FoP3B Part II Lecture 2: Electrons and holes

The primary application for semiconductor materials is electronic devices, such as computers, mobile phones etc. It is therefore important to understand how a semiconductor conducts electricity at a fundamental level. Here we explain how **electrons** and **holes** carry charge in a material (see below if you are not familiar with holes). We shall do this using electronic band structure diagrams, relying on **three key equations**:

$$\mathbf{j} = ne\mathbf{v} \qquad \dots (1)$$

$$\mathrm{v} = \frac{1}{\hbar}\frac{dE}{dk} \qquad \dots (2)$$

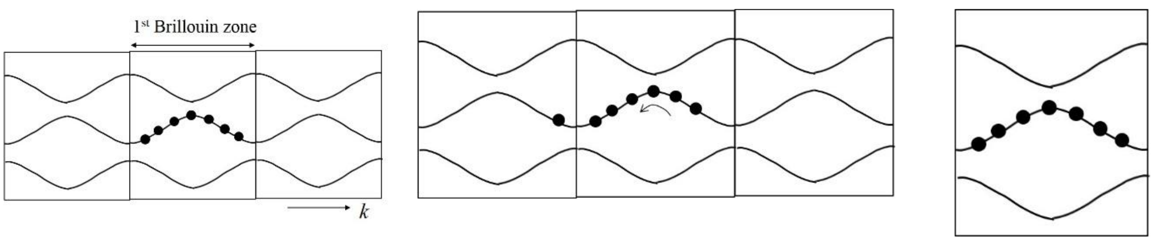
$$\mathbf{F} = \hbar\frac{d\mathbf{k}}{dt} \qquad \dots (3)$$

Equation (1) is the current density **j** expressed as a vector, with *n* being the number density of charge carriers of charge *e* per unit volume that have velocity **v**. Equations (2) and (3) represent the group velocity and force on electrons respectively (you came across the last two equations in Lecture 1). The velocity of an electron is proportional to the gradient of the *E*-*k* diagram.

From Equation (1) it follows that for net electrical conduction $\Sigma\mathbf{v} \neq 0$, *where the summation is over all electrons. Similarly we must have* $\Sigma\mathbf{k} \neq 0$, *where* **k** *is the electron wavevector; this means that electrons have a net momentum when conducting electricity.*

Conduction in a completely full band

Let us apply the above principles to electrons in a completely full band under an applied electric field (the driving force for producing an electric current). *Since the electron is negatively charged the force will be in the opposite direction to the electric field*. Before the electric field is applied the entire band is full and therefore $\Sigma\mathbf{v} = 0$ and $\Sigma\mathbf{k} = 0$, i.e. there is no net current as required (Figure 1a). Assume the electric field is applied in the +*k* direction, so that from Equation (3) the electron **k**-vector would decrease (Figure 1b). Because we only need to consider electrons in the first Brillouin zone the Reduced Zone scheme still gives a full band with $\Sigma\mathbf{v} = 0$ and $\Sigma\mathbf{k} = 0$ (Figure 1c). **A completely full band cannot therefore conduct electricity**. **Insulators (e.g. wood, plastic) do not conduct electricity due to filled bands.**

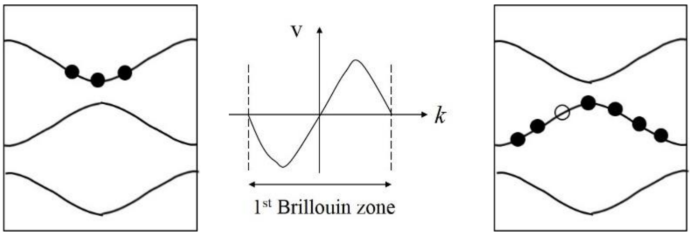


(a) **(b)** **(c)**

Figure 1: Completely full band (a) before and (b) after applying an electric field in +*k* direction. (c) is the Reduced Zone scheme representation of (b)

Conduction in a nearly empty band

Consider the case where only a few electronic states in a band are occupied (Figure 2a). Examples are (i) metals and (ii) semiconductor conduction band after light absorption. Going through the same arguments described previously it should be clear that even in the Reduced Zone scheme $\Sigma\mathbf{v} \neq 0$ and $\Sigma\mathbf{k} \neq 0$ under an applied electric field, which is the condition for conduction. However, there is a subtlety. If Equation (3) is integrated over time the electron wavevector will cycle through all **k**-values within the first Brillouin zone. Now from Equation (2) the velocity of electrons change sign in opposite halves of the first Brillouin zone (Figure 2b). *The <u>time integrated</u> electron velocity and hence electric current is therefore zero!* We do however know that metals are good conductors, so something is missing from our model.



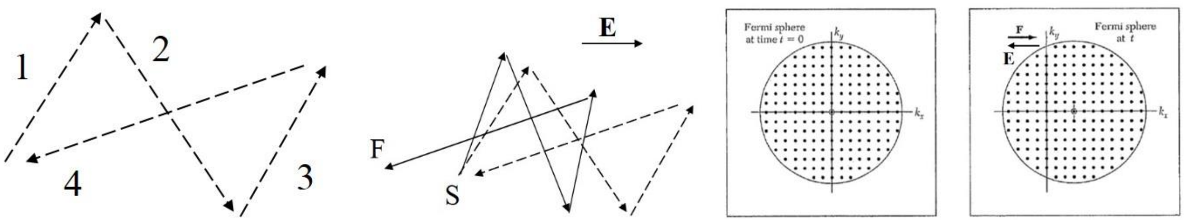
(a) (b) (c)

Figure 2: (a) nearly empty band and (b) the electron velocity within the first Brillouin zone. (c) shows a nearly full band, with the missing electron denoted by an empty circle.

The answer lies in electron **scattering**. *In real materials thermal energy cause atoms to vibrate, and electrons can scatter off them such that there is no change in the <u>time averaged</u> position (Figure 3a)*. This is however not the case when an electric field is applied (Figure 3b). Then the electrons acquire a **drift velocity** ($\mathbf{v}_\mathrm{d}$) given by:

$$\mathbf{v}_\mathrm{d} = -\mu\mathbf{E}$$

where μ is the **mobility**. *The negative sign indicates that the negatively charged electrons drift in the opposite direction to the electric fiel*d **E**. **The fact that electrons acquire a drift velocity and hence net momentum means that the Fermi surface shifts when an electric field is applied (Figure 3c)**. *Hence* $\Sigma\langle\mathbf{v}\rangle \neq 0$ *and* $\Sigma\langle\mathbf{k}\rangle \neq 0$, *where the* $\langle\ \rangle$ *sign represents a time averaged quantity*. **We conclude that electrons in a nearly empty band can conduct electricity with the aid of scattering**.



(a) (b) (c)

Figure 3: (a) Electron scattering in a material with no electric field. The numeral represents successive trajectories between scattering events. The solid lines in (b) show how the same trajectories are modified under an applied electric field **E**. 'S' and 'F' denote the electron start and finish positions. The shifting of the Fermi surface under an electric field is shown in (c).

Conduction in a nearly full band- the concept of holes

A full band cannot conduct electricity. Let us however consider a nearly full band (Figure 2c). This may occur in (i) metals and (ii) semiconductor valence band after light absorption. Inspecting Figure 2c it is clear that $\Sigma\mathbf{v} \neq 0$ and $\Sigma\mathbf{k} \neq 0$ under an applied field, so that a nearly full band can conduct electricity with the aid of scattering. However, **instead of describing conduction in terms of *all* electrons in the band it is possible to model it using a *single* pseudo-particle called a hole**.

This is best illustrated using Figure 4. The missing electron is initially at the top of the band when an electric field is applied in the $+k$ direction. From Equation (3) this results in the electrons shifting to lower k-values (recall that electrons are negatively charged). The same is also true for the missing electron. *We have* $\Sigma\mathbf{k} = -\mathbf{k}_e$, *where* $\mathbf{k}_e$ *is the wavevector of the missing electron*. Since the hole describes motion of all electrons in the band its wavevector will be $\Sigma\mathbf{k}$ or $-\mathbf{k}_e$. We now consider the energy of the hole so that we may construct a (fictitious) E-k diagram for the **hole band**. **A band with a missing electron is in an excited state and the fact that the missing electron moves into progressively lower energy states with applied field means that the hole band must be a mirror reflection of the nearly full electron band**. This is illustrated in Figure 4. It is also clear from the figure that the hole moves in the opposite direction to electrons under an applied field, i.e. a hole has *positive* charge.

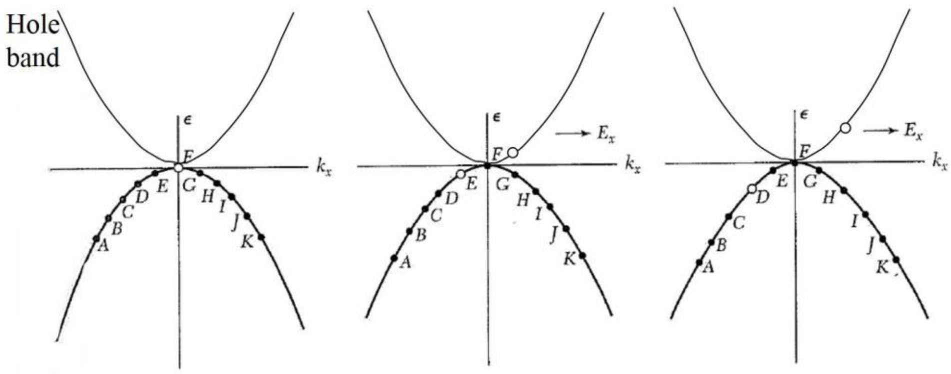


Figure 4: Electrons in a nearly full band under an electric field applied in the $+k$ direction and their description using a pseudo-particle hole band.

NB: A hole arises due to a missing electron in a nearly full electron band. However, it is NOT the missing electron itself. Instead it is a pseudo-particle of positive charge that we use for our own convenience to describe the net motion of all other electrons in the band.

For this reason it should be clear to you that a completely empty band does not consist of holes and therefore is not conducting.