ELECTRONS AND HOLES

Lecture 21

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Electrons and Holes

8 Electrons and Holes

8.1 Equations of motion

In one dimension, an electron with wave-vector k has group velocity

$$v = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{1}{\hbar}\frac{\mathrm{d}E}{\mathrm{d}k}. \tag{1}$$

If an electric field $\mathcal{E}$ acts on the electron, then in time δt it will do work

$$\delta E = \text{force times distance} = -e\mathcal{E}v\,\delta t. \tag{2}$$

But

$$\delta E = \frac{\mathrm{d}E}{\mathrm{d}k}\,\delta k = \hbar v\,\delta k, \tag{3}$$

so, comparing eq 2 with 3 we have

$$\delta k = -\frac{e\mathcal{E}}{\hbar}\delta t,$$

or

$$\hbar\frac{\mathrm{d}k}{\mathrm{d}t} = -e\mathcal{E}.$$

In terms of force, $\mathcal{F}$,

$$\hbar\frac{\mathrm{d}k}{\mathrm{d}t} = \mathcal{F}. \tag{4}$$

Generalising to three dimensions:

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

where

$$\nabla_{\mathbf{k}} = \hat{i}\frac{\mathrm{d}}{\mathrm{d}k_x} + \hat{j}\frac{\mathrm{d}}{\mathrm{d}k_y} + \hat{k}\frac{\mathrm{d}}{\mathrm{d}k_z},$$

and

$$\hbar\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} = \mathcal{F}.$$

Similarly, if there is a magnetic field acting,

$$\hbar\frac{\mathrm{d}k}{\mathrm{d}t} = -ev \times \mathcal{B},$$

or

$$\frac{\mathrm{d}k}{\mathrm{d}t} = -\frac{e}{\hbar^2}(\nabla_{\mathbf{k}}E) \times \mathcal{B}.$$

Remember that as k **moves in a direction *perpendicular* to the gradient of energy with respect to** k**, the electron stays on a surface of constant energy in** k**-space.**

8.2 Effective mass

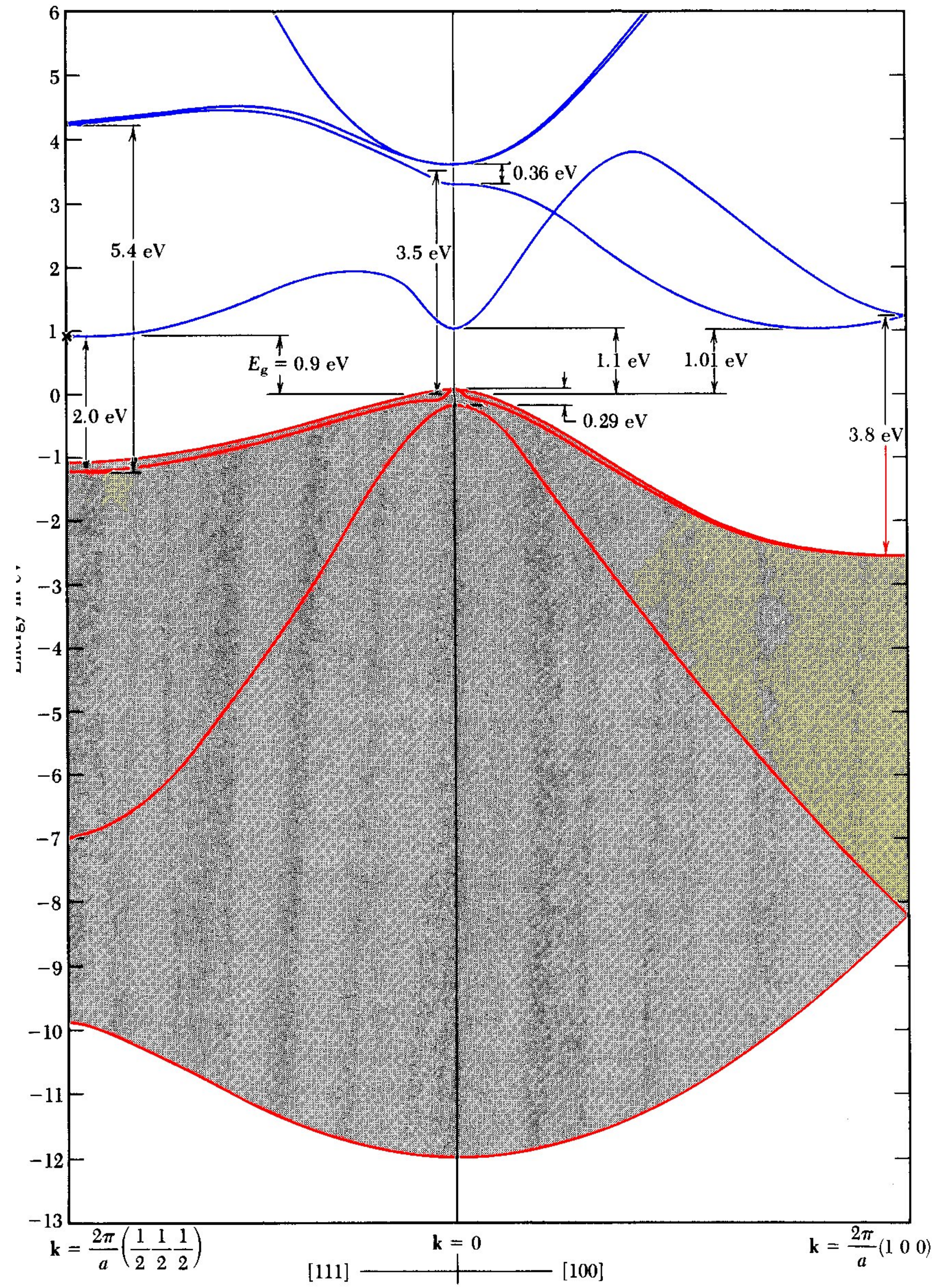
We saw in Lecture 20 that the energy near the bottom of a tight binding band could be written as

$$E(\mathbf{k}) \approx E_0 + A|\mathbf{k}|^2,$$

and near the top of the band (the corner of the Brillouin zone in our two-dimensional example) as

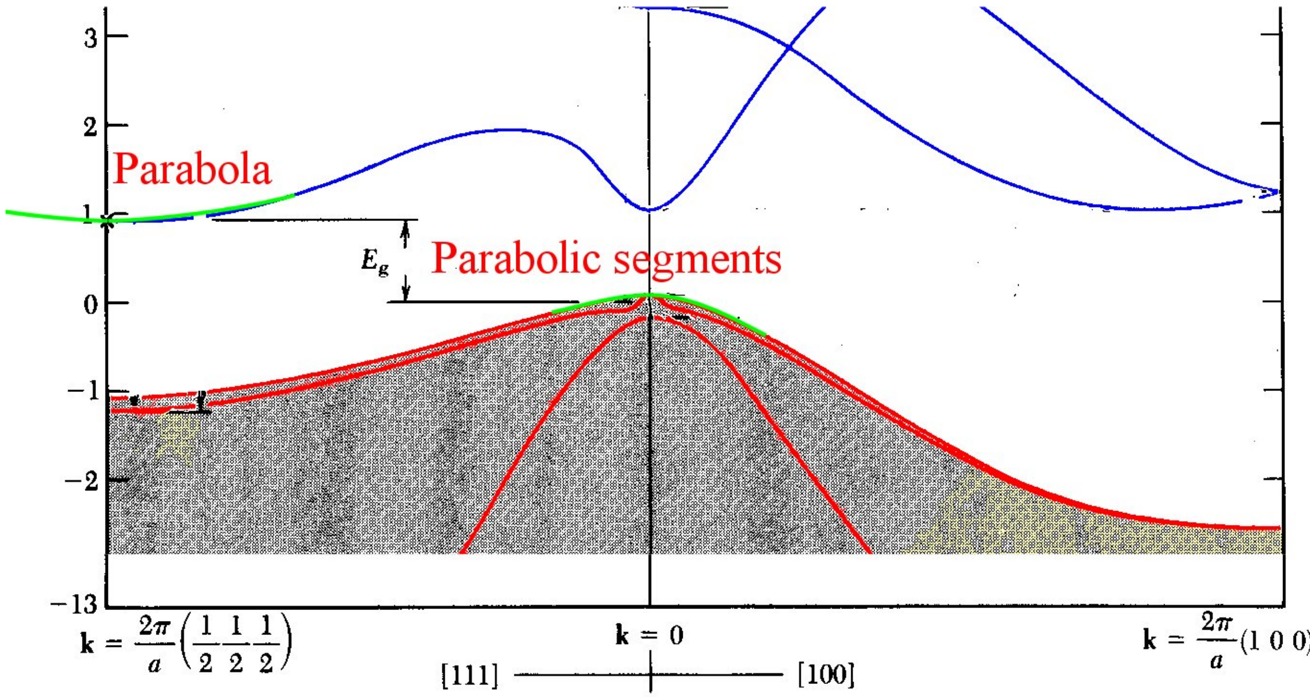
$$E(\mathbf{k}) \approx E_1 - B|\mathbf{k}_{\max} - \mathbf{k}|^2,$$

$\mathbf{k}_{\max}$ **being the** k **value where the energy was a maximum. We can see similar behaviour in more complicated band structures. For example, Germanium:**



We call the lower set of states, fully occupied at $T = 0$, the valence

band, and the upper set, empty at $T = 0$, the conduction band.



In a region close to the maxima and minima, a parabolic approximation can be accurate.

From equation 1

$$v = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{1}{\hbar}\frac{\mathrm{d}E}{\mathrm{d}k}, \tag{5}$$

differentiating with respect to time

$$\frac{\mathrm{d}v}{\mathrm{d}t} = \frac{1}{\hbar}\frac{\mathrm{d}^2E}{\mathrm{d}k\mathrm{d}t} = \frac{1}{\hbar}\frac{\mathrm{d}^2E}{\mathrm{d}k^2}\frac{\mathrm{d}k}{\mathrm{d}t}. \tag{6}$$

But from equation 4

$$\hbar\frac{\mathrm{d}k}{\mathrm{d}t} = \mathcal{F}, \tag{7}$$

so

$$\frac{\mathrm{d}v}{\mathrm{d}t} = \frac{1}{\hbar^2}\frac{\mathrm{d}^2E}{\mathrm{d}k^2}\mathcal{F}. \tag{8}$$

But from Newton's equation we expect

$$\frac{\mathrm{d}v}{\mathrm{d}t} = \frac{1}{m}\mathcal{F}, \tag{9}$$

which leads us to define an effective mass

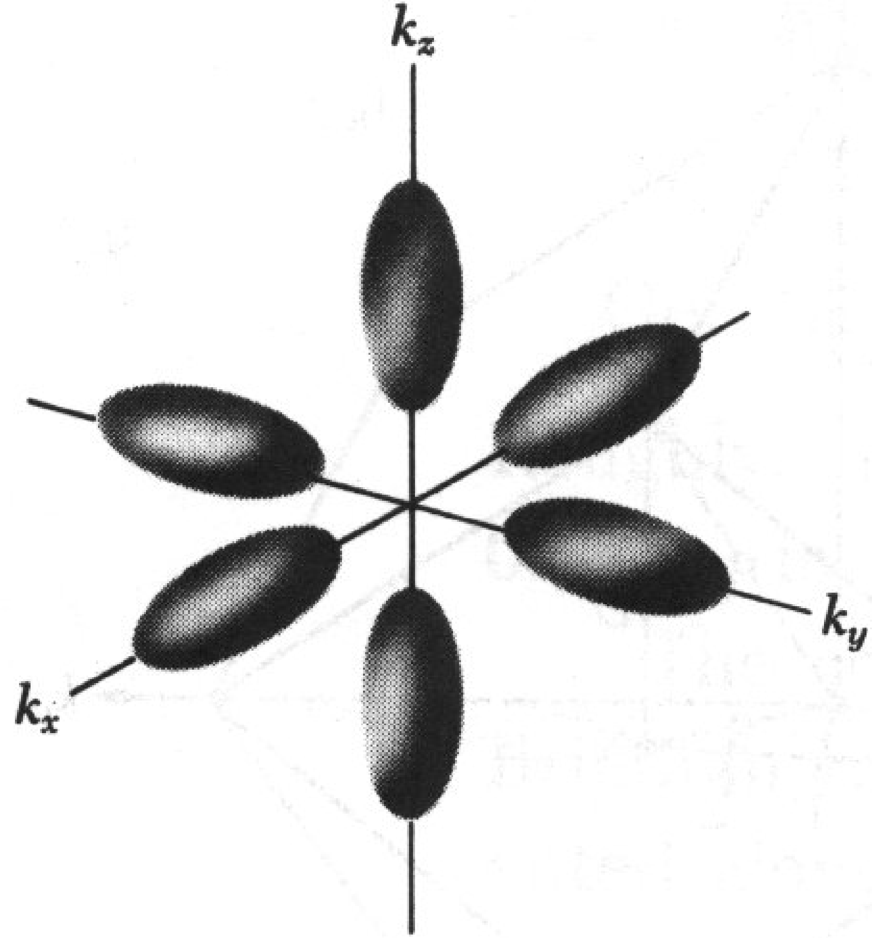
$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\mathrm{d}^2E}{\mathrm{d}k^2}.$$

That is

- **the effective mass depends on the *curvature* of the bands;**
- **flat bands (in tight-binding, small overlap matrix elements, e.g. d-bands or f-bands) have large effective masses;**
- **near the bottom of a band, m^* is positive, near the top of a band, m^* is negative.**

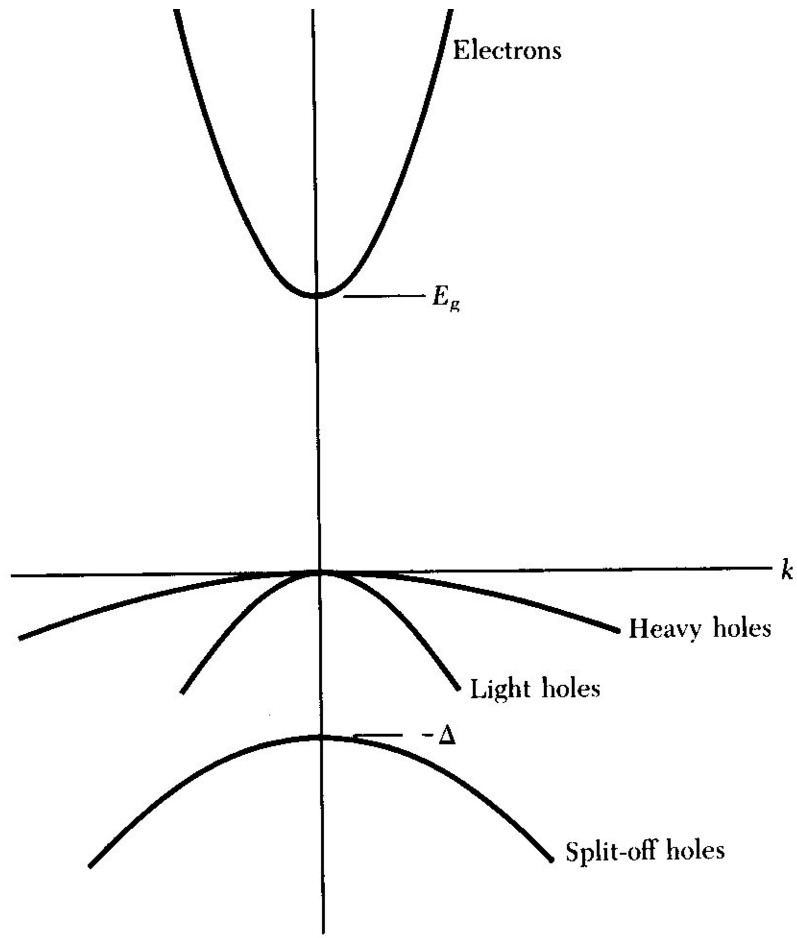
In three dimensions, constant energy surfaces are not necessarily spherical, and the effective mass is a tensor:

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\frac{\mathrm{d}^2 E}{\mathrm{d}k_i \mathrm{d}k_j}.$$



k_z
k_y
k_x

8.2.1 Typical effective masses for semiconductors



Note that the top of the valence band is often degenerate, with heavy and light holes and a split-off hole band arising from spin-orbit coupling.

	Mass relative to free electron				
	Electron	**Heavy hole**	**Light hole**	**Split-off hole**	**Δ/eV**
Si	**0.19-0.92**	**0.52**	**0.16**		
Ge	**0.082-1.59**	**0.34**	**0.043**	**-**	**0.29**
InSb	**0.015**	**0.39**	**0.021**	**0.11**	**0.82**
InAs	**0.026**	**0.41**	**0.025**	**0.08**	**0.43**
InP	**0.073**	**0.4**	**0.078**	**0.15**	**0.11**
GaSb	**0.047**	**0.3**	**0.06**	**0.14**	**0.80**
GaAs	**0.066**	**0.5**	**0.082**	**0.17**	**0.34**

8.3 Electrons and holes

We have discussed (in lecture 20) a full band (a full Brillouin zone) in terms of Bragg reflection, and shown that it does not respond to electric fields to produce an electric current. We can use our tight binding model to show this: in one dimension

$$E_{\mathbf{k}} = -\alpha - 2\gamma\cos(ka),$$

so the electron velocity is

$$2\gamma a$$

(Note that the effective mass is

$$m^* = \frac{\hbar^2}{2\gamma a^2 \cos(ka)},$$

which is negative near the top of the band, $k = \pm\pi/a$**.) It is clear that if we integrate** v **over a Brillouin zone (**$-\pi/a \leq k \leq \pi/a$**) we are integrating** $\sin$ **over a period, and we get zero. Even if the electrons drift under the influence of an electric field, there as many electrons at the top of the band moving against the field as there are at the top of the band moving with the field. But if the band is not full, we can have a nett current. If we have somehow managed to excite a few electrons from the valence bands into the conduction bands, leaving a few holes in the valence bands, it may be easier to focus on the behaviour of the holes.**

8.3.1 Hole wavevector

The total k **of a full band is zero: if we remove an electron with wavevector** k_e **the total** k **of the band is**

$$\mathrm{k}_h = 0 - \mathrm{k}_e = -\mathrm{k}_e.$$

8.3.2 Hole energy

Take the energy zero to be the top of the valence band. The lower the electron energy, the more energy it takes to remove it: thus

$$E_h(\mathbf{k}_e) = -E_e(\mathbf{k}_e),$$

but bands are usually symmetric,

$$E(\mathbf{k}) = E(-\mathbf{k})$$

so

$$E_h(\mathbf{k}_h) = E_h(-\mathbf{k}_h) = -E_e(\mathbf{k}_e).$$

8.3.3 Hole velocity

$$v_h = \frac{1}{\hbar}\nabla_{\mathbf{k}_h} E_h,$$

but

$$\mathbf{k}_h = -\mathbf{k}_e$$

so

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

and so

$$\frac{1}{\hbar}\nabla \ldots (-E_e)$$

The group velocity of the hole is the same as that of the electron.

8.3.4 Hole effective mass

The curvature of E is just the negative of the curvature of $-E$, so

$$m_h^* = -m_e^*.$$

Note that this has the pleasant effect that if the electron effective mass is negative, as it is at the top of the band, the equivalent hole has a positive effective mass.

8.3.5 Hole dynamics

We know that

$$\hbar\frac{\mathrm{d}\mathbf{k}_e}{\mathrm{d}t} = -e(\mathcal{E} + \mathbf{v}_e \times \mathcal{B}),$$

so substituting $\mathbf{k}_h = -\mathbf{k}_e$ and $\mathbf{v}_h = \mathbf{v}_e$ gives

$$\hbar\frac{\mathrm{d}\mathbf{k}_h}{\mathrm{d}t} = e(\mathcal{E} + \mathbf{v}_h \times \mathcal{B}),$$

or *exactly the equation of motion for a particle of positive charge.* Un-

opposite directions, but both give electric current in the direction of the field.

8.3.6 Experimental

Under a magnetic field $\mathcal{B}$, electrons move in helical paths (orbits around the field direction, uniform motion parallel to $\mathcal{B}$), with angular frequency

$$\omega_c = \frac{e\mathcal{B}}{m^*},$$

the *cyclotron frequency*. Electrons can absorb energy from an electromagnetic field of the appropriate frequency – *cyclotron resonance* – this is how effective masses can be measured.

8.3.7 Mobility and conductivity

We define mobilities for electrons and holes in the relaxation time approximation as

$$\mu_e = \frac{e\tau}{m_e^*}, \qquad \mu_h = \frac{e\tau}{m_h^*}$$

and then the total current is the sum of electron and hole currents,

$$J = -en_e v_e + en_h v_h,$$

so the conductivity is

or

$$\sigma = n_e \frac{e^2 \tau}{m_e^*} + n_h \frac{e^2 \tau}{m_h^*}.$$

Note that we have assumed equal relaxation times, τ, for electrons and holes – this is not necessarily true.