The change $\Delta \mathbf{p}_{\text{lat}}$ in the lattice momentum resulting from the change of state of the electron may be derived by an elementary physical consideration. An electron reflected by the lattice transfers momentum to the lattice. If an incident electron with plane wave component of momentum $\hbar\mathbf{k}$ is reflected with momentum $\hbar(\mathbf{k}+\mathbf{G})$, the lattice acquires the momentum $-\hbar\mathbf{G}$, as required by momentum conservation. The momentum transfer to the lattice when the state ψ goes over to $\psi_{\mathbf{k}+\Delta\mathbf{k}}$ is

$$\Delta \mathbf{p}_{\text{lat}} = -\hbar \sum_{\mathbf{G}} \mathbf{G}[(\nabla_{\mathbf{k}}|C(\mathbf{k}+\mathbf{G})|^2 \cdot \Delta\mathbf{k}] \ , \tag{7f}$$

as the portion

$$\nabla_{\mathbf{k}}|C(\mathbf{k}+\mathbf{G})|^2 \cdot \Delta\mathbf{k} \tag{7g}$$

of each individual component of the initial state is reflected during the state change $\Delta\mathbf{k}$.

The total momentum change is therefore

$$\Delta \mathbf{p}_{\text{el}} + \Delta \mathbf{p}_{\text{lat}} = \mathbf{J} = \hbar\Delta\mathbf{k} \ , \tag{7h}$$

exactly as for free electrons, Eq. (7c). Thus from the definition of $\mathbf{J}$, we have

$$\hbar d\mathbf{k}/dt = \mathbf{F} \ , \tag{7i}$$

derived in (5) by a different method.

Holes

The properties of vacant orbitals in an otherwise filled band are important in semiconductor physics and in solid state electronics. Vacant orbitals in a band are commonly called holes. A hole acts in applied electric and magnetic fields as if it has a positive charge $+e$. The reason is given in five steps in the boxes that follow. (One test of a solid state course is that it should treat holes correctly.)

I.

$$\mathbf{k}_h = -\mathbf{k}_e \ . \tag{8}$$

The total wavevector of the electrons in a filled band is zero: $\Sigma\mathbf{k} = 0$. This result follows from the geometrical symmetry of the Brillouin zone: every fundamental lattice type has symmetry under the inversion operation $\mathbf{r} \rightarrow -\mathbf{r}$ about any lattice point; it follows that the Brillouin zone of the lattice also has inversion symmetry. If the band is filled all pairs of orbitals $\mathbf{k}$ and $-\mathbf{k}$ are filled, and the total wavevector is zero. If an electron is missing from an orbital of wavevector $\mathbf{k}_e$, the total wavevector of the system is $-\mathbf{k}_e$ and is attributed to the hole. This result is surprising: the electron is missing from $\mathbf{k}_e$ and the position of the hole is usually indicated graphically as situated at $\mathbf{k}_e$, as in Fig. 7. But the true wavevector $\mathbf{k}_h$ of the hole is $-\mathbf{k}_e$, which is the wavevector of the point G if the hole is at E. The wavevector $-\mathbf{k}_e$ enters into selection rules for photon absorption. The hole is an alternate description of a band with one missing electron, and we either say that the hole has wavevector $-\mathbf{k}_e$ or that the band with one missing electron has total wavevector $-\mathbf{k}_e$.

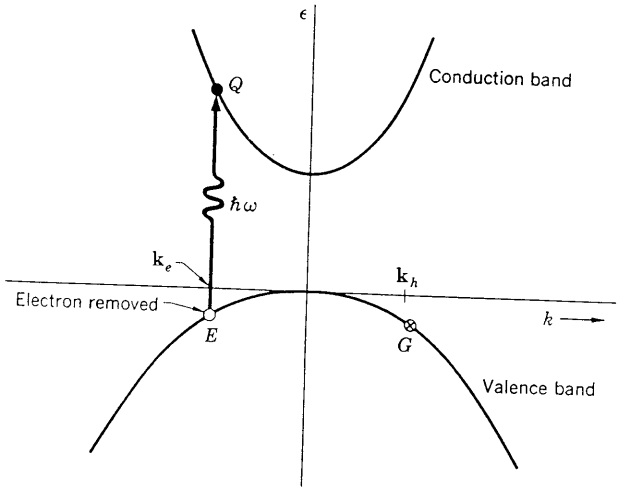

Figure 7 Absorption of a photon of energy $\hbar\omega$ and negligible wavevector takes an electron from E in the filled valence band to Q in the conduction band. If $\mathbf{k}_e$ was the wavevector of the electron at E, it becomes the wavevector of the electron at Q. The total wavevector of the valence band after the absorption is $-\mathbf{k}_e$, and this is the wavevector we must ascribe to the hole if we describe the valence band as occupied by one hole. Thus $\mathbf{k}_h = -\mathbf{k}_e$; the wavevector of the hole is the same as the wavevector of the electron which remains at G. For the entire system the total wavevector after the absorption of the photon is $\mathbf{k}_e + \mathbf{k}_h = 0$, so that the total wavevector is unchanged by the absorption of the photon and the creation of a free electron and free hole.

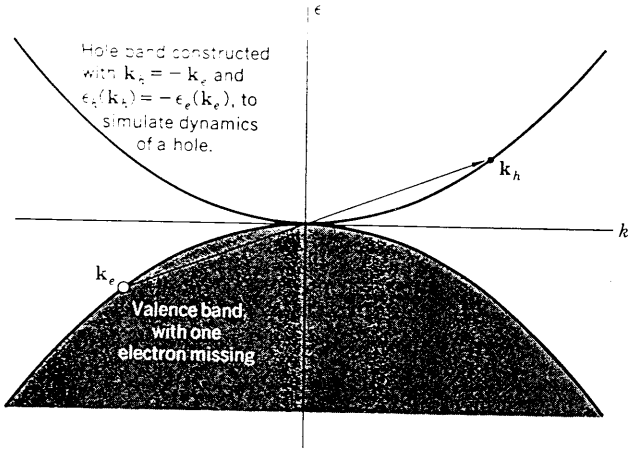

Figure 8 The upper half of the figure shows the hole band that simulates the dynamics of a hole, constructed by inversion of the valence band in the origin. The wavevector and energy of the hole are equal, but opposite in sign, to the wavevector and energy of the empty electron orbital in the valence band. We do not show the disposition of the electron removed from the valence band at $\mathbf{k}_e$.

2. $$\epsilon_h(\mathbf{k}_h) = -\epsilon_e(\mathbf{k}_e) \ . \tag{9}$$

Let the zero of energy of the valence band be at the top of the band. The lower in the band the missing electron lies, the higher the energy of the system. The energy of the hole is opposite in sign to the energy of the missing electron, because it takes more work to remove an electron from a low orbital than from a high orbital. Thus if the band is symmetric,[2] $\epsilon_e(\mathbf{k}_e) = \epsilon_e(-\mathbf{k}_e) = -\epsilon_h(-\mathbf{k}_e) = -\epsilon_h(\mathbf{k}_h)$. We construct in Fig. 8 a band scheme to represent the properties of a hole. This hole band is a helpful representation because it appears right side up.

3. $$\mathbf{v}_h = \mathbf{v}_e \ . \tag{10}$$

The velocity of the hole is equal to the velocity of the missing electron. From Fig. 8 we see that $\nabla\epsilon_h(k_h) = \nabla\epsilon_e(k_e)$, so that $v_h(k_h) = v_e(k_e)$.

4. $$m_h = -m_e \ . \tag{11}$$

We show in (19) below that the effective mass is inversely proportional to the curvature $d^2\epsilon/dk^2$, and for the hole band this has the opposite sign to that for an electron in the valence band. Near the top of the valence band m_e is negative, so that m_h is positive.

[2] Bands are always symmetric under the inversion $\mathbf{k} \rightarrow -\mathbf{k}$ if the spin-orbit interaction is neglected. Even with spin-orbit interaction, bands are always symmetric if the crystal structure permits the inversion operation. Without a center of symmetry, but with spin-orbit interaction, the bands are symmetric if we compare subbands for which the spin direction is reversed: $\epsilon(k, \uparrow) = \epsilon(-k, \downarrow)$. See *QTS*, Chap. 9.

5. $$\hbar \frac{d\mathbf{k}_h}{dt} = e(\mathbf{E} + \frac{1}{c}\mathbf{v}_h \times \mathbf{B}) \ . \tag{12}$$

This comes from the equation of motion

(CGS) $$\hbar \frac{d\mathbf{k}_e}{dt} = -e(\mathbf{E} + \frac{1}{c}\mathbf{v}_e \times \mathbf{B}) \tag{13}$$

that applies to the missing electron when we substitute $-\mathbf{k}_h$ for $\mathbf{k}_e$ and $\mathbf{v}_h$ for $\mathbf{v}_e$. **The equation of motion for a hole is that of a particle of positive charge *e*.** The positive charge is consistent with the electric current carried by the valence band of Fig. 9: the current is carried by the unpaired electron in the orbital G:

$$\mathbf{j} = (-e)\mathbf{v}(G) = (-e)[-\mathbf{v}(E)] = e\mathbf{v}(E) \ , \tag{14}$$

which is just the current of a positive charge moving with the velocity ascribed to the missing electron at E. The current is shown in Fig. 10.

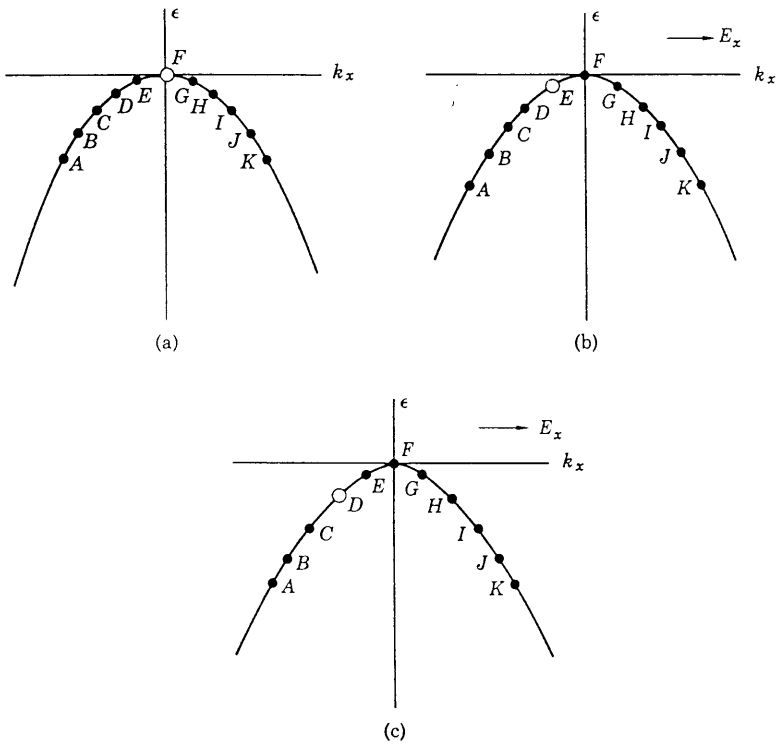

Figure 9 (a) At $t = 0$ all states are filled except F at the top of the band; the velocity v_x is zero at F because $d\epsilon/dk_x = 0$. (b) An electric field E_x is applied in the $+x$ direction. The force on the electrons is in the $-k_x$ direction and all electrons make transitions together in the $-k_x$ direction, moving the hole to the state E. (c) After a further interval the electrons move farther along in k space and the hole is now at D.