Theory of Semiconductor Devices
(반도체 소자 이론)

Lecture 9

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Contents

Crystal Imperfections

Perfect or Not ?

- Up to now we have considered only the properties of ***perfect*** crystals .
- We assumed that the atoms of the crystal were arranged at the sites of a mathematically ***precise*** Bravais lattice.
- This resulted in a ***perfectly*** periodic lattice potential energy for the electrons and we were able to establish relationships between the energy and wavevector of an electron on this basis.
- We also found, incidentally, that electrons can have a constant average velocity in a perfect periodic potential *without* the application of external forces. This, of course, is ***contrary*** to experimental observation.

- Because of this and other important experimental results, we realize that the perfect crystal is an ***overly simplified*** picture of a more complicated situation.
- Thus, to take into account many of the more important properties of semiconductors, we *must* examine possible crystal ***imperfections***.

- We will base our analysis of these imperfections on the assumption that they can be, in general, regarded as perturbations in a perfect crystal.

Electrons and Holes

- Let us first consider the situation where one of the bonds between atoms in a perfect crystal is broken. From a ***chemical*** point of view, sufficient energy has been given to an electron to move it from a bonding state to an antibonding state.
- In the ***energy band*** picture, an electron is excited from somewhere near the top of a completely filled valence band to somewhere near the bottom of a completely empty conduction band.
- After the excitation, of course, the valence band is ***missing*** one electron and the conduction band has ***acquired*** one.

- We will assume for the time being that the conduction band electron is ***spatially*** removed from the empty state it left in the valence band a sufficient distance that interaction between them can be neglected.
-This broken-bond situation represents an excited state of the one-electron energy bands discussed in Chapter 2.

-To understand what will happen in this situation, let us first look at the electrons in a ***completely filled*** valence band under the influence of an external force applied at $t = 0$.
- As indicated in Fig. 3.1, we assume only eight allowed values of k for each energy band in the first Brillouin zone.

Electrons and Holes

- According to (2.111),

$$\hbar \frac{d\mathbf{k}}{dt} = \mathbf{F} \qquad (3.1)$$

which tells us that the **k** vectors for all the electrons in the valence band will increase continually in the direction of F for *t* greater than zero.

- Thus the electron in state 0 will move to state 1, the electron in state 1 will move to state 2, and so on. *What will happen to the electron in state 8?* It can move to the ***first*** state in the ***second*** Brillouin zone. However, since we want to have a ***unique*** wavevector for every electron state, we flip it over (Umklapp process) to state 0 in the first Brillouin zone by adding to it a reciprocal lattice vector - K.

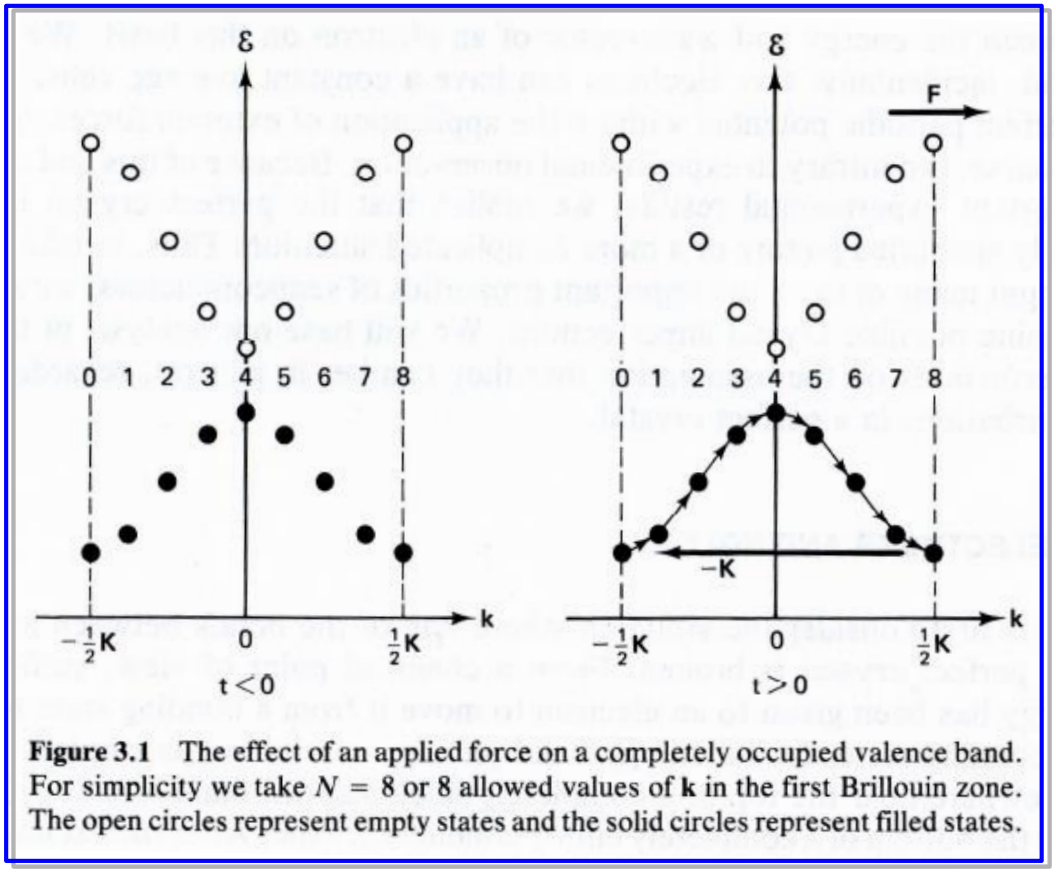


Figure 3.1 The effect of an applied force on a completely occupied valence band. For simplicity we take $N = 8$ or 8 allowed values of **k** in the first Brillouin zone. The open circles represent empty states and the solid circles represent filled states.

Electrons and Holes

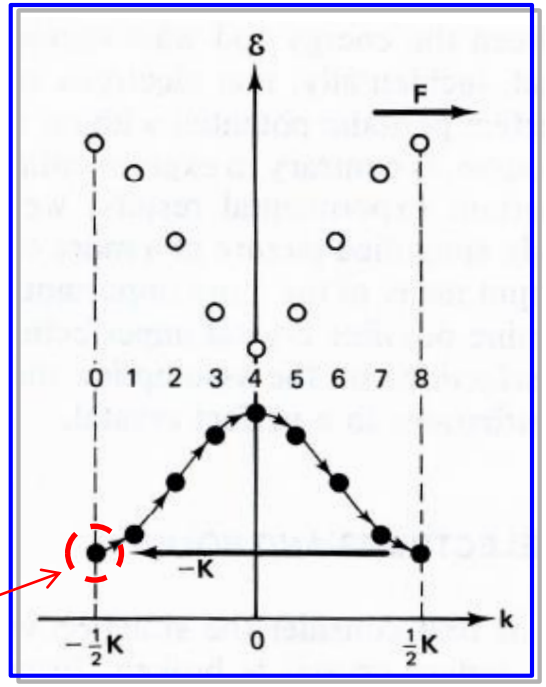
-As long as the force is applied, this process is repeated for each electron and they cycle continuously through the first Brillouin zone.

- Let us look at the velocity and acceleration of an electron as it goes through one of these cycles. From (2 .109) the velocity is given by

$$\mathbf{v} = \frac{1}{\hbar}\frac{\partial \mathscr{E}}{\partial \mathbf{k}} \qquad (3.2)$$

- If we consider a parabolic band, the effective mass tensor of (2.115) reduces to a scalar, and from (2.113) the acceleration is

$$\mathbf{a} = \frac{1}{m^*}\mathbf{F} \qquad (3.3)$$



- From (3.2) and. (3.3) an electron starting at **state 0** has ***zero*** velocity, and since m^* is ***positive*** at the bottom of a band, ***maximum*** acceleration in the direction of the force .
- It thus proceeds to state 1 and then state 2, increasing its velocity.
- **At state 2** : ***maximum*** velocity, and since m^* is ***infinite***, ***zero*** acceleration.
- As the electron goes to state 3 its velocity starts to decreas, since m^* becomes negative, and the acceleration is opposite to the direction of the force.

Electrons and Holes

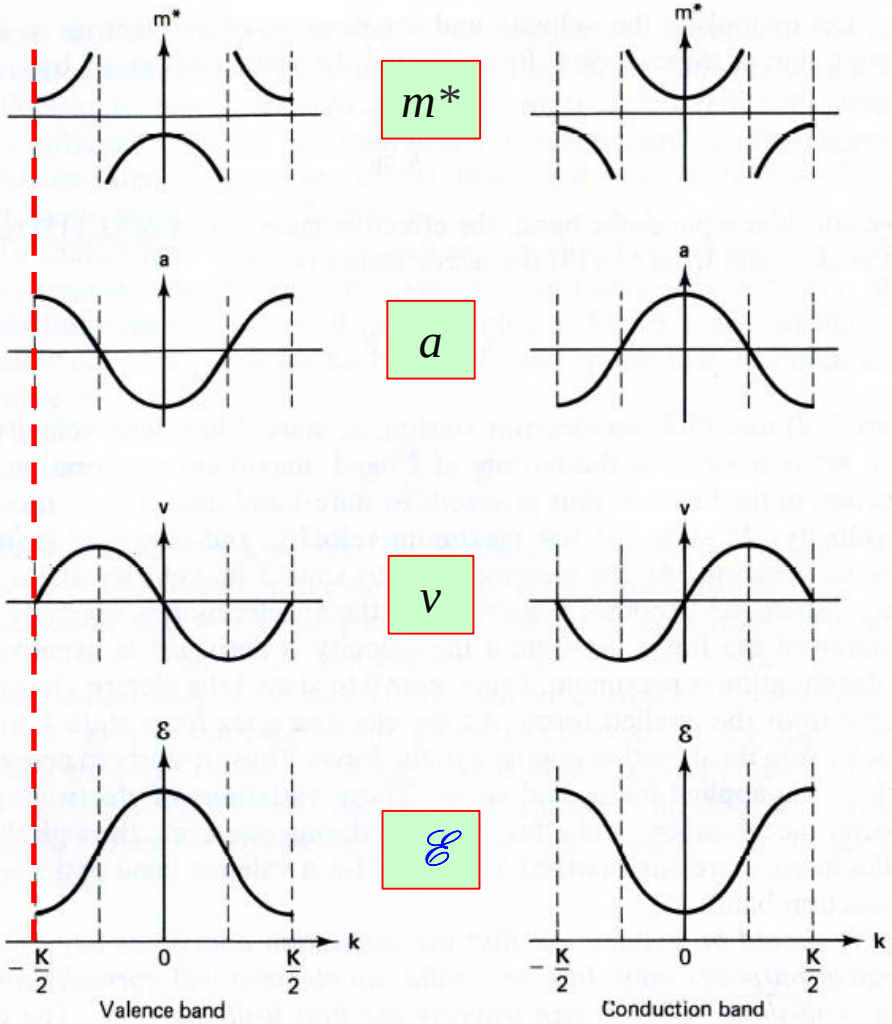


Figure 3.2 Variation of electron energy, $\mathscr{E}$, velocity, **v**, acceleration, **a**, and effective mass, m^*, with wavevector, **k**, in the first Brillouin zone for both valence and conduction bands.

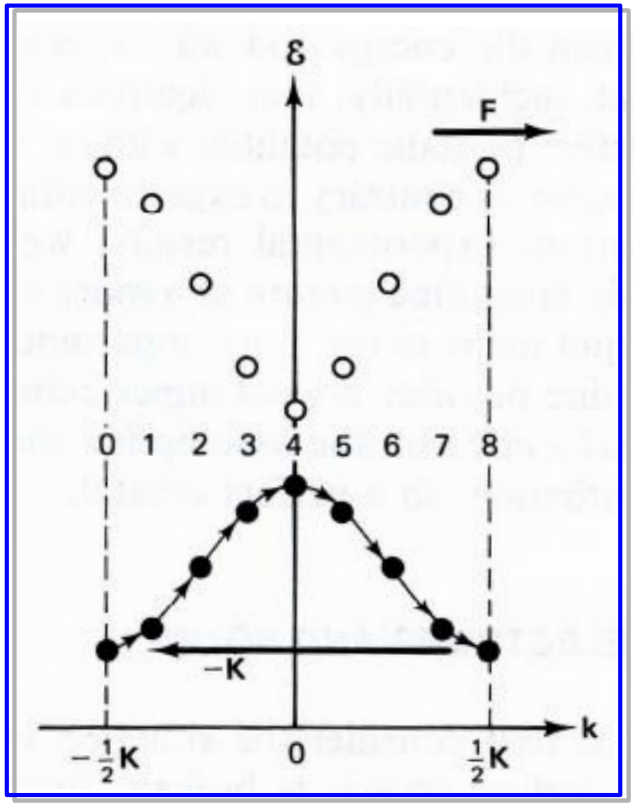
- **<u>At state 4</u>** the velocity is ***zero***, m^* is ***negative*** and the deceleration is ***maximum***.
- From state 0 to state 4 the electron has gained energy from the applied force.
- These variations of electron energy, velocity, acceleration, and effective mass during one cycle through the first Bnlloulll zone are summarized in Fig. 3.2 for a valence band and also for a conduction band.

It should be pointed out that the discussion above has been for pedagogical purposes only. In a ***real*** *solid, an electron will normally undergo many collisions before it can traverse the first Brillouin zone.*

The effects of these collisions on carrier transport are discussed in Chapters 5 and 6.

Electrons and Holes

- From Figs. 3.1 and 3.2 we can see that for a ***filled*** valence band there is no net energy transfer from the applied force to the electrons through either part or all of a cycle.
- If we sum all the values of k in Fig. 3.1, we find $k_4 = 0$, $k_3 = -k_5$, $k_2 = -k_6$, $k_1 = -k_7$, *and* $\frac{1}{2}k_0 = -\frac{1}{2}k_8$, so there is also no net gain in k from the applied force . (To avoid counting states twice, the sum is over only one-half of states 0 and 8.)



- It should be pointed out that these results are *independent* of the specific form of the energy bands, because of the *equivalence* of zone edge points in a given direction.

- Therefore, *the only effect* of an applied force on a filled valence band is to cause the electrons to accelerate and decelerate ***cyclically*** from one state to another.

- Without the force the electrons *would* stay in their states defined by constant wavevector **k** at a constant average velocity **v**.

Electrons and Holes

- Let us now examine the effect of an applied force at $t = 0$ on a conduction band with ***one electron*** and a valence band with ***one missing electron*** at **k = 0**.
- This situation is shown in Fig. 3.3 .
- For $t < 0$ we assume that the electron in valence band state 4 has been excited into conduction band state 4.

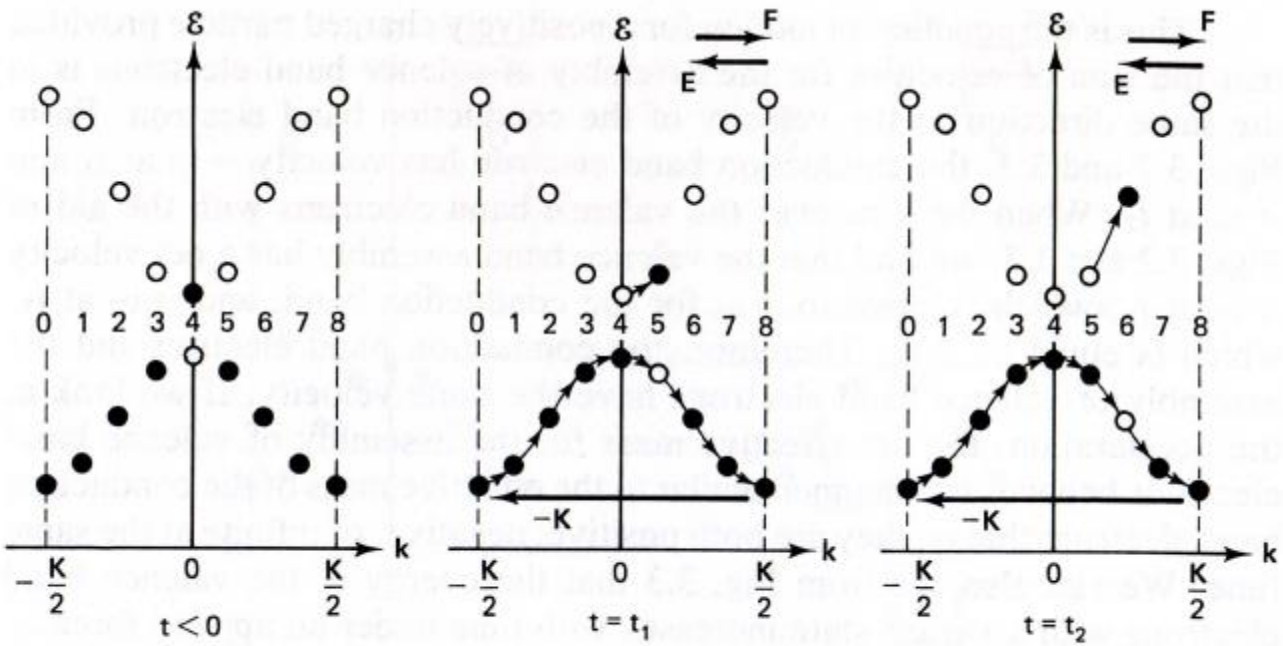


Figure 3.3 The effect of an applied force on a conduction band with one electron and a valence band with one missing electron.

-When the force is turned on, according to (3.1), the **k** vectors for *all* electrons increase simultaneously.
- Thus, at t_1 the electron in conduction band state 4 has ***moved*** to state 5, the electron in valence band state 8 has been Umklapped to state 0, the electron in state 0 has moved to state 1, and so on.

Electrons and Holes

- The ***net*** effect of the valence band electron motion is that the empty state has moved from 4 to 5. At t_2 the conduction band electron has moved from state 5 to state 6, and the empty valence band state has moved from 5 to 6.
- Therefore, we see that the conduction band electron and the empty valence band state ***both*** increase their **k** value in the direction of the applied force F.

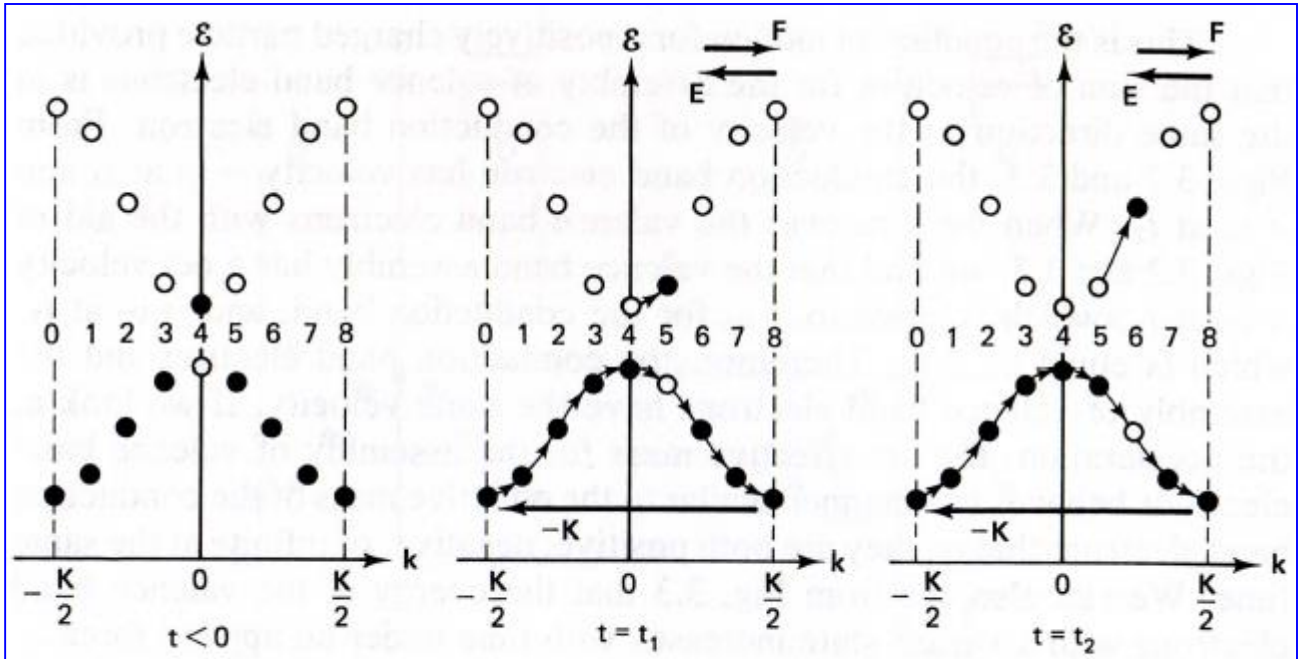


Figure 3.3 The effect of an applied force on a conduction band with one electron and a valence band with one missing electron.

Electrons and Holes

- If we sum the **k** vectors for the conduction band at t_1, the result is obviously k_5. For the valence band, the sum of the **k** vectors is $-k_3$.
- At time t_2 the electron in the conduction band has wavevector k_6, while the sum of the electron wavevectors in the valence band is $-k_2$.

- The interpretation of this behavior for the **electron** in the ***conduction*** band is *straightforward*: Its **k** vector increases with time under an applied force , F, according to (3.1).
- An interpretation of the behavior for the **electron assembly** in the ***valence*** band, however, is *not as obvious*: the sum of **k** vectors for the assembly decreases (becomes more negative) with time under an applied force, F. If we consider the force on an electron wave packet in an applied electric field, **E**,

$$\hbar \frac{d\mathbf{k}}{dt} = \mathbf{F} \qquad (3.1)$$

$$\mathbf{F} = -q\mathbf{E} \qquad (3.4)$$

$$\hbar \frac{d\mathbf{k}}{dt} = -q\mathbf{E}$$

we see that the direction of the force depends on the charge of the particle, $-q$. Since E is in the $-$ **k** direction in Fig. 3.3 (F in the + k direction), the electron in the conduction band follows (3.4) ***nicely***.

Electrons and Holes

- The assembly of electrons in the valence band, however, has a **k** vector that ***decreases*** with time, so that (3.4) for them is

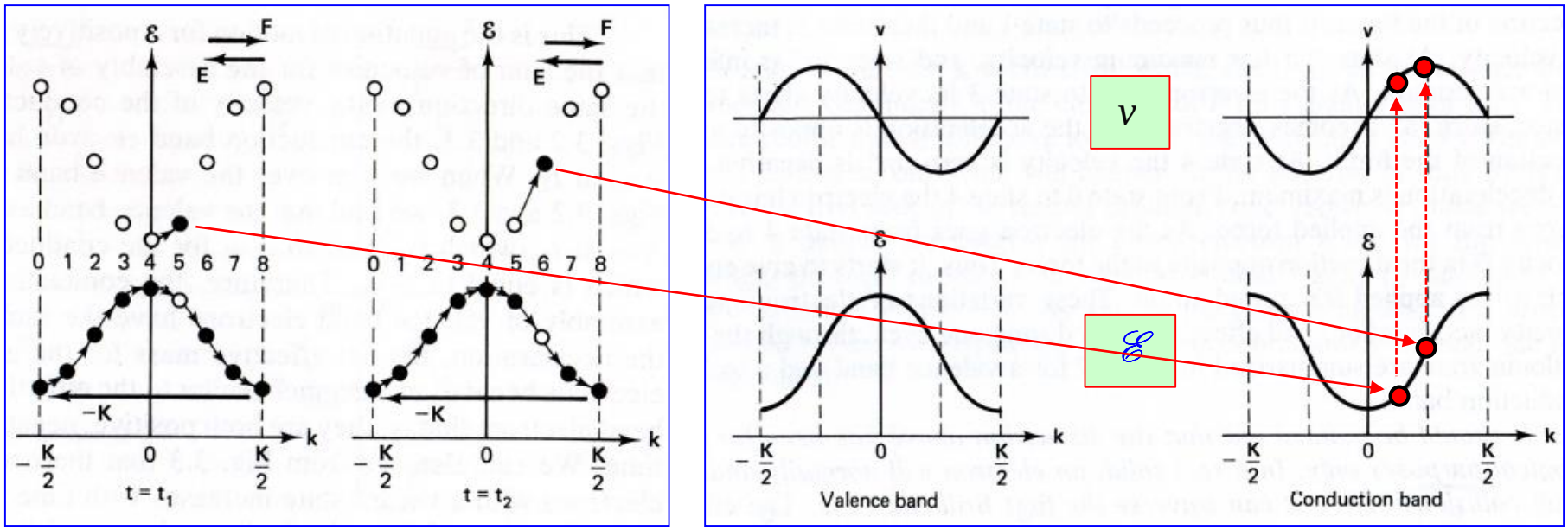
$$-\hbar \frac{d\mathbf{k}}{dt} = -q\mathbf{E}$$
$$h \frac{d\mathbf{k}}{dt} = +q\mathbf{E} \qquad (3.5)$$

-This is the equation of motion for a ***positively*** charged particle provided that the sum of velocities for the assembly of valence band electrons is in the ***same*** direction as the velocity of the ***conduction*** band electron.

- From Figs. 3.2 and 3.3, the conduction band electron has velocity + v_5 at t_1 and + v_6 at t_2. When we sum over the valence band electrons with the aid of Figs. 3.2 and 3.3, we find that the valence band assembly has a net velocity + v_3 at t_1, which is equal to + v_5 for the conduction band, and + v_2 at t_2, which is equal to + v_6.

Electrons and Holes

- The conduction band: electron has **velocity** + v_5 at t_1 and + v_6 at t_2.
- The valence band assembly: net velocity + v_3 at t_1, which is equal to + v_5 for the conduction band, and + v_2 at t_2, which is equal to + v_6.



- Therefore, the conduction band electron and the assembly of valence band electrons have the same velocity.

Electrons and Holes

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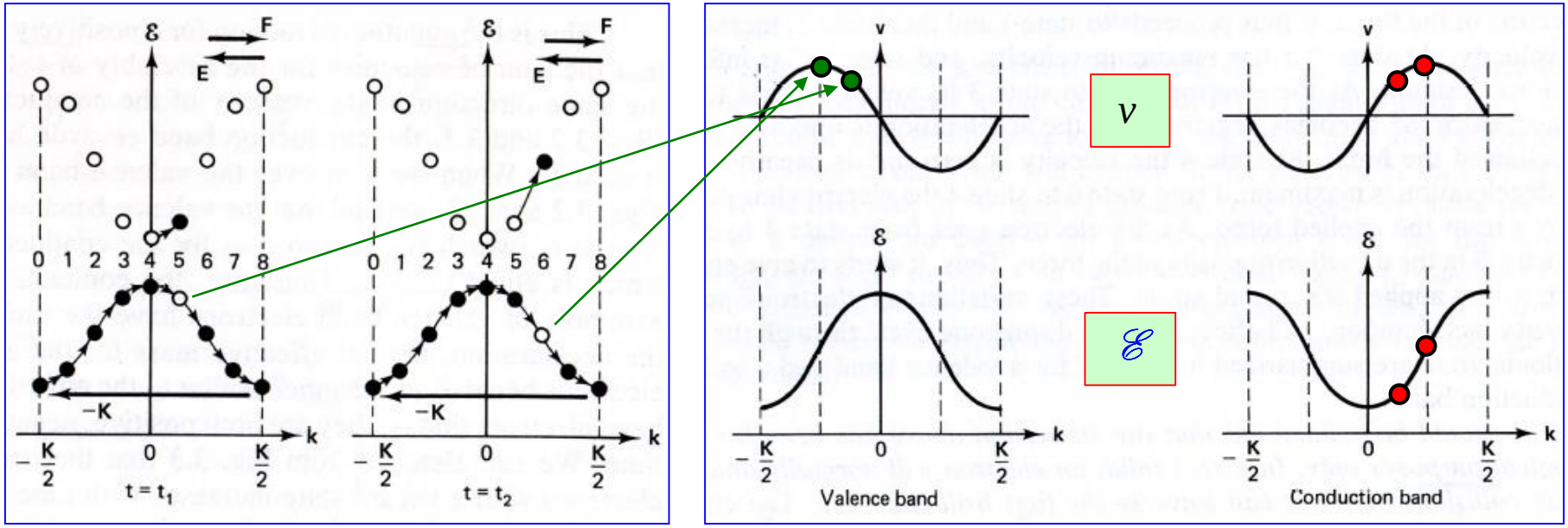
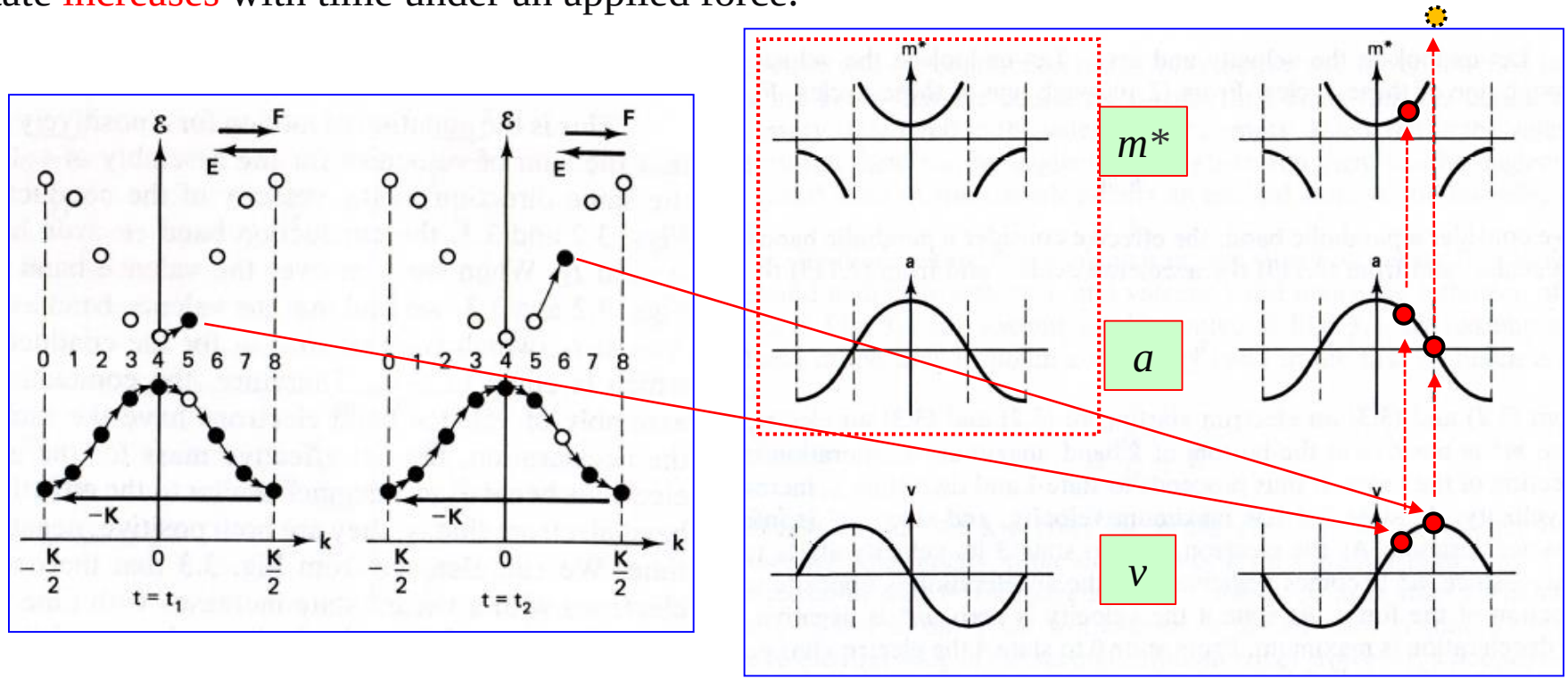


- Therefore, the conduction band electron and the assembly of valence band electrons have the same velocity.

Electrons and Holes

- If we look at the acceleration, the net effective mass for the assembly of valence band electrons behaves in a manner similar to the effective mass of the conduction band electron: that is, they are ***both*** positive, negative, or infinite at the same time.

- We can also see from Fig. 3.3 that the energy of the valence band electrons with a vacant state increases with time under an applied force.



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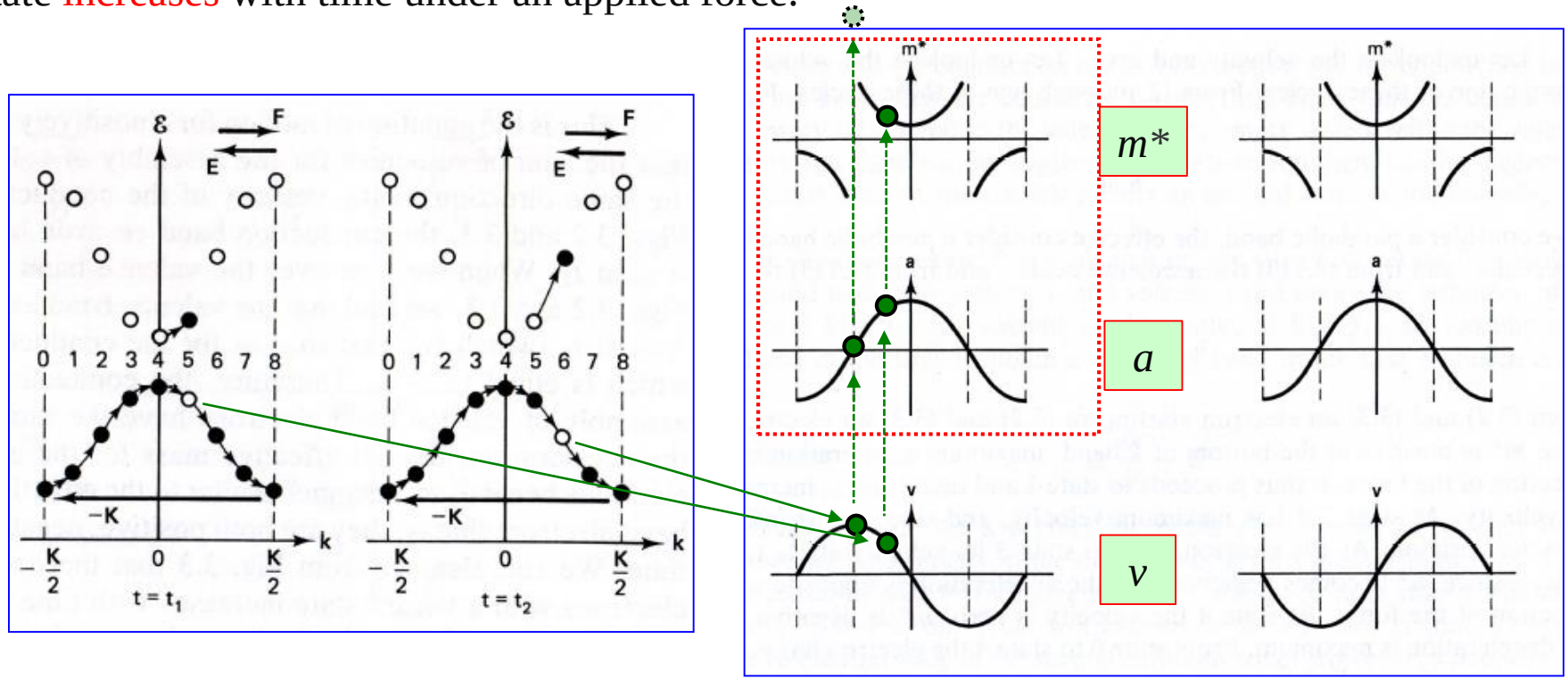

Electrons and Holes

- If we have followed this discussion carefully, we can see that there is nothing particularly unusual (other than the effective mass) about the behavior of the electron in the ***conduction*** band under an applied external force.
- These are usually referred to as conduction electrons, electrons, or sometimes, inappropriately, as "free" electrons.
- The assembly of ***valence*** band electrons with an empty state, however, is another matter. In an applied force we have seen that this ***entity*** has an increasing energy when the empty state goes to lower energy, a decreasing wavevector when the empty state goes to higher wavevector, a positive velocity when the empty state is in a negative velocity region, a positive effective mass when the empty state is in the top of the valence band, and a negative effective mass when the empty state is at the bottom of the band.

- In fact, the assembly of valence band electrons acts as a ***positively*** charged particle in an otherwise empty band. This particle would have positive m^* near the ***top*** of the band and negative m* near the ***bottom***.
- It would also travel from state 4 to 3 to 2 in Fig. 3.3 as the empty site traveled from 4 to 5 to 6. To avoid a tedious summation over N values of wave vector every time we wish to examine the properties of a valence band with empty states, it is ***convenient*** to invent an equivalent particle.
- Such a particle with the properties of the ***assembly of valence band electrons*** is called a **hole**.

Electrons and Holes

- At time t_2 in the electron energy band diagram of Fig. 3.3, the empty valence band state was at 6, moving in the direction of ***increasing* k**, while the fictitious hole appeared to be at 2, moving in the direction of ***decreasing* k**. This is the situation shown in Fig. 3.4(a).
- Equation (3.5) tells us, however, that the wavevector for the hole ***should increase*** in the direction of E because of its positive charge. Also, we saw that the valence band energy increased as the vacant state went toward decreasing electron energy.
-Thus the direction of increasing energy for the hole is ***opposite*** to the electron energy.

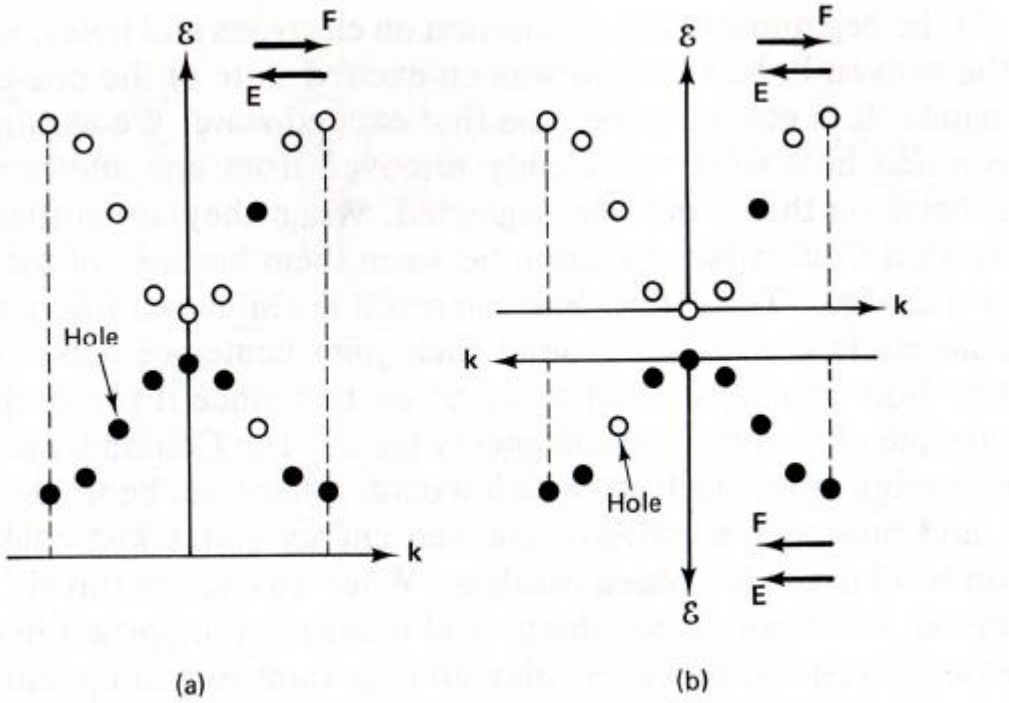

Figure 3.4 Conduction band electrons, empty valence band state, and hole in (a) an electron representation and (b) a mixed electron and hole representation.

- For these reasons it is *convenient* to use ***two separate*** $\mathscr{E}$ versus **k** diagrams simultaneously, as indicated in Fig. 3.4(b): one to represent the behavior of **electrons** in the **conduction** band and another to represent the behavior of **holes** in the **valence** band.

Electrons and Holes

- Although we have demonstrated that the assembly of valence band electrons with an empty state behaves as a positively charged particle, it is somewhat difficult to see the physical origin of this charge in the energy band scheme. In the bond diagram for a covalent semiconductor in Fig. 3.5, however, the origin of the positive charge is obvious.
- An examination of the unit cell that contains the broken bond or hole has a net charge of + 1 from the atomic cores.

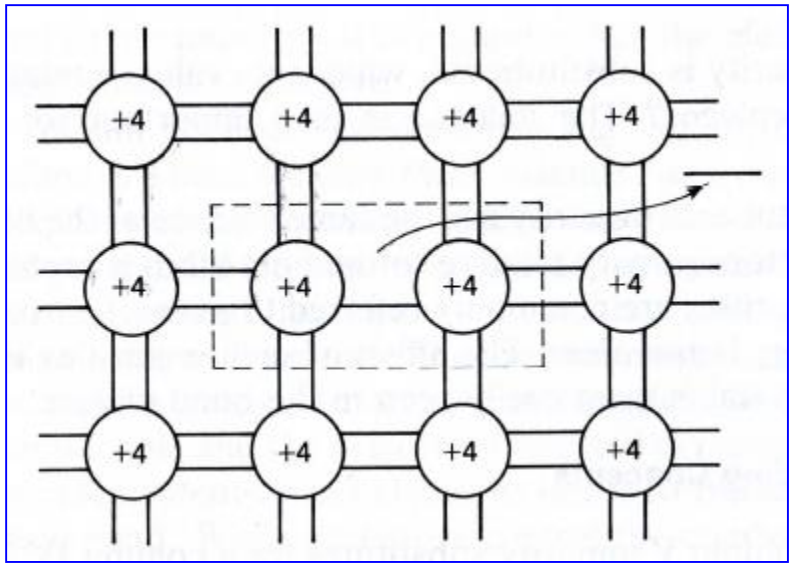

Figure 3.6 (a) Column V substitutional donor impurity and (b) column III substitutional acceptor impurity in Ge.

- The broken-bond situation was an excited state of the one-electron energy bands. It is *not*, however, the first excited state. We **assumed** that the electron and hole were *sufficiently* removed from one another that interaction between them could be neglected. When they are sufficiently close we expect a Coulombic attraction between them because of their opposing effective charges. This interaction can result in a situation where the electron and hole circle each other around their joint center of mass. This bound electron-hole pair is referred to as an ***exciton*** since it represents the first excited state of the one-electron energy bands.