Band of Silicon - II

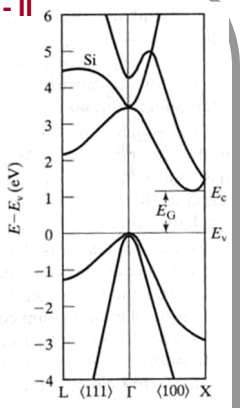
Now we look at the conduction band minimum that occurs along the Γ-X(0,2π/a,0) direction:

$$\vec{k}_o = 0.85\left(0,\frac{2\pi}{a},0\right) \qquad E_c(\vec{k}_o) = E_c$$

$$M^{-1} = \begin{bmatrix} 1/m_t & 0 & 0 \\ 0 & 1/m_\ell & 0 \\ 0 & 0 & 1/m_t \end{bmatrix}$$

Not isotropic!

$m_\ell = 0.92\ m$
$m_t = 0.19\ m$



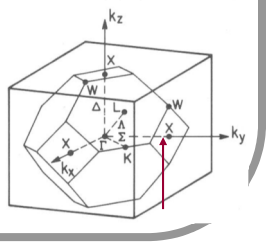
This implies:

$$E_c(\vec{k}) = E_c + \frac{\hbar^2(k_x - k_{ox})^2}{2m_t} + \frac{\hbar^2(k_y - k_{oy})^2}{2m_\ell} + \frac{\hbar^2(k_z - k_{oz})^2}{2m_t}$$

The average velocity of an electron in a Bloch state near the conduction band bottom is given by:

$$\vec{v}_c(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}} E_c(\vec{k})$$

$$= \frac{\hbar(k_x - k_{ox})}{m_t} + \frac{\hbar(k_y - k_{oy})}{m_\ell} + \frac{\hbar(k_z - k_{oz})}{m_t}$$



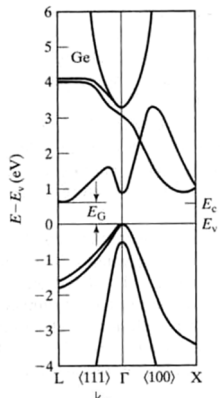
Example: Conduction Band of Germanium - I

In germanium there are eight conduction band minima that occur at the L-points. For the one that occurs at the L(π/a, π/a, π/a) point:

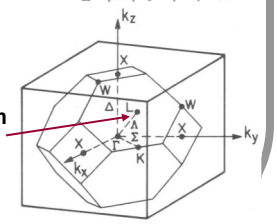
$$\vec{k}_o = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right) \qquad E_c(\vec{k}_o) = E_c$$

$$M^{-1} = \begin{bmatrix} 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t & 1/3m_\ell - 1/3m_t \\ 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t \\ 1/3m_\ell - 1/3m_t & 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t \end{bmatrix}$$

Not isotropic! Not even diagonal!
$m_\ell = 1.6\ m$
$m_t = 0.08\ m$



Since the inverse effective mass tensor is symmetric (it always is) one can rotate the co-ordinate system such that the inverse effective mass tensor is diagonal in the new co-ordinate system (Recall from linear algebra that a symmetric matrix can always be diagonalized by a rotation of the basis)



Example: Conduction Band of Germanium - II

Define a new rotated co-ordinate system, call it the primed co-ordinate system, in which the x'-axis points in the $(1,1,1)/\sqrt{3}$ direction. Co-ordinate rotation is accomplished by a rotation matrix R:

$$E_c(\vec{k}) = E_c + \frac{\hbar^2}{2}(\vec{k} - \vec{k}_o)^T . M^{-1} . (\vec{k} - \vec{k}_o)$$

$$\Rightarrow E_c(\vec{k}) = E_c + \frac{\hbar^2}{2}(\vec{k} - \vec{k}_o)^T . R^{-1} R M^{-1} R^{-1} R . (\vec{k} - \vec{k}_o)$$

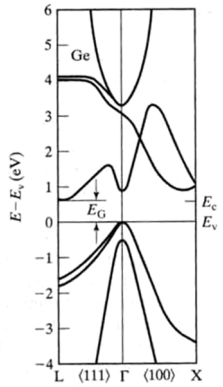
$$\Rightarrow E_c(\vec{k}) = E_c + \frac{\hbar^2}{2}\left[R . (\vec{k} - \vec{k}_o)\right]^T . R M^{-1} R^{-1} . \left[R . (\vec{k} - \vec{k}_o)\right]$$

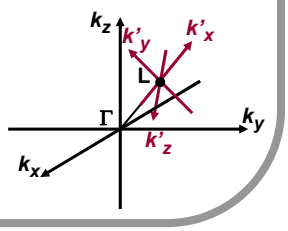
$$\Rightarrow E_c(\vec{k}') = E_c + \frac{\hbar^2}{2}(\vec{k}' - \vec{k}'_o)^T . M'^{-1} . (\vec{k}' - \vec{k}'_o)$$

$$M'^{-1} = \begin{bmatrix} 1/m_\ell & 0 & 0 \\ 0 & 1/m_t & 0 \\ 0 & 0 & 1/m_t \end{bmatrix}$$

In Ge:
$m_\ell = 1.6\ m$
$m_t = 0.08\ m$

Effective mass along the Γ-L direction is m_ℓ and in the two directions perpendicular to this direction it is m_t



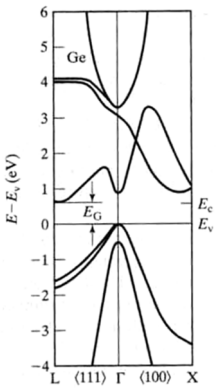


Example: Conduction Band of Germanium - III

In the primed (rotated) co-ordinate system, we have at the L-point:

$$E_c(\vec{k}') = E_c + \frac{\hbar^2}{2}(\vec{k}'-\vec{k}'_o)^T \,.\, M'^{-1} \,.\, (\vec{k}'-\vec{k}'_o)$$

$$\Rightarrow E_c(\vec{k}') = E_c + \frac{\hbar^2(k'_x-k'_{ox})^2}{2m_\ell} + \frac{\hbar^2(k'_y-k'_{oy})^2}{2m_t} + \frac{\hbar^2(k'_z-k'_{oz})^2}{2m_t}$$

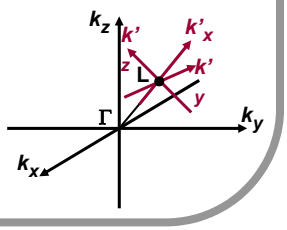


The average velocity of an electron in a Bloch state near the conduction band bottom is then given by:

$$\vec{v}_c(\vec{k}') = \frac{1}{\hbar}\nabla_{\vec{k}'} E_c(\vec{k}')$$

$$= \frac{\hbar(k'_x-k'_{ox})}{m_\ell} + \frac{\hbar(k'_y-k'_{oy})}{m_t} + \frac{\hbar(k'_z-k'_{oz})}{m_t}$$

Same procedure can be applied to the conduction band minima at the other L-points



Average Momentum and Crystal Momentum

The wavevector $\vec{k}$ associated with a Bloch state $\psi_{n,\vec{k}}(\vec{r})$ is not the momentum of the electron and it is not even the average momentum of the electron in the Bloch state

The average momentum of an electron in a Bloch state is given as:

$$\left\langle \psi_{n,\vec{k}} \left| \hat{\vec{P}} \right| \psi_{n,\vec{k}} \right\rangle = \frac{m}{\hbar}\nabla_{\vec{k}} E_n(\vec{k})$$

Near a band extrema, assuming:

$$E_n(\vec{k}) = E_n(\vec{k}_o) + \frac{\hbar^2}{2}(\vec{k}-\vec{k}_o)^T \,.\, M^{-1} \,.\, (\vec{k}-\vec{k}_o)$$

We have for the average momentum:

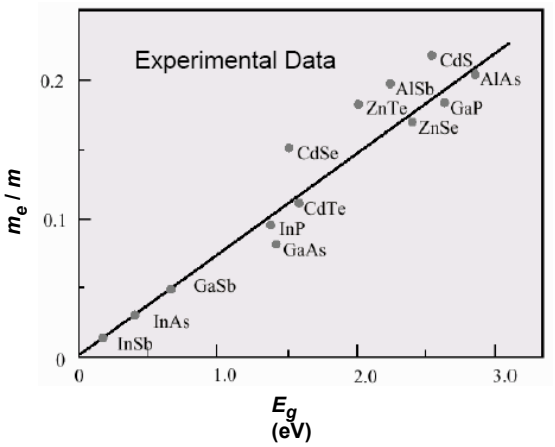
$$\left\langle \psi_{n,\vec{k}} \left| \hat{\vec{P}} \right| \psi_{n,\vec{k}} \right\rangle = m\, M^{-1} \,.\, \hbar(\vec{k}-\vec{k}_o)$$

Example: For GaAs conduction band, the average momentum of an electron near the band bottom equals:

$$\left\langle \psi_{n,\vec{k}} \left| \hat{\vec{P}} \right| \psi_{n,\vec{k}} \right\rangle = \left(\frac{m}{m_e}\right) \hbar\vec{k}$$

The quantity $\hbar\vec{k}$ is called the crystal momentum of an electron in an energy band. As we will see, it satisfies several conservation rules just like the actual momentum does for a free-electron.

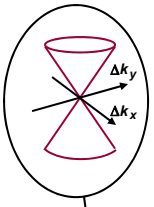
Effective Mass vs Bandgap



Energy Band Dispersion Near Band Extrema: When Taylor Expansion Fails

Graphene is a classical example of the case when Taylor expansion fails
So a different strategy is needed near band extrema

$$\begin{bmatrix} E_p & -V_{pp\pi} f(\vec{k}) \\ -V_{pp\pi} f^*(\vec{k}) & E_p \end{bmatrix} \begin{bmatrix} c_{pzA}(\vec{k}) \\ c_{pzB}(\vec{k}) \end{bmatrix} = E(\vec{k}) \begin{bmatrix} c_{pzA}(\vec{k}) \\ c_{pzB}(\vec{k}) \end{bmatrix}$$



Suppose one is interested in band dispersion near $\vec{k}_o = \vec{K} = \left(0, \frac{4\pi}{3a}\right)$

Expand the function $f(\vec{k})$ near $\vec{K}$ as follows:

$$\vec{k} = \vec{K} + \Delta\vec{k}$$

$$f(\vec{k} = \vec{K} + \Delta\vec{k}) = \left[e^{i\,\vec{k}.\vec{n}_1} + e^{i\,\vec{k}.\vec{n}_2} + e^{i\,\vec{k}.\vec{n}_3} \right]_{\vec{k}=\vec{K}+\Delta\vec{k}}$$

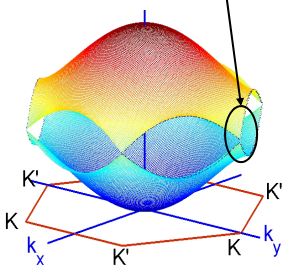
$$\approx i\frac{\sqrt{3}}{2} a \left[\Delta k_x + i\Delta k_y\right]$$

$$E(\vec{k} = \vec{K} + \Delta\vec{k}) = E_p \pm V_{pp\pi} \left| f(\vec{k} = \vec{K} + \Delta\vec{k}) \right|$$

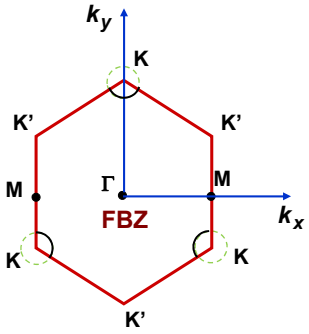
$$\approx E_p \pm \frac{\sqrt{3}}{2} a V_{pp\pi} \sqrt{\Delta k_x^2 + \Delta k_y^2}$$

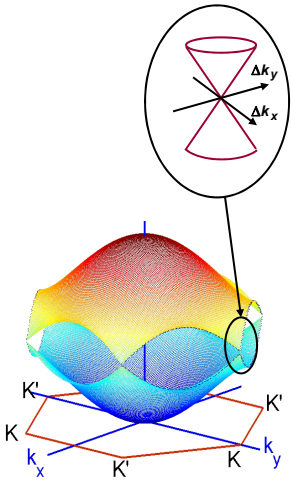
$$E(\vec{k} = \vec{K} + \Delta\vec{k}) \approx E_p \pm \hbar v \sqrt{\Delta k_x^2 + \Delta k_y^2}$$

$$v = \frac{\sqrt{3}}{2} \frac{a V_{pp\pi}}{\hbar} \approx 10^6 \text{ m/s}$$



Energy Band Dispersion Near Band Extrema





- There are 6 one-third cones sitting inside the FBZ

⇒ There are 2 full cones sitting inside the FBZ: one at the K-point and one at the K'-point

Energy Band Dispersion in Graphene: Massless Dirac Fermions

$$E_c\left(\vec{k}=\vec{K}+\Delta\vec{k}\right)\approx E_p+\hbar v\sqrt{\Delta k_x^2+\Delta k_y^2}$$ Conduction band dispersion

$$E_v\left(\vec{k}=\vec{K}+\Delta\vec{k}\right)\approx E_p-\hbar v\sqrt{\Delta k_x^2+\Delta k_y^2}$$ Valence band dispersion

The average velocity of an electron in a Bloch state near the conduction band bottom is then given by:

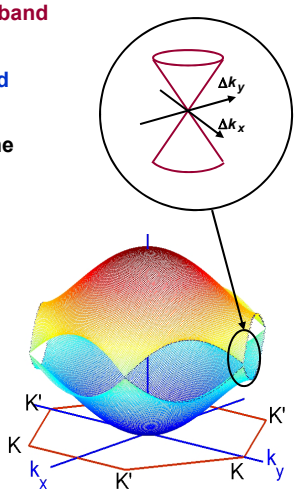
$$\vec{v}_c\left(\vec{k}\right)=\frac{1}{\hbar}\nabla_{\vec{k}}\,E_c\left(\vec{k}\right)=v\,\frac{\Delta k_x\hat{x}+\Delta k_y\hat{y}}{\sqrt{\Delta k_x^2+\Delta k_y^2}}$$

Similarly,

$$\vec{v}_v\left(\vec{k}\right)=\frac{1}{\hbar}\nabla_{\vec{k}}\,E_v\left(\vec{k}\right)=-v\,\frac{\Delta k_x\hat{x}+\Delta k_y\hat{y}}{\sqrt{\Delta k_x^2+\Delta k_y^2}}$$

Note that: $\left|\vec{v}_c\left(\vec{k}\right)\right|=\left|\vec{v}_v\left(\vec{k}\right)\right|=v\approx 10^6$ m/s

All electrons in the conduction band (and in the valence band as well) move with the same speed (i.e. magnitude of the velocity) !!



This is similar to how massless particles, such as photons, behave