### Equilibrium Distributions Chap. 4

- (a) What is the concentration of acceptors? (Assume that  $N_d = 0$ .)
- (b) How many donors  $(g_d = 2, \Delta \mathscr{E}_d = 6 \text{ meV})$  must be introduced to reduce the hole concentration to  $1 \times 10^{17} \text{ cm}^{-3}$ ?
- (c) Consider a sample having the impurity concentrations calculated in parts (a) and (b). If the temperature increases slightly, will the hole concentration increase or decrease? Why?
- **4.13.** A semiconductor sample is made quite thin in its Z dimension so that  $k_z$  may assume very few discrete values. What is the concentration of electrons in the conduction band at equilibrium (electrons per unit area)? Assume that the conduction band is spherically symmetric, the material is nondegenerate, and the effective mass approximation is valid. If the Fermi energy is 4kT below the conduction band energy, what is the concentration of conduction band electrons per unit area in GaAs at 300 K? ( $m_e = 0.067m$ .)

Physical Properties of Semiconductors: Wolfe, Holonyak, Stillman



# Transport Properties

When electrons are in thermal equilibrium with the lattice, they are distributed among possible energy levels in a manner given by the Fermi–Dirac function of (4.41). Under these conditions no net transport of charge or energy occurs since the probability that a state with wavevector k is occupied is the same as that for a state with wavevector  $-\mathbf{k}$ . That is, the equilibrium distribution function,  $f_0$ , is symmetrical about the origin in k-space.

When external forces or temperature gradients are applied to the material, however, this is no longer true. Under these conditions we can, in principle, determine the nonequilibrium distribution function, f, in a manner similar to that used for  $f_0$  in Section 4.1. In the nonequilibrium case, however, we would have to maximize (4.10) for the most probable distribution subject to the additional constraints that a steady flow of charge and energy be maintained. That is,

$$\mathbf{J} = -q \sum_{k} n_k \mathbf{v}_k \tag{5.1}$$

$$\mathbf{W} = \sum_{k} e_k n_k \mathbf{v}_k \tag{5.2}$$

where J is the electrical current density, W is the heat flow density, and  $e_k$  is the heat content per electron. These additional constraints produce an asymmetry in the nonequilibrium distribution function which shifts its center away from the origin in k-space. In this chapter we examine this nonequilibrium distribution of electrons and use it to determine the transport of charge and energy in semiconductors.

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### Sec. 5.1 Boltzmann's Equation

# 5.1 BOLTZMANN'S EQUATION

The approach we take in determining the transport properties of semiconductors is to first construct an electron wave packet from plane wave solutions to the time-dependent Schrödinger equation. This is the same method as that used in Section 2.8. Then, from the correspondence principle, we can use a semiclassical approach.

On this basis, let  $f(\mathbf{k}, \mathbf{r}, t)$  be the probability that a state with wavevector  $\mathbf{k}$  is occupied by an electron with position  $\mathbf{r}$  at time t. The electrons are continually changing their position according to (2.109) and, under the influence of forces  $\mathbf{F}_t$  (other than the periodic crystal forces), are continually changing their wavevector according to (2.111).  $\mathbf{F}_t$  includes applied forces  $\mathbf{F}$  and forces  $\mathbf{F}_c$  due to electron collisions with lattice vibrations and other imperfections in the crystal. Therefore, at time t + dt the probability that a state with wavevector  $\mathbf{k} + d\mathbf{k}$  is occupied by an electron with position  $\mathbf{r}$  $+ d\mathbf{r}$  is given by

$$f\left(\mathbf{k} + \frac{1}{\hbar}\mathbf{F}_{t} dt, \mathbf{r} + \mathbf{v} dt, t + dt\right)$$

The total rate of change in the distribution function in the region of the point  $\mathbf{r}$  is then

$$\frac{df}{dt} = \frac{1}{\hbar} \mathbf{F}_t \cdot \nabla_k f + \mathbf{v} \cdot \nabla_r f + \frac{\partial f}{\partial t}$$
(5.3)

On the right side of (5.3), the first term takes into account changes in the distribution due to forces, the second term accounts for changes due to concentration gradients, and the last term is the local change in the distribution at the point **r**. Equation (5.3) is referred to as Boltzmann's transport equation.

Since the total number of states in the crystal is constant, the total rate of change of the distribution function must be zero (Liouville's theorem), and

$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar} \mathbf{F}_t \cdot \nabla_k f - \mathbf{v} \cdot \nabla_r f = \frac{\partial f}{\partial t} \Big|_c - \frac{1}{\hbar} \mathbf{F} \cdot \nabla_k f - \mathbf{v} \cdot \nabla_r f \qquad (5.4)$$

Because of the difficulty of finding a value for  $\mathbf{F}_c$ , we separate the collision forces from the applied forces by defining a local change in the distribution due to collisions only as

$$\frac{\partial f}{\partial t}\Big|_{c} = -\frac{1}{\hbar} \mathbf{F}_{c} \cdot \nabla_{k} f \tag{5.5}$$

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Let us examine this collision term. The action of applied forces and gradients tends to disturb the distribution function f from its equilibrium value  $f_0$ . If

this disturbance is removed, the scattering processes will tend to restore equilibrium. When the change in the distribution is not large compared to its initial value, it is reasonable to assume that

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial t} \Big|_{c} = \frac{-(f - f_{0})}{\tau_{m}}$$
(5.6)

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where  $\tau_m$  is a constant of proportionality called the *momentum relaxation time*. In general,  $\tau_m$  depends on the electron energy and is different for different scattering mechanisms. We examine  $\tau_m$  for various scattering processes in some detail in Chapter 6. In the meantime, integrating (5.6), we find that

$$f(t) - f_0 = [f(0) - f_0] \exp\left(-\frac{t}{\tau_m}\right)$$
 (5.7)

That is, the momentum relaxation time  $\tau_m$  characterizes an exponential relaxation of the distribution function f to its equilibrium value  $f_0$ .

In the steady state  $\partial f/\partial t = 0$  and using this and (5.6) in (5.4), we obtain the steady-state Boltzmann equation in the relaxation time approximation,

$$f = f_0 - \frac{\tau_m}{\hbar} \mathbf{F} \cdot \nabla_k f - \tau_m \mathbf{v} \cdot \nabla_r f$$
(5.8)

Since

$$\nabla_k f = \frac{\partial f}{\partial \mathfrak{E}} \nabla_k \mathfrak{E} \tag{5.9}$$

the Boltzmann equation can be put in the form

$$f = f_0 - \frac{\tau_m}{\hbar} \frac{\partial f}{\partial \mathcal{E}} \mathbf{F} \cdot \nabla_k \mathcal{E} - \tau_m \mathbf{v} \cdot \nabla_r f$$
(5.10)

From (2.109)

 $\mathbf{v} = \frac{1}{\hbar} \, \boldsymbol{\nabla}_k \boldsymbol{\mathscr{E}}$ 

so that (5.10) is finally

$$f = f_0 - \tau_m \mathbf{v} \cdot \left(\frac{\partial f}{\partial \mathcal{E}} \mathbf{F} + \nabla_r f\right)$$
(5.11)

or

$$f = f_0 - \frac{\tau_m}{\hbar} \nabla_k \mathscr{E} \cdot \left( \frac{\partial f}{\partial \mathscr{E}} \mathbf{F} + \nabla_r f \right)$$
(5.12)

The Boltzmann equation in the form of (5.12) tells us that the nonequilibrium distribution of electrons depends on the scattering processes through the

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term  $\tau_m$ , on the band structure through  $\nabla_k \mathcal{E}$ , on applied forces through  $(\partial f/\partial \mathcal{E})F$ , and on concentration gradients through  $\nabla_r f$ . Therefore, we have, in general, a rather difficult partial differential equation to solve for f, the nonequilibrium distribution function.

## **5.2 DISTRIBUTION FUNCTION**

Before looking at a more general solution for f, let us look at the simplest possible case. We will assume that the only applied force is a small electric field **E** and that there are no concentration or temperature gradients. Under these conditions (5.11) becomes

$$f = f_0 + q\tau_m \frac{\partial f}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{E}$$
(5.13)

Equation (5.13) can be integrated to obtain an analytical expression for f provided that the energy dependence of  $\tau_m$  is known. The solution, however, is nonlinear in E. Under the relaxation time assumption that the change in distribution function is not large, we can also make the approximation that

$$\frac{\partial f}{\partial \mathcal{E}} \simeq \frac{\partial f_0}{\partial \mathcal{E}} \tag{5.14}$$

so that

$$f = f_0 + q\tau_m \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{E}$$
(5.15)

This retains only a linear term in E, which is consistent with our initial assumption of a small electric field.

Let us now look at a more general situation, where we include a small electric field E and an arbitrary magnetic field B in the force term and retain the term for concentration and temperature gradients. Under these conditions (5.8) is

$$\frac{f - f_0}{\tau_m} = \frac{+q}{\hbar} \left( \mathbf{E} + \mathbf{v} \times \mathbf{B} \right) \cdot \nabla_k f - \mathbf{v} \cdot \nabla_r f \tag{5.16}$$

We will assume that the solution for (5.16) has the form of (5.15),

$$f = f_0 + \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{G}$$
 (5.17)

and then solve for the unknown vector G. Inserting (5.17) into (5.16) the term on the left-hand side of (5.16) is simply

Sec. 5.2 Distribution Function

$$\frac{f - f_0}{\tau_m} = \frac{1}{\tau_m} \frac{\partial f_0}{\partial \mathscr{E}} \mathbf{v} \cdot \mathbf{G}$$
(5.18)

The terms on the right-hand side of (5.16) are more difficult to evaluate.

Ignoring  $+q/\hbar$  for the moment, the first term on the right-side of (5.16) is

$$(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_k f = \mathbf{E} \cdot \nabla_k f_0 + (\mathbf{v} \times \mathbf{B}) \cdot \nabla_k f_0$$

+ 
$$\mathbf{E} \cdot \nabla_k \left( \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{G} \right)$$
 +  $(\mathbf{v} \times \mathbf{B}) \cdot \nabla_k \left( \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{G} \right)$  (5.19)

In (5.19) the third term on the right has both E and G and is thus a secondorder term in E. Neglecting this third term and making the substitution

$$\nabla_k f_0 = \frac{\partial f_0}{\partial \mathcal{E}} \hbar \mathbf{v} \tag{5.20}$$

in the first and second term on the right, (5.19) becomes

$$(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_k f = \hbar \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{E} + \hbar \frac{\partial f_0}{\partial \mathcal{E}} (\mathbf{v} \times \mathbf{B}) \cdot \mathbf{v} + (\mathbf{v} \times \mathbf{B}) \cdot \nabla_k \left( \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{G} \right)$$
(5.21)

Since  $(\mathbf{v} \times \mathbf{B}) \cdot \mathbf{v}$  is identically zero, the second term on the right in (5.21) is zero. When we perform the gradient operation in the third term, (5.21) is

$$(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_k f = \hbar \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{E} + \frac{\partial f_0}{\partial \mathcal{E}} (\mathbf{v} \times \mathbf{B}) \cdot \nabla_k (\mathbf{v} \cdot \mathbf{G}) + (\mathbf{v} \cdot \mathbf{G}) (\mathbf{v} \times \mathbf{B}) \cdot \nabla_k \frac{\partial f_0}{\partial \mathcal{E}} \quad (5.22)$$

From (5.20) we see that

$$\nabla_k \frac{\partial f_0}{\partial \mathscr{C}} = \frac{\partial^2 f_0}{\partial \mathscr{C}^2} \hbar \mathbf{v}$$

and the third term on the right in (5.22) vanishes because of  $(\mathbf{v} \times \mathbf{B}) \cdot \mathbf{v}$ . The second term on the right in (5.22) can be resolved into Cartesian components and rearranged to obtain the result,

$$\frac{-q}{\hbar} \left( \mathbf{E} + \mathbf{v} \times \mathbf{B} \right) \cdot \nabla_k f = -q \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{E} - \frac{q}{\hbar^2} \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \left[ \mathbf{B} \times (\mathbf{G} \cdot \nabla_k) \nabla_k \mathcal{E} \right] \quad (5.23)$$

This is the desired form for the first term on the right in (5.16).

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Let us now examine the second term on the right in (5.16),

$$\mathbf{v} \cdot \nabla_{\mathbf{r}} f = \mathbf{v} \cdot \nabla_{\mathbf{r}} f_0 + \mathbf{v} \cdot \nabla_{\mathbf{r}} \left( \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{G} \right)$$
(5.24)

For our purposes we can assume that the spatial dependence of G is small and consider only the first term in (5.24). We then have

$$\mathbf{v} \cdot \nabla_r f = \frac{\partial f_0}{\partial ((\mathscr{E} - \boldsymbol{\mu})/kT)} \mathbf{v} \cdot \nabla_r \left(\frac{\mathscr{E} - \boldsymbol{\mu}}{kT}\right)$$
$$= kT \frac{\partial f_0}{\partial \mathscr{E}} \mathbf{v} \cdot \nabla_r \left(\frac{\mathscr{E} - \boldsymbol{\mu}}{kT}\right)$$
(5.25)

where  $\mu$  is the chemical potential.

Using (5.18), (5.23), and (5.25), Boltzmann's equation is now

$$\frac{1}{\tau_m} \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{G} = +q \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{E} + \frac{q}{\hbar^2} \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot [\mathbf{B} \times (\mathbf{G} \cdot \nabla_k) \nabla_k \mathcal{E}] - kT \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \nabla_r \left(\frac{\mathcal{E} - \mu}{kT}\right) \quad (5.26)$$

Since each term in (5.26) has a common factor  $(\partial f_0/\partial \mathscr{E})v$  on the left, it can be eliminated to obtain

$$\frac{1}{\tau_m} G = +q\mathbf{E} - kT \, \nabla_r \left(\frac{\mathscr{E} - \mu}{kT}\right) + \frac{q}{\hbar^2} \left[\mathbf{B} \times (\mathbf{G} \cdot \nabla_k) \nabla_k \mathscr{E}\right] \quad (5.27)$$

Defining an electrothermal field for electrons,  $\mathcal{F}$ , by

$$q\mathcal{F} = +q\mathbf{E} - T\nabla_r \left(\frac{\mathcal{E} - \mu}{T}\right)$$
(5.28)

(5.27) has the form

$$\mathbf{G} = q\tau_m \mathcal{F} + \frac{q\tau_m}{\hbar^2} \left[ \mathbf{B} \times (\mathbf{G} \cdot \nabla_k) \nabla_k \mathcal{E} \right]$$
(5.29)

Equation (5.29) can be solved for G by using an explicit expression for the conduction band minima. For this purpose we will assume ellipsoidal minima with a quadratic dispersion relationship as given by (2.117). In vector notation we have

$$\mathscr{E} = \mathscr{E}_c + \frac{1}{2}\hbar^2 \mathbf{k} \cdot \mathbf{M} \cdot \mathbf{k} \tag{5.30}$$

where

$$\mathbf{M} = \begin{bmatrix} \frac{1}{m_1^*} & 0 & 0\\ 0 & \frac{1}{m_2^*} & 0\\ 0 & 0 & \frac{1}{m_3^*} \end{bmatrix}$$
(5.31)

is the effective mass tensor, the k on its left is a row vector, and the k on its right is a column vector. From (5.30),

$$(\mathbf{G} \cdot \boldsymbol{\nabla}_k) \boldsymbol{\nabla}_k \mathscr{E} = \hbar^2 \mathbf{M} \cdot \mathbf{G} \tag{5.32}$$

and (5.29) takes the form

$$\mathbf{G} = q\tau_m \mathcal{F} + q\tau_m \mathbf{B} \times (\mathbf{M} \cdot \mathbf{G}) \tag{5.33}$$

Reducing this equation to its components and solving for G, we have, finally,

$$\mathbf{G} = q\tau_m \left[ \frac{\mathcal{F} - q\tau_m \mathbf{M} \cdot (\mathcal{F} \times \mathbf{B}) + (q\tau_m)^2 (\det \mathbf{M}) (\mathcal{F} \cdot \mathbf{B}) (\mathbf{M}^{-1} \cdot \mathbf{B})}{1 + (q\tau_m)^2 (\det \mathbf{M}) (\mathbf{M}^{-1} \cdot \mathbf{B}) \cdot \mathbf{B}} \right]$$
(5.34)

The nonequilibrium distribution function for electrons in ellipsoidal conduction band minima is obtained by using G from (5.34) in (5.17). For spherical minima the distribution function is

$$f = f_0 + \frac{\partial f_0}{\partial \mathscr{E}} q \tau_m \mathbf{v} \cdot \left[ \frac{\mathscr{F} - (q \tau_m/m^*)(\mathscr{F} \times \mathbf{B}) + (q \tau_m/m^*)^2 (\mathscr{F} \cdot \mathbf{B}) \mathbf{B}}{1 + (q \tau_m/m^*)^2 \mathbf{B} \cdot \mathbf{B}} \right]$$
(5.35)

We can see that there are four components to the distribution function. The first is simply the equilibrium function  $f_0$  given by (4.41), which does not contribute to the transport of charge and energy. The term that involves  $\mathcal{F}$  is the ohmic contribution to the transport properties. This term accounts for electrical and thermal conductivity as well as the Seebeck, Peltier, and Thomson effects. The term with  $\mathcal{F} \times \mathbf{B}$  is the Hall contribution to transport and accounts for the Hall, Ettinghausen, Nernst, and Righi–Leduc effects. The  $\mathbf{B}^2$  terms in the numerator and denominator of (5.35) account for magnetoresistive effects. We discuss these various effects in more detail later.

The distribution function derived above for electrons can also be used for holes when the appropriate parameters of q,  $m^*$ , and  $\tau_m$  are substituted in the equations.

From (5.1) and (5.2) we can determine the current density J and heat flow density W by summing (or integrating)  $n_k v_k$  and  $e_k n_k v_k$ , respectively, over the first Brillouin zone. In (4.68), however, we have already obtained

an expression for n, the number of electrons in the conduction band minima. For this reason we can approach the problem from a different point of view. That is, the current density can be determined by

$$\mathbf{J} = -qn\langle \mathbf{v} \rangle \tag{5.36}$$

where  $\langle \mathbf{v} \rangle$  is the average velocity of the *n* electrons in the nonequilibrium distribution. In a similar manner the heat flow density can be obtained from

$$\mathbf{W} = n\langle e\mathbf{v} \rangle \tag{5.37}$$

where the heat content per electron and the velocity are averaged over the distribution. The problem is to determine how this averaging should be performed.

### 5.3 CHARGE TRANSPORT

For this purpose let us examine the current density for spherical conduction band minima in a small electric field. The average velocity is obtained by summing the velocities of all the electrons in the distribution and normalizing the result. That is,

$$\langle \mathbf{v} \rangle = \frac{\int_{-\infty}^{\infty} \mathbf{v} f \, d\mathbf{v}}{\int_{-\infty}^{\infty} f \, d\mathbf{v}}$$
(5.38)

where f is given by (5.15). Inserting (5.15) in (5.38), we have

$$\langle \mathbf{v} \rangle = \frac{\int_{-\infty}^{\infty} \mathbf{v} f_0 \, d\mathbf{v} + q \, \int_{-\infty}^{\infty} \tau_m(\partial f_0 / \partial \mathcal{E}) \mathbf{v}(\mathbf{v} \cdot \mathbf{E}) \, d\mathbf{v}}{\int_{-\infty}^{\infty} f_0 \, d\mathbf{v} + q \, \int_{-\infty}^{\infty} \tau_m(\partial f_0 / \partial \mathcal{E}) (\mathbf{v} \cdot \mathbf{E}) \, d\mathbf{v}}$$
(5.39)

The term on the left in the numerator of this equation is an average over the equilibrium distribution. Since there is no transport of charge in equilibrium, this term is zero. The term on the right in the denominator provides for additional nonequilibrium carriers over the equilibrium concentration. We will take this term to be zero as well. Equation (5.39) is therefore

$$\langle \mathbf{v} \rangle = \frac{+q \int_{-\infty}^{\infty} \tau_m (\partial f_0 / \partial \mathscr{E}) \mathbf{v} (\mathbf{v} \cdot \mathbf{E}) \, d\mathbf{v}}{\int_{-\infty}^{\infty} f_0 \, d\mathbf{v}}$$
(5.40)

For spherical conduction band minima we can replace the integrals over three-dimensional velocity space by integrals over energy with relative

### Sec. 5.3 Charge Transport

ease. From (2.109) and (2.118) the relationship between & and v is

$$\mathscr{E} - \mathscr{E}_c = \frac{1}{2}m^* \mathbf{v}^2 = \frac{1}{2}m^* v^2 \tag{5.41}$$

and the differential volume in velocity space is

$$d\mathbf{v} = 4\pi v^2 \, dv \tag{5.42}$$

With (5.41) and (5.42), (5.40) becomes

$$\langle \mathbf{v} \rangle = \frac{+q \int_{\mathscr{E}_c}^{\infty} \tau_m (\partial f_0 / \partial \mathscr{E}) \mathbf{v} (\mathbf{v} \cdot \mathbf{E}) (\mathscr{E} - \mathscr{E}_c)^{1/2} d\mathscr{E}}{\int_{\mathscr{E}_c}^{\infty} f_0 (\mathscr{E} - \mathscr{E}_c)^{1/2} d\mathscr{E}}$$
(5.43)

If we consider an electric field in the x direction, the term

$$\mathbf{v}(\mathbf{v} \cdot \mathbf{E}) = + v_x^2 E_x \tag{5.44}$$

Assuming equipartition of energy, each degree of freedom has the same average kinetic energy and

$$v^2 = v_x^2 + v_y^2 + v_z^2 = 3v_x^2 \tag{5.45}$$

Using (5.44) and (5.45), (5.43) is then

$$\langle v_x \rangle = \frac{2qE_x}{3m^*} \frac{\int_{\mathscr{K}_c}^{\infty} \tau_m (\partial f_0 / \partial \mathscr{E}) (\mathscr{E} - \mathscr{E}_c)^{3/2} \, d\mathscr{E}}{\int_{\mathscr{K}_c}^{\infty} f_0 (\mathscr{E} - \mathscr{E}_c)^{1/2} \, d\mathscr{E}}$$
(5.46)

Defining a drift velocity  $v_d$  as the average velocity of the carriers over the distribution, and introducing the dimensionless variables of (4.65), (5.46) becomes

$$v_{dx} = \frac{-qE_x}{m^*} \langle \tau_m \rangle \tag{5.47}$$

where

$$\langle \tau_m \rangle = \frac{2}{3} \frac{\int_0^\infty \tau_m (-\partial f_0 / \partial x) x^{3/2} \, dx}{\int_0^\infty f_0 x^{1/2} \, dx}$$
(5.48)

Equation (5.48) gives the proper form for the averaging procedure over the distribution of electrons. By evaluating the average momentum relaxation time in the manner proscribed, we can determine the drift velocity from (5.47). Equation (5.47) tells us that for small electric fields, the drift velocity is directly proportional to the field. The constant of proportionality

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where  $\tau_0$  is independent of energy. Equation (5.54) is then

$$\langle \tau_{m}^{s} x' \rangle = \frac{2}{3} \tau_{0}^{s} \frac{\int_{0}^{\infty} (-\partial f_{0}/\partial x) x^{sr+t+3/2} dx}{\int_{0}^{\infty} f_{0} x^{1/2} dx}$$
(5.56)

This equation can be solved by integrating by parts.

Let  $u = x^{sr+t+3/2}$  and  $dv = (-\partial f_0/\partial x) dx$ . Then  $du = (sr + t + \frac{3}{2})x^{sr+t+1/2} dx$  and  $v = -f_0$ . Using these expressions in the numerator of (5.56) gives us

$$\langle \tau_m^s x' \rangle = \frac{2}{3} \tau_0^s \frac{-[f_0 x^{sr+t+3/2}]_0^\infty + (sr+t+\frac{3}{2}) \int_0^\infty f_0 x^{sr+t+1/2} \, dx}{\int_0^\infty f_0 x^{1/2} \, dx}$$
(5.57)

or

$$\langle \tau_m^s x^t \rangle = \frac{2}{3} \left( sr + t + \frac{3}{2} \right) \tau_0^s \frac{\int_0^\infty f_0 x^{sr + t + 1/2} \, dx}{\int_0^\infty f_0 x^{1/2} \, dx}$$
(5.58)

The integral in the numerator is a Fermi-Dirac integral of order j given by

$$F_{j}(\eta) = \frac{1}{j!} \int_{0}^{\infty} f_{0} x^{j} dx$$
 (5.59)

The integral in the denominator is simply a Fermi-Dirac integral of order  $\frac{1}{2}$  which we saw before in (4.67). Values for these integrals are tabulated in Appendix B. Using (5.59) and (4.67), we obtain

$$\langle \tau_m^s x^t \rangle = \frac{4}{3\sqrt{\pi}} \left( sr + t + \frac{3}{2} \right)! \, \tau_0^s \frac{F_{sr+t+1/2}(\eta)}{F_{1/2}(\eta)} \tag{5.60}$$

which is the final form for the average.

To determine transport parameters, we will use expressions of the form  $\langle \tau_m^s x' \rangle$ , which can then be evaluated with (5.60). As an example, the conductivity mobility in (5.50) and the conductivity in (5.52) can be obtained from

$$\langle \tau_m \rangle = \frac{4(r+\frac{3}{2})! \tau_o}{3\sqrt{\pi}} \frac{F_{r+1/2}(\eta)}{F_{1/2}(\eta)}$$
(5.61)

when the value of r for the appropriate scattering mechanism is known.

Let us now look at the transport of electrons in both electric and magnetic fields. Assuming no concentration or temperature gradients, (5.34)

is called the *conductivity mobility*,  $\mu_c$ . Thus (5.47) can be put in the form

$$v_{dx} = -\mu_c E_x \tag{5.49}$$

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where

$$\mu_c = \frac{q\langle \tau_m \rangle}{m^*} \tag{5.50}$$

From (5.36) and (5.47) the current density in the x direction is

$$J_x = \frac{q^2 n \langle \tau_m \rangle}{m^*} E_x \tag{5.51}$$

Since the constant of proportionality between current density and electric field is referred to as the conductivity, we have

$$\sigma = \frac{q^2 n \langle \tau_m \rangle}{m^*} \tag{5.52}$$

and

$$\sigma = qn\mu_c \tag{5.53}$$

Thus, for the simple case of a small applied electric field, we can define all the transport parameters in terms of the average momentum relaxation time,  $\langle \tau_m \rangle$ . Once  $\langle \tau_m \rangle$  has been obtained, the transport problem is solved.

In general, however, the quantity to be averaged is more complex. For example, to determine the energy transport from (5.37), an extra energy term is included in the average. Also, from (5.34) the vector G depends on multiple powers of  $\tau_m$  and depends on energy through both  $\tau_m$  and  $\mathcal{F}$ . Thus the quantity that must be averaged over the electron distribution in more complex transport problems has the form  $\tau_m^s x'$ , where s and t are to be determined. Equation (5.48) shows that the averaging procedure for this quantity is

$$\langle \tau_m^s x' \rangle = \frac{2}{3} \frac{\int_0^\infty \tau_m^s (-\partial f_0 / \partial x) x'^{+3/2} \, dx}{\int_0^\infty f_0 x^{1/2} \, dx}$$
(5.54)

Equation (5.54) can be evaluated if we know the dependence of  $\tau_m$  on electron energy. In Chapter 6 we will find that  $\tau_m$  can be represented as having a simple power dependence on energy for most scattering mechanisms. Therefore, let us take the momentum relaxation time as having the form

$$\tau_m = \tau_0 x^r \tag{5.55}$$

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reduces to

$$\mathbf{G} = +q\tau_m \left[ \frac{\mathbf{E} - (q\tau_m/m^*)(\mathbf{E} \times \mathbf{B}) + (q\tau_m/m^*)^2 \mathbf{B}(\mathbf{E} \cdot \mathbf{B})}{1 + (q\tau_m/m^*)^2 \mathbf{B} \cdot \mathbf{B}} \right]$$
(5.62)

From (5.47) and (5.48) the drift velocity is

$$\mathbf{v}_{d} = \frac{2}{3m^{*}} \frac{\int_{0}^{\infty} \mathbf{G}(-\partial f_{0}/\partial x) x^{3/2} dx}{\int_{0}^{\infty} f_{0} x^{1/2} dx}$$
(5.63)

and the current density is given by (5.36). Because of (5.58), it is not necessary to average each term of **G** to obtain the current density. We simply have, by inspection,

$$\mathbf{J} = \frac{q^2 n}{m^*} \left\langle \frac{\tau_m}{1 + (\omega_c \tau_m)^2} \right\rangle \mathbf{E} - \frac{q^3 n}{m^{*2}} \left\langle \frac{\tau_m^2}{1 + (\omega_c \tau_m)^2} \right\rangle (\mathbf{E} \times \mathbf{B}) + \frac{q^4 n}{m^{*3}} \left\langle \frac{\tau_m^3}{1 + (\omega_c \tau_m)^2} \right\rangle \mathbf{B}(\mathbf{E} \cdot \mathbf{B})$$
(5.64)

where we have introduced the cyclotron frequency

$$\omega_c \equiv \frac{q \mid \mathbf{B} \mid}{m^*} \tag{5.65}$$

The first term in (5.64) is the ohmic term. The factor  $1 + (\omega_c \tau_m)^2$  in the denominator of the average in this term reflects the magnetoresistance or reduction in conductivity due to the magnetic field. The second term reflects the Hall effect; it also has magnetoresistance associated with it. The third term is an additional magnetoresistance term.

Let us look at (5.64) for small magnetic fields. Under this condition the second-order terms in **B**, which produce the magnetoresistance, are small and

$$\mathbf{J} = \frac{q^2 n}{m^*} \langle \tau_m \rangle \mathbf{E} - \frac{q^3 n}{m^{*2}} \langle \tau_m^2 \rangle (\mathbf{E} \times \mathbf{B})$$
(5.66)

If we take  $\mathbf{B} = \hat{z}B_z$ , (5.66) becomes

$$J_x = \frac{q^2 n}{m^*} \langle \tau_m \rangle E_x - \frac{q^3 n}{m^{*2}} \langle \tau_m^2 \rangle E_y B_z$$
(5.67)

$$J_{y} = \frac{q^{2}n}{m^{*}} \langle \tau_{m} \rangle E_{y} + \frac{q^{3}n}{m^{*2}} \langle \tau_{m}^{2} \rangle E_{x} B_{z}$$
(5.68)

$$J_z = \frac{q^2 n}{m^*} \langle \tau_m \rangle E_z \tag{5.69}$$

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When  $J_y = 0$ , (5.68) gives us

$$E_x = -\frac{m^*}{qB_z} \frac{\langle \tau_m \rangle}{\langle \tau_m^2 \rangle} E_y \tag{5.70}$$

Using (5.70) in (5.67) and neglecting a second-order term in  $B_z$ , we have

$$J_x = \frac{-qn}{B_z} \frac{\langle \tau_m \rangle^2}{\langle \tau_m^2 \rangle} E_y$$
(5.71)

That is,  $J_x$  and  $B_z$  induce a field  $E_y$ . This is the Hall effect. These geometric constraints are obtained experimentally by applying a magnetic field in the z direction, a current in the x direction, and measuring the voltage in the y direction with a high-impedance voltmeter, so that the current in the y direction is negligible.

The Hall constant is defined as

$$R_{H} \equiv \frac{E_{y}}{J_{x}B_{z}} = -\frac{1}{qn} \frac{\langle \tau_{m}^{2} \rangle}{\langle \tau_{m} \rangle^{2}}$$
(5.72)

From (5.72) we can see that the concentration of electrons in the conduction band can be obtained from an experimental determination of the Hall constant. If the charge carriers are holes in the valence bands, the negative q's in (5.28), (5.34), and (5.36) are replaced by positive q's. The resulting Hall constant is

$$R_H = \frac{1}{qp} \frac{\langle \tau_m^2 \rangle}{\langle \tau_m \rangle^2} \tag{5.73}$$

Thus the sign of the Hall constant (and Hall field) indicates the sign of the charge carriers and Hall measurements can be used to distinguish between n- and p-type material. With (5.53) for the conductivity, we can define a *Hall mobility* as

$$\mu_{\rm H} = R_{\rm H}\sigma = \mu_c \frac{\langle \tau_m^2 \rangle}{\langle \tau_m \rangle^2}$$
(5.74)

This mobility differs from the conductivity mobility  $\mu_c$  by the factor

$$r_{\rm H} \equiv \frac{\langle \tau_m^2 \rangle}{\langle \tau_m \rangle^2} \tag{5.75}$$

which is referred to as the *Hall factor*. For a nondegenerate semiconductor, we find, from (5.60),

$$r_{\rm H} = \frac{3\sqrt{\pi}}{4} \frac{(2r+\frac{3}{2})!}{[(r+\frac{3}{2})!]^2}$$
(5.76)

(In the analysis of experimental data, the Hall factor is often assumed to be

### Sec. 5.3 Charge Transport

1. Depending on the relevant scattering mechanisms and temperature, this can produce about an 80% error in the carrier concentration.)

Let us next examine the flow of charge for small electric fields in the presence of electron concentration gradients. We will assume there are no magnetic fields or temperature gradients. Under these conditions the electrothermal field (5.28) for electrons is

$$\mathcal{F} = +\mathbf{E} + \frac{1}{q} \nabla_r \mu = + \frac{1}{q} \nabla_r \zeta \qquad (5.77)$$

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and from (5.34),

$$\mathbf{G} = q\tau_m \mathbf{E} + \tau_m \nabla_r \mu = + \tau_m \nabla_r \zeta \tag{5.78}$$

Equations (5.36), (5.47), and (5.34) tell us that the electron current density is given by

$$\mathbf{J} = \frac{+qn}{m^*} \langle \mathbf{G} \rangle \tag{5.79}$$

or

$$\mathbf{J} = \frac{q^2 n}{m^*} \langle \tau_m \rangle \mathbf{E} + \frac{q n}{m^*} \langle \tau_m \rangle \nabla_r \mu$$
(5.80)

Using (5.50) for the conductivity mobility. (5.80) becomes

$$\mathbf{J} = qn\mu_n \mathbf{E} + n\mu_n \, \nabla_r \mu \tag{5.81}$$

where  $\mu_n$  indicates conductivity mobility for electrons.

The gradient of the chemical potential can be written in terms of a concentration gradient as

$$\nabla_r \mu = \frac{\partial \eta}{\partial n} \frac{\partial \mu}{\partial \eta} \nabla_r n \qquad (5.82)$$

Since

$$\frac{d}{d\eta}F_j(\eta) = F_{j-1}(\eta)$$
(5.83)

[J. McDougall and E. C. Stoner, *Philos. Trans. R. Soc. London 237*, 67 (1938)], (4.68) gives us

$$\frac{\partial n}{\partial \eta} = N_c F_{-1/2}(\eta) \tag{5.84}$$

Also, from (4.65),

$$\frac{\partial \eta}{\partial \mu} = \frac{1}{kT} \tag{5.85}$$

Using (5.84), (5.85), and (4.68) the chemical potential gradient is

$$\nabla_r \mu = \frac{kT}{N_c F_{1/2}(\eta)} \nabla_r n \tag{5.86}$$

and the electron current density is

$$\mathbf{J} = qn\mu_n \mathbf{E} + kT\mu_n \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)} \nabla_r n$$
(5.87)

Equation (5.87) shows that in the presence of an electric field and a concentration gradient, the electron current density consists of two components: The first component is proportional to the electric field and is called the *drift* term. The second component is directly related to the concentration gradient and is referred to as the *diffusion* term. Notice that the electron current density is in the same direction as the concentration gradient, which is in the direction of increasing concentration.

The diffusion component of current is usually obtained from Fick's first law as  $qD_n \nabla_r n$ , where  $D_n$  is the diffusion constant of the electrons. In comparison with (5.87), we find that

$$D_n = \frac{kT}{q} \mu_n \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)}$$
(5.88)

Equation (5.88) is the Einstein relationship between the diffusion coefficient and the conductivity mobility. Although this relationship is easily derived for an equilibrium condition where the total current density is zero, the approach we have taken shows that Einstein's relation is also valid under nonequilibrium conditions.

Following similar arguments for valence band holes, the current density is

$$\mathbf{J} = qp\mu_p \mathbf{E} - kT\mu_p \frac{F_{1/2}(\boldsymbol{\eta})}{F_{-1/2}(\boldsymbol{\eta})} \nabla_r p$$
(5.89)

where  $\mu_p$  is the conductivity mobility for holes. Notice that the diffusion component of hole current is opposite to the direction of the hole gradient. From Fick's law the diffusion coefficient for holes is also of the form of (5.88). When the Fermi energy is in the energy gap at least 4kT removed from either band edge, (5.88) reduces to

$$D_n = \frac{kT}{q} \mu_n \tag{5.90}$$

The equations we have derived for the mobility (5.50), conductivity (5.52), and Hall constant (5.72) are applicable for electrons in spherical conduction band minima. When the electrons transport charge in an ellipsoidal minimum, the situation is somewhat more complicated. Consider one ellipsoidal

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soldal conduction band minimum at  $\Gamma$  given by (5.30). If the x direction is taken as one of the axes of the constant energy ellipsoids, an electric field in the x direction will produce a current in the x direction,

$$J_x = \frac{q^2 n \langle \tau_m \rangle}{m_1^*} E_x \tag{5.91}$$

Similar expressions containing  $m_2^*$  and  $m_3^*$  are obtained in the y and z directions. The total current density is therefore

$$\mathbf{J} = q^2 n \langle \mathbf{\tau}_m \rangle \mathbf{M} \cdot \mathbf{E} \tag{5.92}$$

where the effective mass tensor M is given by (5.31). This can also be put in the form

$$\mathbf{J} = \boldsymbol{\sigma} \cdot \mathbf{E} \tag{5.93}$$

where  $\sigma$  is a conductivity tensor and E is a column vector. Thus, for an ellipsoidal minimum at  $\Gamma$ , the current density is not necessarily in the same direction as the applied electric field.

When there are  $g_c$  equivalent ellipsoidal conduction band minima, it is necessary to account for the fact that the concentration of electrons in each minimum is  $n/g_c$ . In this case the current density is obtained by summing the concentration of electrons in each minimum, while allowing for the effective mass each minimum has in the direction of the current. For a semiconductor with conduction band minima in the direction of X, such as Si, this is relatively easy. As shown in Fig. 5.1, when the current is in the x direction, the two minima along the  $k_x$  axis each contribute n/6 electrons with effective mass  $m_1^*$ , while the two minima along the  $k_y$  axis contribute n/6 electrons each with effective mass  $m_2^*$ . In the third dimension, the two minima along the k<sub>z</sub> axis also contribute n/6 electrons of mass  $m_3^*$ . The total

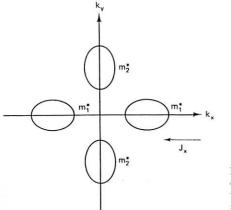


Figure 5.1 Diagram showing how equivalent ellipsoidal minima contribute to conduction along one of their principal axes.

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current density in the x direction is therefore

$$J_x = \frac{q^2 n \langle \tau_m \rangle}{6} \left( \frac{2}{m_1^*} + \frac{2}{m_2^*} + \frac{2}{m_3^*} \right) E_x$$
(5.94)

Similar expressions are obtained for the components of current in the y and z directions. Thus the total current can be put in the form

$$\mathbf{J} = \frac{q^2 n \langle \tau_m \rangle}{m_c} \mathbf{E}$$
(5.95)

where

$$\frac{1}{m_c} \equiv \frac{1}{3} \left( \frac{1}{m_1^*} + \frac{1}{m_2^*} + \frac{1}{m_3^*} \right)$$
(5.96)

defines the conductivity effective mass.

Equation (5.96) is also valid for semiconductors, such as Ge, which have equivalent minima in directions other than X. Notice that the conductivity effective mass defined by (5.96) is a scalar, so that the current density and the electric field are always in the same direction. Comparing (5.95) with (5.92), we see that equivalent ellipsoidal minima result in isotropic conductivity, while an ellipsoidal minimum at  $\Gamma$  produces anisotropic conductivity. This difference due to the position of ellipsoidal minima is reflected in the conductivity of sphalerite crystals with indirect bandgaps as compared to wurtzite crystals with direct bandgaps.

When the Hall effect in ellipsoidal minima is examined, similar results are obtained. That is, an ellipsoidal conduction band minimum at  $\Gamma$  produces an anisotropic Hall effect, while equivalent minima produce an isotropic Hall effect. In the latter case, for simplicity, a Hall effective mass can be defined to reduce the expression for the Hall mobility to the form of (5.74).

# 5.4 CHARGE AND ENERGY TRANSPORT

To determine the heat flow density, (5.37) tells that we must find the average

$$\langle e\mathbf{v}\rangle = \frac{\int_{-\infty}^{\infty} e\mathbf{v}f \, d\mathbf{v}}{\int_{-\infty}^{\infty} f \, d\mathbf{v}}$$
 (5.97)

where e is heat content per electron. This equation has the same form as (5.38) except that, in this case, we must include e in the average since edepends on the electron energy. We have already solved this problem with (5.60), so in the same way we obtained (5.79) we can simply write

$$\mathbf{W} = \frac{-n}{m^*} \langle e\mathbf{G} \rangle \tag{5.98}$$

where the minus sign indicates that W is opposite in direction to G and thus J for electrons. It is now necessary to obtain e in terms of  $\mathcal{E}$ , so that the average in (5.98) can be determined.

Since heat is that portion of the total electron energy which can be added or removed in disordered form, the heat content of all the electrons in the system is given by the entropy term in Euler's equation (4.28). Thus the heat content per electron is

$$e = \left[\frac{\partial}{\partial n'} \left(TS\right)\right]_{T,V}$$
(5.99)

From (4.29) for the Helmholtz function,

$$TS = \mathcal{E}' - F \tag{5.100}$$

where  $\mathscr{E}'$  is the total energy of all the electrons. Using (5.100) in (5.99), we have

$$e = \left(\frac{\partial \mathscr{E}'}{\partial n'}\right)_{T,V} - \left(\frac{\partial F}{\partial n'}\right)_{T,V}$$
(5.101)

The first term in (5.101) is simply the energy per electron,  $\mathcal{E}$ . From (4.39) the second term is simply the chemical potential,  $\mu$ . The heat content per electron is therefore

$$e = \mathscr{E} - \mu \tag{5.102}$$

Let us now obtain the equations that determine the transport of charge and energy under the following conditions. We will assume that the electric and magnetic fields are small and allow for temperature and concentration gradients. Also, for simplicity we will assume spherical energy band extrema. From (5.79) and (5.34) the equation for the electron current density is

$$\mathbf{J} = \frac{+q^2 n}{m^*} \left[ \langle \tau_m \mathcal{F} \rangle - \frac{q}{m^*} \langle \tau_m^2 (\mathcal{F} \times \mathbf{B}) \rangle \right]$$
(5.103)

Using (5.98), (5.102), and (5.34), the electron heat current density is

$$W = \frac{-qn}{m^*} \left[ \langle \tau_m e \mathcal{F} \rangle - \frac{q}{m^*} \langle \tau_m^2 e (\mathcal{F} \times \mathbf{B}) \rangle \right]$$
(5.104)

where from (5.28),

$$\mathcal{F} = +\mathbf{E} - \frac{1}{q} \nabla_r e + \frac{e}{qT} \nabla_r T \qquad (5.105)$$

We will use (5.103), (5.104), and (5.105) to examine various effects that involve the transport of charge and energy in semiconductors.

## Sec. 5.4 Charge and Energy Transport

### 5.4.1 Thermal Conductivity

One of the more important thermal transport parameters is the thermal conductivity. Although in lightly doped semiconductors most of the heat is carried by lattice vibrations or phonons, in heavily doped semiconductors a substantial proportion is carried by electrons. The thermal conductivity,  $\kappa$ , is defined as the proportionality factor between the heat current density and the temperature gradient,

$$\mathbf{W} = -\kappa \, \boldsymbol{\nabla}_r T \tag{5.106}$$

The minus sign is required because the heat flows from higher to lower temperatures. To determine the thermal conductivity, we examine a sample under open-circuit conditions (J = 0) with no magnetic field. For small temperature gradients, (5.103) is

$$0 = +\langle \tau_m \rangle \left( \mathbf{E} + \frac{1}{q} \, \boldsymbol{\nabla}_r \boldsymbol{\mu} \right) + \frac{1}{qT} \langle \tau_m e \rangle \, \boldsymbol{\nabla}_r T \tag{5.107}$$

and (5.104) is

$$\mathbf{W} = \frac{-qn}{m^*} \left[ \langle \tau_m e \rangle \left( \mathbf{E} + \frac{1}{q} \, \nabla_r \mu \right) + \frac{1}{qT} \langle \tau_m e^2 \rangle \, \nabla_r T \right]$$
(5.108)

Using (5.107) in (5.108) yields

$$W = \frac{-n}{m^*T} \left[ \langle \tau_m e^2 \rangle - \frac{\langle \tau_m e \rangle^2}{\langle \tau_m \rangle} \right] \nabla_r T$$
(5.109)

and the thermal conductivity due to electrons is

$$\kappa = \frac{n}{m^* T} \left[ \langle \tau_m e^2 \rangle - \frac{\langle \tau_m e \rangle^2}{\langle \tau_m \rangle} \right]$$
(5.110)

Numerical values for the averages in (5.110) can be obtained with (5.60).

# 5.4.2 Thermoelectric Effects

We can see from (5.107) that under open-circuit conditions, the electrons diffuse down the temperature gradient and set up an electric field that opposes the motion of electrons due to the gradient. The production of an electric field by a temperature gradient is referred to as the *Seebeck* or *thermoelectric* effect. In the steady state the electric field is given by (5.107) as

$$\mathbf{E} = -\frac{1}{q} \, \nabla_r \mu \, - \frac{1}{q \langle \tau_m \rangle T} \langle \tau_m e \rangle \, \nabla_r T \tag{5.111}$$

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$$\nabla_{r}\mu = \frac{\partial\mu}{\partial T} \nabla_{r}T \qquad (5.112)$$

(5.111) gives us

$$\mathbf{E} = -\frac{1}{qT} \left[ T \frac{\partial \mu}{\partial T} + \frac{\langle \tau_m e \rangle}{\langle \tau_m \rangle} \right] \nabla_r T \qquad (5.113)$$

or

$$\mathbf{E} = T \frac{d}{dT} \left[ \frac{\langle \tau_m e \rangle}{qT \langle \tau_m \rangle} \right] \nabla_r T$$
(5.114)

Thus the electric field is related to the temperature gradient by means of the equation

$$\mathbf{E} = \mathcal{T} \, \boldsymbol{\nabla}_r T \tag{5.115}$$

where

$$\mathcal{T} = T \frac{d}{dT} \left[ \frac{\langle \tau_m e \rangle}{qT \langle \tau_m \rangle} \right]$$
(5.116)

is the Thomson coefficient.

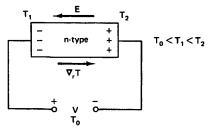
As indicated in Fig. 5.2, the Seebeck effect can be examined by measuring the voltage across a semiconductor in a temperature gradient. The voltage is given by

$$V = -\oint \mathbf{E} \cdot d\mathbf{r} = \oint \mathcal{F} \nabla_r T \cdot d\mathbf{r}$$

$$V = \int_{T_0}^{T_1} \mathcal{T}_m \, dT + \int_{T_1}^{T_2} \mathcal{T}_s \, dT + \int_{T_2}^{T_0} \mathcal{T}_m \, dT \qquad (5.117)$$

$$V = \int_{T_1}^{T_2} (\mathcal{T}_s - \mathcal{T}_m) \, dT$$

where  $\mathcal{T}_s$  and  $\mathcal{T}_m$  are the Thomson coefficients for the semiconductor and



**Figure 5.2** Determination of Seebeck effect for *n*-type semiconductor. *V* is negative.

metal, respectively. If the metal is chosen to have 
$$\mathcal{T}_m = 0$$
, the Seebeck voltage is directly related to the Thomson coefficient of the semiconductor and the temperature difference across the sample. Notice that the Thomson coefficient for electrons is negative, as indicated by (5.115). For holes under the same conditions, the Thomson coefficient is positive, so that the field and temperature gradients are in the same direction.

A transport parameter closely related to the Thomson coefficient is the absolute *thermoelectric power*,  $\mathcal{P}$ . The relationship is

$$\mathcal{T} = -T\frac{d}{dT}\mathcal{P} \tag{5.118}$$

or from (5.116),

$$\mathcal{P} = -\frac{\langle \tau_m e \rangle}{qT \langle \tau_m \rangle} \tag{5.119}$$

Notice that the thermoelectric power for electrons and holes have opposing signs, due to the dependence on q. Because of this the sign of the thermoelectric power can be used to determine whether a material exhibits *n*-or *p*-type conductivity.

When the electric current density is not constrained to be zero, it adds an additional component to the heat current density. Under these conditions (5.103) can be written in the form

$$\mathbf{E} + \frac{1}{q} \nabla_r \mu = \frac{m^*}{q^2 n \langle \tau_m \rangle} \mathbf{J} - \frac{1}{qT} \frac{\langle \tau_m e \rangle}{\langle \tau_m \rangle} \nabla_r T \qquad (5.120)$$

Substituting this into (5.108), the heat current density is

$$\mathbf{W} = \frac{-\langle \tau_m e \rangle}{q \langle \tau_m \rangle} \mathbf{J} - \frac{n}{m^* T} \left[ \langle \tau_m e^2 \rangle - \frac{\langle \tau_m e \rangle^2}{\langle \tau_m \rangle} \right] \nabla_r T \qquad (5.121)$$

Using (5.110) and (5.119), this is simply

$$\mathbf{W} = T \mathcal{P} \mathbf{J} - \kappa \, \nabla_r T \tag{5.122}$$

Thus the electric current density carries heat in addition to that transported by the temperature gradient. This is referred to as the *Peltier effect*. The constant of proportionality between heat current density and electric current density is the Peltier coefficient,  $\Pi$ , where

$$\Pi \equiv T \mathcal{P} \tag{5.123}$$

$$\Pi = -\frac{\langle \tau_m e \rangle}{q \langle \tau_m \rangle} \tag{5.124}$$

Because of the dependence on q, the Peltier coefficient is negative for electrons and positive for holes.

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Figure 5.4 Schematic of a thermoelec-

tric cooler. The heat sinks and cold junc-

tions are metals that form ohmic con-

tacts.

In addition to transporting heat, the electric current density also generates heat. The net rate at which heat is generated per unit volume is equal to the rate generated per unit volume minus the rate at which it is transported away, or

$$P = \mathbf{J} \cdot \mathbf{E} - \nabla_r \cdot \mathbf{W} \tag{5.125}$$

From (5.120), (5.52), and (5.115),

$$\mathbf{E} = \frac{1}{\sigma} \mathbf{J} + \mathcal{T} \, \boldsymbol{\nabla}_r T \tag{5.126}$$

Also, from (5.122) and (5.123),

$$\mathbf{W} = \Pi \mathbf{J} - \kappa \, \boldsymbol{\nabla}_r T \tag{5.127}$$

Using (5.126) and (5.127) in (5.125), we have

$$P = \frac{\mathbf{J} \cdot \mathbf{J}}{\sigma} + \mathcal{T} \mathbf{J} \cdot \nabla_r T - \Pi \nabla_r \cdot \mathbf{J} + \kappa \nabla_r \cdot \nabla_r T \qquad (5.128)$$

Thus the net rate at which heat is generated per unit volume, P, has several components. The first term in (5.128) is simply the Joule heat. The second term is referred to as the *Thomson heat*. The third term, which involves the divergence of the electric current, allows for the generation or recombination of electrons in the unit volume and will not be considered further. Finally, the last term provides for the transport of heat out of the volume by thermal conduction.

Notice that the Thomson heat term in (5.128) changes sign when either the current density or the temperature gradient is reversed. Since the Thomson coefficient is negative for electrons, in *n*-type material heating is produced when J and  $\nabla_r T$  are in the same direction. That is, the electrons going from a higher to a lower temperature have to give heat to the lattice. When J and  $\nabla_r T$  are in opposite directions, the electrons produce cooling since they take heat from the lattice in going from a lower to a higher temperature. These effects are indicated schematically in Fig. 5.3. Since the Thomson coefficient for holes is positive, cooling is produced when J and  $\nabla_r T$  are in

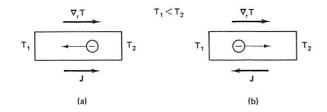
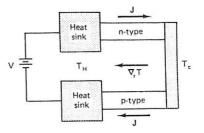


Figure 5.3 The Thomson term in an *n*-type semiconductor produces (a) heating when J and  $\nabla_r T$  are in the same direction and (b) cooling when they are in opposite directions.



the same direction. These results can be used to construct a thermoelectric cooler in the manner shown in Fig. 5.4.

Similar effects are obtained for electrons in concentration gradients. In the absence of a temperature gradient, the electric field for n-type material is given from (5.87) as

$$\mathbf{E} = \frac{\mathbf{J}}{\sigma} - \frac{kT}{qN_cF_{-1/2}(\eta)} \nabla_r n \tag{5.129}$$

In this case, (5.125) is

$$\mathbf{P} = \frac{\mathbf{J} \cdot \mathbf{J}}{\sigma} - \frac{kT}{qN_c F_{-1/2}(\eta)} \mathbf{J} \cdot \nabla_r n - \Pi \nabla_r \cdot \mathbf{J}$$
(5.130)

Thus, when J and  $\nabla_r n$  are in the same direction, the electrons take heat from the lattice as they go from higher to lower concentrations and cooling is produced.

### 5.4.3 Thermomagnetic Effects

When we allow for a small magnetic field, in addition to small electric fields and temperature gradients, the transport of heat produces several thermomagnetic effects. We examine these in the Hall configuration shown in Fig. 5.5. In Section 5.3 we examined the Hall effect assuming that no tem-

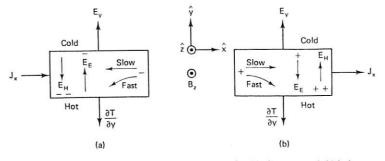


Figure 5.5 Hall and Ettinghausen effects  $(0 \le r)$  for (a) electrons and (b) holes.

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perature gradients were present (isothermal conditions) and that there was no electric current in the  $\hat{y}$  direction. That is,  $J_y = \partial T/\partial x = \partial T/\partial y = 0$ . Under these conditions, the electrons were deflected by the magnetic field in the direction shown in Fig. 5.5(a) and an electric field,  $E_H$ , was induced in the negative  $\hat{y}$  direction to balance the Lorentz force. However, this Hall field can only exactly balance the Lorentz force on electrons with average velocity. If we assume that the momentum relaxation time increases with energy ( $\tau_m = \tau_0 x'$ , where  $0 \le r$ ), the faster or hotter electrons are deflected more and the slower ones less by the magnetic field. As a result, the side of the sample where the faster carriers are deflected becomes warmer and the opposite side cooler, inducing a temperature gradient. In a manner similar to the thermoelectric effect, the warmer electrons tend to diffuse to the cooler surface, where they set up an electric field, as in (5.115), to oppose the diffusion. The mechanism that produces this electric field is referred to as the *Ettinghausen effect*.

The Ettinghausen coefficient is defined under conditions such that no heat current is transferred to the surroundings (adiabatic conditions). For  $J_y = \partial T/\partial x = W_y = 0$ , this coefficient is

$$P_{\rm E} \equiv \frac{\partial T/\partial y}{J_x B_z} \tag{5.131}$$

Applying these conditions to (5.103) and (5.104), we can eliminate the electric field and the chemical potential gradient,

$$P_{\rm E} = \frac{\mu_c}{q\kappa} \left[ \frac{\langle \tau_m^2 \mathscr{E} \rangle}{\langle \tau_m \rangle^2} - \frac{\langle \tau_m^2 \rangle \langle \tau_m \mathscr{E} \rangle}{\langle \tau_m \rangle^3} \right]$$
(5.132)

From this equation we expect the Ettinghausen field to change sign when the sign of the charge carrier is reversed. Figure 5.5(b) for holes shows that this is, indeed, what occurs. In either case, however, the direction of the Ettinghausen field depends on the energy dependence of the momentum relaxation time. It can be verified by (5.132) that when r in (5.55) is less than zero, the slower carriers are deflected more than the faster ones and the direction of the Ettinghausen field in Fig. 5.5 are reversed. Thus the direction of the Ettinghausen field depends on the sign of the carrier and the scattering mechanism.

Two other thermomagnetic effects we will mention are the *Nernst* and *Righi-Leduc effects*. As indicated in Fig. 5.6, these effects are the thermal analogues of the Hall and Ettinghausen effects, respectively. The Nernst coefficient is defined under isothermal conditions  $(J_x = J_y = \partial T/\partial y = 0)$  as

$$Q_N \equiv \frac{E_y}{(\partial T/\partial x)B_z} \tag{5.133}$$

Thus we see that the Nernst effect is a process whereby a transverse electric

### Sec. 5.5 High-Frequency Transport

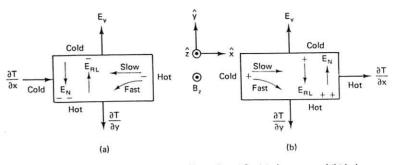


Figure 5.6 Nernst and Righi-Leduc effects  $(0 \le r)$  for (a) electrons and (b) holes.

field is produced by a temperature gradient. This equation can be compared to (5.72) for the Hall constant. Under these conditions (5.103) and (5.104) give us

$$Q_{\rm N} = \frac{\mu_c}{qT} \left[ \frac{\langle \tau_m^2 \mathcal{E} \rangle}{\langle \tau_m \rangle^2} - \frac{\langle \tau_m^2 \rangle \langle \tau_m \mathcal{E} \rangle}{\langle \tau_m \rangle^3} \right]$$
(5.134)

ог

$$Q_{\rm N} = \frac{\kappa}{T} P_{\rm E} \tag{5.135}$$

The Righi-Leduc coefficient is defined under adiabatic conditions  $(J_x = J_y)$ =  $W_y = 0$  as

$$S_{\rm RL} = \frac{\partial T/\partial y}{(\partial T/\partial x)B_z} \tag{5.136}$$

which gives

$$S_{\rm RL} = \frac{n\mu_c^2}{qT\kappa} \left[ \frac{\langle \tau_m^2 \mathscr{E}^2 \rangle}{\langle \tau_m^2 \rangle} + \frac{\langle \tau_m^2 \rangle \langle \tau_m \mathscr{E} \rangle^2}{\langle \tau_m \rangle^4} - \frac{2\langle \tau_m^2 \mathscr{E} \rangle \langle \tau_m \mathscr{E} \rangle}{\langle \tau_m \rangle^3} \right]$$
(5.137)

Arguments regarding the sign of these coefficients are similar to those made for the sign of the Ettinghausen coefficient.

### 5.5 HIGH-FREQUENCY TRANSPORT

The dc theory of charge and energy transport developed in this chapter can be applied to transport at high frequencies with only slight modification. Let us apply a small sinusoidal electric field,

$$\mathbf{E} = \mathbf{E}_0 \exp\left(-i\omega t\right) \tag{5.138}$$

to a semiconductor sample where  $\omega$  is the angular frequency of the field.

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Assuming no other applied forces and no temperature or concentration gradients, we can examine the form of the nonequilibrium distribution function. In the same manner in which (5.15) was obtained, we have

$$f = f_0 + q\tau_m \frac{\partial f_0}{\partial \mathcal{E}} \mathbf{v} \cdot \mathbf{E}_0 \exp(-i\omega t)$$
 (5.139)

The time-dependent Boltzmann equation in the relaxation time approximation from (5.4), (5.5), and (5.9) is

$$\frac{\partial f}{\partial t} = -\mathbf{v} \cdot \left(\frac{\partial f}{\partial \mathscr{C}} \mathbf{F} + \nabla_r f\right) - \frac{f - f_0}{\tau_m}$$
(5.140)

Taking the time derivative of (5.139), we have

$$\frac{\partial f}{\partial t} = +q\tau_m \frac{\partial f_0}{\partial \mathscr{E}} \left( -i\omega \mathbf{v} + \frac{d\mathbf{v}}{dt} \right) \cdot \mathbf{E}_0 \exp\left(-i\omega t\right)$$
(5.141)

Since

$$\frac{d\mathbf{v}}{dt} = -q\mathbf{M}\cdot\mathbf{E}_0 \exp\left(-i\omega t\right) \tag{5.142}$$

the last term in (5.141) is second order in E and can be neglected. We now have

$$\frac{\partial f}{\partial t} = -i\omega(f - f_0) \tag{5.143}$$

and the Boltzmann equation is

$$f - f_0 = \frac{-\tau_m}{(1 - i\omega\tau_m)} \mathbf{v} \cdot \left(\frac{\partial f}{\partial \mathscr{C}} \mathbf{F} + \nabla_r f\right)$$
(5.144)

Except for the term  $(1 - i\omega\tau_m)$ , (5.144) has the same form as (5.11). Because of this, all of the dc transport equations can be used at high frequency if we replace  $\tau_m$  by  $\tau_m^*$  where

$$\tau_m^* \equiv \frac{\tau_m}{1 - i\omega\tau_m} \tag{5.145}$$

The general solution of the Boltzmann equation (5.144) for ellipsoidal minima is

$$f = f_{0} + \frac{\partial f_{0}}{\partial \mathscr{C}} q \tau_{m}^{*} \mathbf{v} \cdot \left[ \frac{\mathscr{F} - q \tau_{m}^{*} \mathbf{M} \cdot (\mathscr{F} \times \mathbf{B}) + (q \tau_{m}^{*})^{2} (\det \mathbf{M}) (\mathscr{F} \cdot \mathbf{B}) (\mathbf{M}^{-1} \cdot \mathbf{B})}{1 + (q \tau_{m}^{*})^{2} (\det \mathbf{M}) (\mathbf{M}^{-1} \cdot \mathbf{B}) \cdot \mathbf{B}} \right]$$
(5.146)

and this is used to determine the transport parameters. Since  $\tau_m^*$  is a complex

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number, all the terms in the distribution function (except for  $f_0$ ) are complex. Thus, in general, the high-frequency components of electric current density and heat current density are not in phase with the applied forces.

A useful effect can be observed when we examine the denominator of the last term in (5.146). If we define a cyclotron frequency as in (5.65) by

$$\omega_c^2 \equiv q^2 (\det \mathbf{M}) (\mathbf{M}^{-1} \cdot \mathbf{B}) \cdot \mathbf{B}$$
 (5.147)

the denominator becomes  $1 + (\omega_c \tau_m^*)^2$ . Using (5.145) gives

$$1 + (\omega_c \tau_m^*)^2 = 1 + \frac{(\omega_c \tau_m)^2}{(1 - i\omega\tau_m)^2}$$
(5.148)

which can be put in the form

$$1 + (\omega_c \tau_m^*)^2 = \frac{(\omega_c^2 - \omega^2)\tau_m^2 - 2i\omega\tau_m + 1}{(1 - i\omega\tau_m)^2}$$
(5.149)

Equation (5.149) tells us that for conditions such that  $\omega \tau_m$  is much greater than 1, 1 +  $(\omega_c \tau_m^*)^2$  exhibits a sharp minimum when  $\omega = \omega_c$ . Thus the transport properties, such as charge current density. J, will exhibit a resonant peak when the applied frequency is equal to the cyclotron frequency. This effect is referred to as *cyclotron resonance*. From (5.65) or (5.147) the frequency at which cyclotron resonance occurs can be used to determine effective mass.

### 5.6 HIGH ELECTRIC FIELD EFFECTS

Up to now we have limited our analysis of transport properties to small electric fields. Under these conditions the energy the carrier distribution gains from the electric field is lost to the lattice through collisions with lowenergy acoustic phonons or impurities. The average energy of the electrons, therefore, remains close to the thermal equilibrium value,  $\frac{3kT}{kT}$ , and the drift velocity of the distribution is linearly related to the electric field. However, because the average electron energy in semiconductors is so small, it is relatively easy to obtain significant deviations from this ohmic behavior. For moderate electric fields the collisions with acoustic phonons and impurities, which serve to maintain the electron distribution and the lattice at the same temperature, become less effective and the electrons gain energy from the field faster than they can lose it to the lattice. In this situation, the electron distribution can be characterized by an effective temperature,  $T_c$ , which is "hotter" than the lattice temperature, T. The relationship between the drift velocity and electric field is no longer linear and nonohmic electrical behavior is observed.

When the electrons have gained sufficient energy from the field, they can transfer energy to the lattice by the generation of high energy optical

phonons. Since this process is an efficient energy loss mechanism for the electrons, the drift velocity of the distribution reaches a limiting value where it no longer increases with the electric field. This value is referred to as the *saturated drift velocity* and is obtained for electron energies of the order of the optical phonon frequencies given in Table 3.2. Figure 5.7(a) and (b) show experimental drift velocity–electric field characteristics of electrons and holes, respectively, for Ge, Si, and GaAs up to the saturated regions. As can be seen, all of these characteristics, except for electrons in GaAs, exhibit, qualitatively, the nonohmic behavior described above. The negative resistance region in the GaAs  $v_d$  versus E curve is due to the transfer of electrons from the  $\Gamma$  to *L* conduction band minima. This forms the basis of the Gunn effect.

Since these hot electron effects play an important role in the operation of several semiconductor devices, let us examine them in more detail. Although there are several approaches to the problem of high electric field transport in semiconductors [Esther M. Conwell, *High Field Transport in Semiconductors* (New York: Academic Press, 1967)], we will use an approach with which analytical results can readily be obtained. Let us assume that the electron distribution can be described by

$$f = \frac{1}{1 + \exp\left[(\mathscr{E} - \zeta)/kT_c\right]}$$
(5.150)

where  $T_e$  is the effective temperature of the electron distribution. Notice that this distribution function has the form of the equilibrium distribution

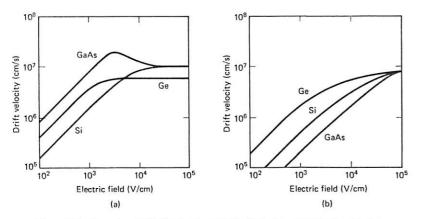


Figure 5.7 Experimental drift velocity-electric field characteristics for (a) electrons and (b) holes in several semiconductors. [After C. B. Norris and J. F. Gibbons, *IEEE Trans. Electron Devices ED-14*, 38 (1967); C. Y. Duk and J. L. Moll, *IEEE Trans. Electron Devices ED-14*, 46 (1967); T. E. Seidel and D. L. Scharfetter, *J. Phys. Chem. Solids 28*, 2563 (1967); J. G. Ruch and G. S. Kino, *Appl. Phys. Lett.* 10, 40 (1967); V. L. Dalal, *Appl. Phys. Lett.* 16, 489 (1970).]

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function,  $f_0$ , derived in (4.41), except for  $T_e$ , which is a function of electric field, E. We will also maintain the form of the low-field relationship between the drift velocity and the electric field (5.49).

$$\mathbf{v}_d = -\mu(T_e)\mathbf{E} \tag{5.151}$$

where the mobility,  $\mu$ , is now a function of  $T_e$  or electric field. In a similar manner,

$$\mu(T_e) = \frac{q\langle \tau_m(T_e) \rangle}{m^*}$$
(5.152)

where

$$\langle \tau_m(T_e) \rangle = \frac{\int_{-\infty}^{\infty} \tau_m(T_e) f \, d\mathbf{v}}{\int_{-\infty}^{\infty} f \, d\mathbf{v}}$$
(5.153)

and f is given by (5.150). Under these assumptions, we can proceed with our examination of high-field transport.

The average over velocity space of the momentum relaxation time in (5.153) can be simplified to an average over energy

$$\langle \tau_m(T_e) \rangle = \tau_0(T_e) \frac{\int_0^\infty f x_e^{r+1/2} \, dx_e}{\int_0^\infty f x_e^{1/2} \, dx_e}$$
(5.154)

or, using (5.59),

$$\langle \tau_m(T_e) \rangle = \frac{2}{\sqrt{\pi}} \left( r + \frac{1}{2} \right)! \tau_0(T_e) \frac{F_{r+1/2}(\eta_e)}{F_{1/2}(\eta_e)}$$
(5.155)

where

$$x_c \equiv \frac{\mathscr{E} - \mathscr{E}_c}{kT_e} \quad \text{and} \quad \eta_e \equiv \frac{\zeta - \mathscr{E}_c}{kT_e}$$
 (5.156)

Equation (5.155) tells us that, in general, the appropriate average is

$$\langle \tau_m^s(T_e) x_e^t \rangle = \frac{2}{\sqrt{\pi}} \left( sr + t + \frac{1}{2} \right)! \, \tau_0^s(T_e) \, \frac{F_{sr+t+1/2}(\eta_e)}{F_{1/2}(\eta_e)} \quad (5.157)$$

To proceed further we need to know the dependence of  $\tau_0$  on  $T_c$ . This dependence, of course, depends on the particular scattering mechanism. For several scattering mechanisms, the low-field momentum relaxation time can be put in the form

$$\tau_m = \tau_0 x^r = C T^u x^r \tag{5.158}$$

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where C is independent of temperature. If we assume that the high-field momentum relaxation time has the same form,

$$\tau_m(T_e) = \tau_0(T_e) x_e^r = C T_e^u x_e^r$$
(5.159)

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then

$$\tau_m(T_e) = \tau_0 \left(\frac{T_e}{T}\right)^{\mu} x_e^{r}$$
 (5.160)

From (5.152), (5.155), and (5.160) the field-dependent mobility is

$$\mu(T_e) = \frac{q\tau_0}{m^*} \left(\frac{T_e}{T}\right)^{\prime\prime} \frac{2}{\sqrt{\pi}} \left(r + \frac{1}{2}\right)! \frac{F_{r+1/2}(\eta_e)}{F_{1/2}(\eta_e)}$$
(5.161)

or simply

$$\mu(T_e) = \mu_0 \left(\frac{T_e}{T}\right)'' \qquad (5.162)$$

Thus if we can determine the dependence of  $T_e$  on E, we can obtain the dependence of  $\mu$  and, from (5.151), the dependence of  $v_d$  on E.

The effective electron temperature can be determined from conservation of energy. From (5.4) and (5.6) the time-dependent Boltzmann equation is

$$\frac{\partial f}{\partial t} = \frac{+q}{\hbar} \mathbf{E} \cdot \nabla_k f - \mathbf{v} \cdot \nabla_r f - \frac{f - f_0}{\tau_m}$$
(5.163)

If we multiply each term of this equation by the electron energy,  $\mathcal{E}$ , and average it over the electron distribution, we obtain

$$\frac{\int_{-\infty}^{\infty} \mathscr{C} \frac{\partial f}{\partial t} d\mathbf{v}}{\int_{-\infty}^{\infty} f d\mathbf{v}} = \frac{\frac{+q}{\hbar} \mathbf{E} \cdot \int_{-\infty}^{\infty} \mathscr{C} \nabla_k f d\mathbf{v}}{\int_{-\infty}^{\infty} f d\mathbf{v}} - \frac{\int_{-\infty}^{\infty} \mathscr{C} \mathbf{v} \cdot \nabla_r f d\mathbf{v}}{\int_{-\infty}^{\infty} f d\mathbf{v}} - \frac{\int_{-\infty}^{\infty} \mathscr{C} \frac{f - f_0}{\tau_m} d\mathbf{v}}{\int_{-\infty}^{\infty} f d\mathbf{v}}$$
(5.164)

With (2.109) and (5.38), the first term on the right-hand side can be reduced to  $qv_d \cdot E$ . Neglecting the diffusion term, (5.164) then reduces to the form

$$\frac{d}{dt} \langle \mathscr{E} \rangle = q \mathbf{v}_{e} \cdot \mathbf{E} - \frac{\langle \mathscr{E} \rangle - \langle \mathscr{E}_{0} \rangle}{\tau_{e}}$$
(5.165)

where we have defined an energy relaxation time,  $\tau_e$ , by

$$\frac{\langle \mathcal{E} \rangle - \langle \mathcal{E}_0 \rangle}{\tau_e} \equiv \frac{\int_{-\infty}^{\infty} \mathcal{E} \left( \frac{f - f_0}{\tau_m} \right) d\mathbf{v}}{\int_{-\infty}^{\infty} f d\mathbf{v}}$$
(5.166)

Equation (5.165) is the energy balance equation for the hot electron distribution. It tells us that the net energy gained per unit time is equal to the power supplied by the electric field minus the energy lost to collisions. Under steady-state conditions the electron distribution attains a temperature  $T_c$  and

$$\frac{\langle \mathcal{E} \rangle - \langle \mathcal{E}_0 \rangle}{\tau_c} = q \mathbf{v}_d \cdot \mathbf{E}$$
 (5.167)

Notice from (5.165) that  $\tau_e$  characterizes the relaxation of the hot electron distribution to its average thermal equilibrium energy  $\langle \mathscr{E}_0 \rangle$  when the electric field is turned off. We see from (5.166) that, since  $\tau_m$  is in general a function of  $\mathscr{E}$ .  $\tau_m$  and  $\tau_e$  are not equal. That is, the times that characterize the relaxation of energy and momentum are different.

From (5.156) and (5.157) the average energy of the hot electron distribution is

$$\langle \mathscr{E} \rangle = kT_c \langle x_c \rangle = \frac{3}{2} kT_c \frac{F_{3/2}(\eta_c)}{F_{1/2}(\eta_c)}$$
(5.168)

In a similar manner the average energy of the equilibrium distribution is

$$\langle \mathscr{E}_0 \rangle = kT \langle x \rangle = \frac{3}{2} kT \frac{F_{3/2}(\eta)}{F_{1/2}(\eta)}$$
 (5.169)

Using (5.156) and (5.166) yields

$$\frac{\langle \mathcal{C} \rangle}{\tau_c} \equiv \left\langle \frac{\mathcal{C}}{\tau_m} \right\rangle = kT_c \left\langle \frac{x_c}{\tau_m} \right\rangle \tag{5.170}$$

The average in this equation can be evaluated with (5.157) and (5.160) as

$$\frac{\langle \mathscr{C} \rangle}{\tau_e} = \frac{2}{\sqrt{\pi}} \left( \frac{3}{2} - r \right)! \frac{kT_e}{\tau_0} \left( \frac{T}{T_e} \right)^{\mu} \frac{F_{3/2-r}(\eta_e)}{F_{1/2}(\eta_e)}$$
(5.171)

and

$$\tau_e = \frac{3\sqrt{\pi}}{4} \frac{\tau_0}{(3/2 - r)!} \left(\frac{T_e}{T}\right)'' \frac{F_{3/2}(\eta_e)}{F_{3/2 - r}(\eta_e)}$$
(5.172)

Under nondegenerate conditions, we can readily obtain an expression

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Thus, for this scattering mechanism the mobility also decreases with electric field, and the drift velocity does not saturate. From (5.176) we see that u must be infinite to obtain a completely saturated drift velocity. This corresponds to scattering by optical phonons, where the energy changes are so large that the use of a momentum relaxation time is a poor approximation.

Under these conditions a reasonable approximation to the saturated drift velocity can be obtained by assuming that the energy of the hot electron distribution is dissipated in the generation of longitudinal optical phonons

$$\frac{\mathcal{E}}{\tau_c} - \frac{\mathcal{E}_0}{\tau_c} \simeq \frac{\hbar\omega_{\rm LO}}{\tau_c} \tag{5.180}$$

and that the proportionality factor between drift velocity and electric field is

$$\mu = \frac{q\tau_c}{m^*} \tag{5.181}$$

Using (5.180) and (5.181) in the energy balance equation (5.167), we find that

$$\tau_e = \frac{(\hbar\omega_{\rm LO}m^*)^{1/2}}{qE} \tag{5.182}$$

and the drift velocity is saturated at the value

$$w_d = \left(\frac{\hbar\omega_{\rm LO}}{m^*}\right)^{1/2} \tag{5.183}$$

Values for the longitudinal optical phonon frequencies from Table 3.2 can be used in (5.183) to obtain saturated drift velocities which are in reasonable agreement with experimental results.

If the electric field is increased further in the saturated region, at some point the charge carriers will have sufficient energy to generate an electronhole pair in a collision with the lattice. This process is known as *impact ionization*. When each of these electron-hole pairs creates an additional pair by impact ionization, an unstable situation is obtained where, in principle, the number of charge carriers increases without limit. This situation is referred to as *avalanche breakdown* and is readily observed in the reversebias current-voltage characteristics of p-n junctions. These phenomena are examined in more detail in Chapter 9.

### PROBLEMS

5.1. Find the nonequilibrium distribution function to second order in  $\mathbf{E} = \pounds E_x$  for a parabolic band. Assume a Maxwellian equilibrium distribution and that  $\tau_m = \tau_0 (\pounds/kT)^{-1/2}$ .

relating 
$$T_c$$
 to E. Using (5.151), (5.161), and (5.171) in (5.167), we have

 $\left(\frac{3}{2}-r\right)!\frac{k}{\tau_0}\left(\frac{T}{T_e}\right)''(T_e-T) = \left(r+\frac{1}{2}\right)!\frac{q^2\tau_0}{m^*}\left(\frac{T_e}{T}\right)''E^2 \quad (5.173)$ 

or

or

$$\frac{T_e}{T} - 1 \left( \frac{T}{T_e} \right)^{2u} = \frac{q^2 \tau_0^2}{m^* k T} \frac{(r + \frac{1}{2})!}{(\frac{3}{2} - r)!} E^2$$
$$= (\beta E)^2$$
(5.174)

For hot electrons  $T_e$  is much greater than T and (5.174) can be solved for  $T_e$ , with the result

$$\frac{T_{\epsilon}}{T} = (\beta E)^{-2/(2u-1)}$$
(5.175)

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From (5.162) the mobility is

 $\mu(T_e) = \mu_0 \left(\frac{T_e}{T}\right)^u$ 

$$(\mathbf{E}) = \mu_0(\beta \mathbf{E})^{-2u/(2u-1)}$$
(5.176)

With (5.176) we can examine the dependence of the mobility on electric field for scattering processes in which the relaxation time approximation can be used.

The temperature dependence of the momentum relaxation time for acoustic phonon scattering is  $u = -\frac{3}{2}$ . Using this value in (5.176), the mobility is

$$\mu(T_e) = \mu_0 \left(\frac{T}{T_e}\right)^{3/2}$$

$$\mu(\mathbf{E}) = \mu_0 \left(\frac{1}{\beta E}\right)^{3/4}$$
(5.177)

Thus the mobility for this scattering mechanism decreases as the electric field increases. From (5.151) and (5.177) the drift velocity,

$$\mathbf{v}_d = -\mu_0 \beta^{-3/4} \mathbf{E}^{1/4} \tag{5.178}$$

does not saturate at high electric fields. For ionized impurity scattering  $u = +\frac{3}{2}$  and the mobility is

$$\mu(T_e) = \mu_0 \left(\frac{T_e}{T}\right)^{3/2}$$

$$\mu(\mathbf{E}) = \mu_0 \left(\frac{1}{\beta E}\right)^{3/2}$$
(5.179)

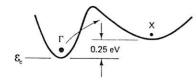
5.2. Derive an expression for the Hall factor assuming Fermi statistics and  $\tau_m =$  $\tau_0 x^r$ . Plot  $r_{\rm H}$  versus  $\eta(-4 \le \eta \le 10)$  for  $r = -\frac{1}{2}$  and  $r = \frac{3}{2}$ . Explain the dependence on m.

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- 5.3. Determine the diffusion coefficient  $(D_n)$  for electrons in a fully degenerate ntype semiconductor, specifically for Ge with  $\mu_n = 300 \text{ cm}^2/\text{V} \cdot \text{s}$ ,  $n = 10^{19} \text{ cm}^{-3}$ . and  $m_n = 0.2m_0$ .
- 5.4. Show how all but one of the following secondary effects can be canceled in a Hall experiment by taking four measurements with B and J reversals: Ettinghausen, Nernst, Righi-Leduc, thermoelectric, and IR drop (probe misalignment).
- 5.5. Assume that a semiconductor has spherical energy surfaces in both the conduction and the valence bands, but with two species of holes. Find an expression for the Hall coefficient in terms of appropriate averages of  $\tau_{p1}, \tau_{p2}, \tau_n$ .  $\mu_{p1}, \mu_{p2}, \mu_n; p_1, p_2, n.$
- 5.6. Consider an *n*-type semiconductor material as shown in Fig. P5.6 of mobility  $10^4$  cm<sup>2</sup>/V·s which is to be used as a fast microwave switch. The device, a conductive bar, is switched from the more conductive to the less conductive state, with an applied electric field, by "heating" electrons from the direct to the indirect conduction band minima. Estimate the applied field needed.

$$m^*(\Gamma) = 0.07m, \qquad \frac{N_c(X)}{N_c(\Gamma)} \simeq 60$$

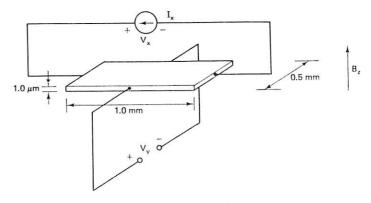
- 5.7. Consider the Righi-Leduc effect in a uniformly doped nondegenerate n-type semiconductor with spherical energy surfaces. A thermal gradient is maintained in the x direction and a magnetic field in the z direction, with  $J_x = J_y$  $= W_y = 0.$  If  $\nabla_y T = S_{RL}B_z \nabla_x T$ :
  - (a) Find  $S_{RL}$  in terms of appropriate averages of  $\tau^s$ .
  - (b) For spherical energy surfaces and  $\tau = \tau_0 \mathscr{E}^p$ , express  $S_{\rm RL}$  in terms of gamma functions.
  - (c) For  $p = -\frac{1}{2}$ , show that  $S_{\rm RL} = -(21\pi/32)(k^2T/q\kappa)n\mu_n^2$ , where  $\kappa$  is the thermal conductivity.







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- 5.8. Hall meaurements are performed on a sample in the configuration shown in Fig. P5.8 with  $I_x = 5$  mA,  $B_z = 0.1$  T, and T = 77 K. Measured values are  $V_x = 10$  V and  $V_y = -5$  V. Assuming that  $m_e = 0.1m$ ,  $m_h = 0.5m$ , and  $\tau_m$ =  $\tau_0 x^{3/2}$  (ionized impurities), determine the following:

  - (a) Type of material
  - (b) Hall constant
  - (c) Carrier concentration
  - (d) Conductivity
  - (e) Conductivity mobility
  - (f) Hall mobility
- 5.9. Calculate the root-mean-square z-directed velocity of conduction band electrons in an isotropic material at equilibrium. Assume that nondegenerate statistics are valid and that the material exhibits spherically symmetric constant energy surfaces about Γ.
- 5.10. Consider a collection of electrons in an isotropic material which are constrained to possess a nonzero z-directed net velocity (e.g., through the application of an electric field  $\mathbf{E} = -E_z \hat{z}$ ,  $\mathbf{J} = \sigma \mathbf{E}$ ). Show that the distribution function has the form

$$f = \frac{1}{1 + \exp \left[\beta(\mathscr{E} - \alpha - \gamma v_z)\right]}$$

where  $v_z$  is the z-directed velocity.

5.11. The steady-state distribution function for a nondegenerate material under certain conditions is

$$f = \exp\left[-\beta(\mathscr{E} - \zeta)\right] \exp\left(\frac{\hbar^2\beta}{m^*}\gamma k_z\right)$$

where  $\beta = 1/kT$ ,  $\zeta$  and  $\gamma$  are constants. The conduction band states near  $\Gamma$ 

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are described by

$$\mathcal{E} = \mathcal{E}_c + \frac{\hbar^2 k^2}{2m^*}$$

Determine the concentration of electrons in the conduction band and their mean z-directed velocity. For the conditions  $\gamma = 10^7 \text{ m}^{-1}$ , T = 300 K,  $m^* = 0.0665m$ , and  $n = 10^{16} \text{ cm}^{-3}$ , what are the z-directed velocity and current density?



# Scattering Processes

In Chapter 5 we used the relaxation time approximation to examine the transport of charge and energy in electric, magnetic, and thermal fields. There it was assumed that a momentum relaxation time,  $\tau_m$ , could be defined for various carrier scattering processes, such that

$$\dot{\tau}_m = \tau_0 x^r \tag{5.55}$$

where x is the electron kinetic energy in units of kT,

$$x \equiv \frac{\mathcal{E} - \mathcal{E}_c}{kT} \tag{4.65}$$

and  $\tau_0$  and the exponent *r* are independent of energy. In this chapter we examine this assumption and discuss the physics of the more important scattering processes. Rather than being all-inclusive, we will derive momentum relaxation times for ionized and neutral impurity scattering, as examples, and then show how these can be combined with values for phonon scattering to model and predict experimental mobility.

# 6.1 SCATTERING POTENTIALS

As discussed in Chapter 2, an electron moving in a perfect periodic crystal potential with no applied force has a constant velocity and is not scattered by the atoms of the crystal. When a force is applied to an electron, its acceleration can be described by a modified Newton's law where the perfect

### Sec. 6.1 Scattering Potentials

periodic crystal potential is taken into account by an effective mass. Therefore, to describe the deceleration or scattering of an electron by a crystal defect, it is convenient to examine the perturbation that the defect produces on the perfect crystal potential. This perturbation is referred to as a *scat*-

*tering potential*,  $\Delta U(\mathbf{r})$ , and has units of energy. In the following section we examine the scattering processes associated with impurities and phonons and derive their scattering potentials.

## 6.1.1 Impurities

For an ionized impurity the scattering process is dominated by the electrical interaction between its charge and the charge of the free carrier. For an ion with charge Zq the perturbation on the perfect crystal potential is simply the Coulomb energy,

$$\Delta U(\mathbf{r}) = \frac{\pm Zq^2}{4\pi\epsilon(0)\mathbf{r}} \tag{6.1}$$

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where r is the distance between the ion and the charge carrier. The plus sign is valid when the charges on the ion and the carrier have the same polarity, and the minus sign is for charges of opposite polarity. As indicated in Fig. 6.1, the scattering trajectories of the free carriers are described by a hyperbola with the ion at a focal point.

In (6.1) the screening of the Coulomb potential by atomic and ionic polarization of the constituent atoms is described by the use of the static permittivity of the material,  $\epsilon(0)$ . Because of the long-range nature of the Coulomb potential, it is also necessary to consider the screening of (6.1) by other free carriers and ionized impurities. We look at this in Section 6.2.

A nonionized or neutral impurity has a scattering potential which is much weaker but more complex than for an ionized impurity. For a hydrogen-like neutral impurity, Coulombic scattering with the ground-state (1s) electron cloud occurs. The free carriers, however, can also interact with a neutral impurity by polarizing it or by changing places with a bound electron

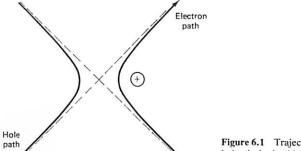


Figure 6.1 Trajectories of electrons and holes in ionized impurity scattering.

or hole. This raises the possibility of a combination of Coulombic, dipole, and exchange scattering which is not easy to analyze.

An empirical analysis [C. Erginsoy, *Phys. Rev.* 79, 1013 (1950)] of electron scattering by hydrogen atoms indicates that neutral impurity scattering can be approximated by a *differential scattering cross section*,

$$\sigma = \frac{20r_{\rm B}}{k} \tag{6.2}$$

where  $r_{\rm B}$  is the ground-state Bohr radius of the impurity, and k is the wavevector of the free electron. It can be shown (see Sections 6.3 and 6.4) that this scattering cross section is approximately equivalent to a scattering potential,

$$\Delta U(\mathbf{r}) \simeq \frac{\hbar^2}{m^*} \left(\frac{r_{\rm B}}{r^5}\right)^{1/2} \tag{6.3}$$

where **r** is the distance between the neutral impurity and the free carrier. It is interesting to note that this  $r^{-5/2}$  dependence is longer ranged than the  $r^{-4}$  dependence expected for dipole scattering.

### 6.1.2 Acoustic Phonons

The acoustic phonons in a crystal can scatter carriers by two different and independent processes. These are called *deformation potential scattering* and *piezoelectric scattering*. These scattering mechanisms can be examined, qualitatively, by means of Fig. 6.2, where the displacements,  $u(\mathbf{r})$ , of a chain of atoms from their Bravais lattice sites are shown for the longitudinal (LA) and transverse (TA) components of (a) zone center and (b) zone edge acoustic phonons.

As can be seen, the distance between adjacent atoms (the size of the unit cell) is strongly affected by the LA phonons, and little affected by the TA phonons. From the tight-binding model of the energy gap variation with lattice constant (see Fig. 2.14), we see that these LA phonons will produce a modulation of the conduction and valence band edges,  $\mathcal{E}_c$  and  $\mathcal{E}_v$ . This modulation in space and time disturbs the periodicity of the crystal potential and produces the so-called deformation potential scattering of the electrons and holes.

For the long-wavelength acoustic phonons, it is convenient to treat the material as an elastic continuum. Then we can see in Fig. 6.2 that the maximum expansion and contraction of the unit cell produced by LA phonons occurs in regions where the divergence of the displacement vector (gradient of the displacement amplitude), or the *strain*, is maximum. Therefore, the scattering potential for deformation potential scattering must be proportional to the strain. Consider the displacement produced by an acoustic phonon



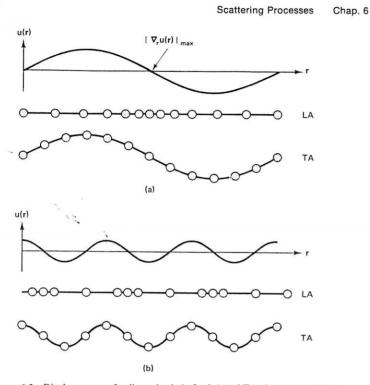


Figure 6.2 Displacements of a diatomic chain for LA and TA phonons at (a) the center and (b) the edge of the Brillouin zone. The lighter mass atoms are indicated by open circles. For zone edge acoustic phonons only the heavier atoms are displaced.

of frequency,  $\omega_s$ , and wavevector,  $\mathbf{q}_s$ ,

$$\mathbf{u}(\mathbf{r}, t) = \mathbf{a}u(\mathbf{r}, t) \tag{6.4}$$

where

$$u(\mathbf{r}, t) = u \exp\left[i(\mathbf{q}_s \cdot \mathbf{r} - \boldsymbol{\omega}_s t)\right]$$
(6.5)

In these equations  $\mathbf{a}$  is the displacement direction, and u is the amplitude. The strain associated with the displacement is

$$\nabla \cdot \mathbf{u}(\mathbf{r}, t) = \mathbf{a} \cdot \nabla u(\mathbf{r}, t) \tag{6.6}$$

$$\nabla \cdot \mathbf{u}(\mathbf{r}, t) = i\mathbf{q}_s \cdot \mathbf{a}u(\mathbf{r}, t) \tag{6.7}$$

Equation (6.7) indicates that for the transverse components of a phonon where the displacement and the wavevector are orthogonal,  $\mathbf{q}_s \cdot \mathbf{a} = 0$ , and no strain is produced. The scattering potential for the longitudinal component

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is, therefore,

$$\Delta U(\mathbf{r}, t) = \mathscr{E}_A \nabla \cdot \mathbf{u}(\mathbf{r}, t) \tag{6.8}$$

where the *deformation potential*,  $\mathscr{C}_A$ , in units of energy, is defined as the proportionality constant between the scattering potential (units of energy) and the strain.

For some semiconductors with two or more atoms per unit cell, there is no crystal inversion symmetry. In these crystals the strain, caused predominantly by the LA phonons, polarizes the ions and produces internal electric fields that vary with time and space. The carrier scattering caused by these electric fields is called *piezoelectric scattering*. The scattering potential for electrons is simply

$$\Delta U(\mathbf{r}, t) = -q\psi(\mathbf{r}, t) \tag{6.9}$$

where  $\psi(\mathbf{r}, t)$  is the electrostatic potential associated with the internal fields,

$$\psi(\mathbf{r}, t) = -\int \mathbf{E}(\mathbf{r}, t) \cdot d\mathbf{r}$$
 (6.10)

To evaluate (6.9), it is thus necessary to determine the fields produced by the piezoelectric interaction.

At a given frequency,  $\omega$ , the relationships among the electric flux density, **D**, the electric field, **E**, and the polarization, **P**, are

$$\mathbf{D}(\omega) = \boldsymbol{\epsilon}(\omega)\mathbf{E} = \boldsymbol{\epsilon}_0\mathbf{E} + \mathbf{P}(\omega) \tag{6.11}$$

where  $\epsilon_0$  is the free-space permittivity. In the low-frequency limit (6.11) become

$$\mathbf{D}(0) = \boldsymbol{\epsilon}(0)\mathbf{E} = \boldsymbol{\epsilon}_0\mathbf{E} + \mathbf{P}(0) \tag{6.12}$$

where  $\epsilon(0) = \epsilon_r(0)\epsilon_0$  is the static permittivity. Physically, the source of D(0) is the "true" charge (i.e., space and surface charges), while the source of P(0) is the "polarization" charge, usually atomic core and ionic dipoles. Since measurements of the so-called "static" dielectric constant do not include piezoelectric polarization, it is necessary to add an additional term to (6.12) to include this effect. [In principle, P(0) should include piezoelectric polarization.]

From Fig. 6.2 we see that this polarization must be proportional to the strain induced by the phonons. Ignoring the tensor nature of this interaction, we have

$$\mathbf{D}(0) = \boldsymbol{\epsilon}(0)\mathbf{E}(\mathbf{r}, t) + e_{\mathrm{pz}} \nabla u(\mathbf{r}, t)$$
(6.13)

where the piezoelectric constant,  $e_{pz}$ , has units of coulomb per square meter. With no true charge, the sources of the electric field are piezoelectric, ionic,

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and atomic polarization,

$$\mathbf{E}(\mathbf{r}, t) = -\frac{e_{pz}}{\epsilon(0)} \nabla u(\mathbf{r}, t)$$
(6.14)

Using (6.9), (6.10), and (6.14), the scattering potential in terms of the displacement is

$$\Delta U(\mathbf{r}, t) = \frac{-qe_{\mathbf{p}z}}{\epsilon(0)} u(\mathbf{r}, t)$$
(6.15)

With (6.5) and (6.6), equation (6.15) can be expressed in terms of the strain as

$$\Delta U(\mathbf{r}, t) = \frac{iqe_{\mathbf{pz}}}{\epsilon(0)q_s} \nabla \cdot \mathbf{u}(\mathbf{r}, t)$$
(6.16)

Comparing (6.8) and (6.16), we see that the scattering potentials for the deformation potential and piezoelectric interactions are separated in phase by 90°. The two acoustic phonon scattering mechanisms therefore operate independently.

### 6.1.3 Optical Phonons

The optical phonons also scatter carriers by two independent processes. These are referred to as *deformation potential scattering* (the same as for acoustic phonons) and *polar mode scattering*. The deformation potential scattering by optical phonons is similar to that for acoustic phonons and the polar mode scattering is due to the polarization of atoms within the unit cell. The displacements,  $u(\mathbf{r})$ , of a chain of atoms from their Bravais lattice sites for longitudinal optical (LO) and transverse optical (TO) phonons are shown in Fig. 6.3.

In a manner similar to acoustic phonons it can be seen that the expansion and contraction of the unit cell is dominated by the longitudinal optical phonons. The main difference in Fig. 6.3 at the zone center is that the atoms in the unit cell vibrate against one another. Because of this, for optical phonon deformation potential scattering, it is necessary to consider the *relative* displacement between atoms in the unit cell,

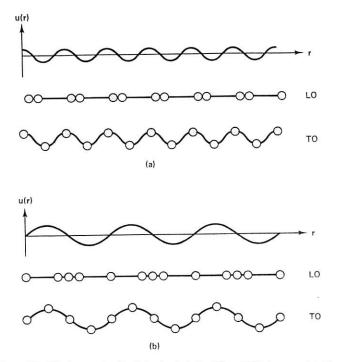
$$\delta \mathbf{u}(\mathbf{r}, t) \equiv \mathbf{u}_1(\mathbf{r}, t) - \mathbf{u}_2(\mathbf{r}, t) \tag{6.17}$$

where  $u_1(\mathbf{r}, t)$  and  $\mathbf{u}_2(\mathbf{r}, t)$  have the form given by (6.4) and (6.5). The scattering potential due to modulation of the conduction and valence edges must then be proportional to this relative displacement and

$$\Delta U(\mathbf{r}, t) = D \,\delta u(\mathbf{r}, t) \tag{6.18}$$

where

$$\delta \mathbf{u}(\mathbf{r}, t) = \mathbf{a} \, \delta u(\mathbf{r}, t) \tag{6.19}$$



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Figure 6.3 Displacements of a diatomic chain for LO and TO phonons at (a) the center and (b) the edge of the Brillouin zone. The lighter mass atoms are indicated by open circles. For zone edge optical phonons only the lighter atoms are displaced.

for optical phonon deformation potential scattering. In (6.18) the deformation potential constant, D, has units of energy per unit length. A similar treatment can be used for intervalley phonon scattering.

The optical phonon polar mode scattering is due to the electric field caused by the polarization of the ions in the unit cell. This polarization is caused mainly by the longitudinal component and is equivalent to the ionic polarization,  $P_i$ , which is discussed in Chapter 7. The scattering potential is obtained from (6.9) and (6.10), where the internal electric field is deduced from the low- and high-frequency limits of (6.11),

$$\mathbf{D}(0) = \boldsymbol{\epsilon}(0)\mathbf{E} = \boldsymbol{\epsilon}_0\mathbf{E} + \mathbf{P}(0) \tag{6.20}$$

and

$$\mathbf{D}(\infty) = \boldsymbol{\epsilon}(\infty)\mathbf{E} = \boldsymbol{\epsilon}_0\mathbf{E} + \mathbf{P}(\infty) \tag{6.21}$$

Note that in (6.20) the total low-frequency polarization is due to atomic and

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ionic polarization,

$$\mathbf{P}(0) = \mathbf{P}(\infty) + \mathbf{P}_i \tag{6.22}$$

Using (6.22) in (6.20) and subtracting (6.21), we obtain

$$\epsilon(0)\mathbf{E} = \epsilon(\infty)\mathbf{E} + \mathbf{P}_i \tag{6.23}$$

or

$$\mathbf{D}(0) = \boldsymbol{\epsilon}(\infty)\mathbf{E} + \mathbf{P}_i \tag{6.24}$$

From (6.24) we can determine the internal fields induced by the optical phonon polarization of the unit cell.

The polarization of a unit cell,  $P_i(\mathbf{r}, t)$ , is determined by the relative displacement of the ions in a unit cell,  $\delta \mathbf{u}(\mathbf{r}, t)$ , and the effective ionic charge,  $e^*$ , such that

$$\mathbf{P}_{i}(\mathbf{r}, t) = \frac{e^{*}}{\Omega} \,\delta \mathbf{u}(\mathbf{r}, t) \tag{6.25}$$

In this equation  $\Omega = V/N$  is the volume of the N primitive or Wigner-Seitz unit cells and  $e^*$  is the Born effective charge given by

$$e^* = \Omega \omega_{\rm LO} \epsilon(\infty) \rho^{1/2} \left[ \frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)} \right]^{1/2}$$
(7.174)

where  $\rho$  is the mass density. This equation is derived in Chapter 7. Assuming no space or surface charges, (6.24) and (6.25) give an internal field,

$$\mathbf{E}(\mathbf{r}, t) = -\frac{e^*}{\Omega\epsilon(\infty)} \,\delta \mathbf{u}(\mathbf{r}, t) \tag{6.26}$$

Using (6.9), (6.10), and (6.26), the scattering potential for polar mode scattering is

$$\Delta U(\mathbf{r}, t) = \frac{-qe^*}{\Omega \epsilon(\infty)} \int \delta \mathbf{u}(\mathbf{r}, t) \cdot d\mathbf{r}$$
(6.27)

or with (6.5) and (6.19),

$$\Delta U(\mathbf{r}, t) = \frac{iqe^*}{\Omega\epsilon(\infty)q_s} \delta u(\mathbf{r}, t)$$
(6.28)

A comparison of (6.18) and (6.28) shows that the scattering potentials for deformation potential and polar mode scattering by optical phonons are out of phase by 90° and are thus independent.

Equation (6.28) is sometimes written in the form

$$\Delta U(\mathbf{r}, t) = \frac{iqe_c}{\Omega\epsilon_0 q_s} \delta u(\mathbf{r}, t)$$
(6.29)

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where a Callen effective charge,  $e_c^*$  is used. The relationship to the Born effective charge is given by

$$e^* = \epsilon_r(\infty) e_c^* \tag{6.30}$$

### 6.2 SCREENING

In the derivations of the scattering potentials we assumed, in all cases, that there were no space charges (also, no surface charges). That is, we assumed that the charge carriers were uniformly distributed in the material such that

$$-\rho = q(n - p + N_a^- - N_d^+) = 0 \tag{6.31}$$

In the vicinity of a crystal potential perturbation caused by an impurity or phonon, however, charge carriers can be accumulated or depleted by the scattering potential. This space charge produces an additional potential given by

$$\nabla^2 \psi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon(0)} \tag{4.99}$$

where

$$-\rho(\mathbf{r}) = q[n(\mathbf{r}) - p(\mathbf{r}) + N_a^{-}(\mathbf{r}) - N_d^{+}(\mathbf{r})]$$
(6.32)

which screens the effects of the scattering potential.

In (6.32),  $n(\mathbf{r})$ ,  $p(\mathbf{r})$ ,  $N_a^-(\mathbf{r})$ , and  $N_d^+(\mathbf{r})$  are the *total* electron, hole, ionized acceptor, and ionized donor concentrations as a function of distance, **r**, from the center of the perturbing potential. These total concentrations can be split into two components,

$$n(\mathbf{r}) = n + \delta n(\mathbf{r})$$

$$N_{+}^{+}(\mathbf{r}) = N_{+}^{+} + \delta N_{+}^{+}(\mathbf{r}), \text{ etc.}$$
(6.33)

a uniform concentration and an excess (or deficit) concentration which varies with **r** according to the variation of  $\psi(\mathbf{r})$ . Excess carriers due to built-in potentials in nonuniform materials are discussed in some detail in Chapter 8. For our purposes here, we assume that  $q\psi(\mathbf{r}) \ll kT$ , so that the excess concentrations are, approximately,

$$\delta n(\mathbf{r}) \simeq \frac{qn}{kT} \psi(\mathbf{r})$$

$$\delta N_d^+(\mathbf{r}) \simeq \frac{-qN_d^+}{kT} \psi(\mathbf{r}), \quad \text{etc.}$$
(6.34)

With this approximation we can define an effective total electron

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concentration,

$$n^*(\mathbf{r}) \equiv n(\mathbf{r}) - p(\mathbf{r}) + N_a^-(\mathbf{r}) - N_d^+(\mathbf{r})$$
(6.35)

which, using (6.33), (6.34), and (6.31), takes the form

$$n^*(\mathbf{r}) = \frac{qn^*}{kT} \psi(\mathbf{r}) \tag{6.36}$$

From (4.99), (6.32), (6.35), and (6.36), Poisson's equation for the potential is

$$\nabla^2 \psi(\mathbf{r}) = \frac{q^2 n^*}{\epsilon k T} \psi(\mathbf{r}) \tag{6.37}$$

where the *effective*, uniform electron concentration,  $n^*$ , is to be determined later. If we define an effective Debye length,

$$x^2 = \frac{\epsilon kT}{q^2 n^*} \tag{6.38}$$

the differential equation for the potential is

$$\nabla^2 \psi(\mathbf{r}) = \frac{1}{\lambda^2} \psi(\mathbf{r}) \tag{6.39}$$

For a spherically symmetric potential, (6.39) is

$$\frac{d^2}{dr^2} \left[ r \psi(r) \right] = \frac{r \psi(r)}{\lambda^2} \tag{6.40}$$

The physically significant solution to this equation is

$$\psi(r) = \frac{C}{r} \exp\left(\frac{-r}{\lambda}\right) \tag{6.41}$$

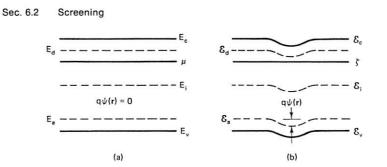
where the constant of integration,

$$C = \frac{Zq^2}{4\pi\epsilon} \tag{6.42}$$

for ionized impurity scattering. From (6.41) we see that the accumulation or depletion of charge carriers produces an exponential decay of the scattering potential with a characteristic length  $\lambda$ . This characteristic length is controlled by  $n^*$ , the effective electron concentration.

### 6.2.1 Degenerate Statistics

To determine  $n^*(\mathbf{r})$  and, subsequently,  $n^*$ , it is necessary to introduce an energy band formalism for nonuniform materials. This formalism is summarized in Fig. 6.4, where we show the terminology for (a) a semiconductor



**Figure 6.4** Energy band diagrams and terminology for (a) uniform material and (b) the same material with potential perturbations.

with uniform charge carrier and ionized impurity distributions, and (b) the same semiconductor with nonuniform distributions caused by perturbing potentials.

For a material with uniform doping and band structure as in Fig. 6.4(a), the Fermi energy is flat in thermal equilibrium and equal to the chemical potential energy,  $\mu$ . For the same material with perturbing potentials due to impurities and phonons as in Fig. 6.4(b), the Fermi energy is flat, also in thermal equilibrium, and equal to the electrochemical potential energy,

$$\zeta = \mu(\mathbf{r}) - q\psi(\mathbf{r}) \tag{6.43}$$

All the other energies have the form

$$\mathscr{E}_c(\mathbf{r}) = E_c - q \psi(\mathbf{r}), \quad \text{etc.}$$
(6.44)

Since the perturbed material is in thermal equilibrium, we can simply modify the equilibrium distributions for n, p,  $N_a^-$ , and  $N_d^+$  derived in Chapter 4 with this formalism to obtain  $n(\mathbf{r})$ ,  $p(\mathbf{r})$ ,  $N_a^-(\mathbf{r})$ , and  $N_d^+(\mathbf{r})$ .

From (4.68) and (4.65) the total electron concentration is

$$n(\mathbf{r}) = N_c F_{1/2}[\eta_c(\mathbf{r})]$$
(6.45)

where

$$\eta_c(\mathbf{r}) = \frac{\mu - E_c + q\psi(\mathbf{r})}{kT} \tag{6.46}$$

Equations (4.78) and (4.76) give the total hole concentration,

$$p(\mathbf{r}) = N_{\nu} F_{1/2}[\eta_{\nu}(\mathbf{r})]$$
(6.47)

where

$$\eta_{v}(\mathbf{r}) = \frac{E_{v} - \mu - q\psi(\mathbf{r})}{kT}$$
(6.48)

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The total ionized acceptor concentration from (4.98) is

$$N_a^{-}(\mathbf{r}) = \frac{N_a}{1 + g_a \exp\{[E_a - \mu - q\psi(\mathbf{r})]/kT\}}$$
(6.49)

while the ionized donor concentration from (4.97) is

$$N_d^+(r) = \frac{N_d}{1 + g_d \exp\left\{[\mu - E_d + q\psi(\mathbf{r})]/kT\right\}}$$
(6.50)

Equations (6.45) and (6.47) for the electron and hole concentrations can be simplified in the following manner. From (4.67) the Fermi-Dirac integral is

$$F_{1/2}[\eta(\mathbf{r})] = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2} \, dx}{1 + \exp\left[x - \eta(\mathbf{r})\right]} \tag{6.51}$$

where  $\eta(\mathbf{r})$  is given by either (6.46) or (6.48). The exponential in the denominator in (6.51) involving  $q\psi(\mathbf{r})/kT$  is then expanded in a Taylor series and the denominator is divided into the numerator. Neglecting terms in  $\psi^2(\mathbf{r})$ and higher, which is equivalent to the assumption  $q\psi(\mathbf{r}) \ll kT$ , (6.45) and (6.47) become

$$n(\mathbf{r}) = n + \frac{q \psi(\mathbf{r})}{kT} \frac{dn}{d\eta_c}$$
(6.52)

and

$$p(\mathbf{r}) = p - \frac{q\psi(\mathbf{r})}{kT} \frac{dp}{d\eta_v}$$
(6.53)

From the recurrence relationship (5.83),

$$\frac{dn}{d\eta_c} = N_c F_{-1/2}(\eta_c) = n \frac{F_{-1/2}(\eta_c)}{F_{1/2}(\eta_c)}$$
(6.54)

and

$$\frac{dp}{d\eta_{\nu}} = N_{\nu}F_{-1/2}(\eta_{\nu}) = p \frac{F_{-1/2}(\eta_{\nu})}{F_{1/2}(\eta_{\nu})}$$
(6.55)

Equations (6.49) and (6.50) for the ionized acceptor and donor concentrations can be simplified in a similar manner to obtain

$$N_a^{-}(\mathbf{r}) = N_a^{-} + \frac{N_a^0 N_a^-}{N_-} \frac{q \psi(\mathbf{r})}{kT}$$
(6.56)

and

$$N_{d}^{+}(\mathbf{r}) = N_{d}^{+} - \frac{N_{d}^{0}N_{d}^{+}}{N_{d}} \frac{q\psi(\mathbf{r})}{kT}$$
(6.57)

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The effective electron concentration,  $n^*$ , which controls the screening is obtained as follows: (6.52), (6.53), (6.56), and (6.57) are substituted into (6.35). Equation (6.31) for charge neutrality is applied to (6.35) and  $n^*$  is then obtained from (6.36) as

$$n^* = \frac{dn}{d\eta_c} + \frac{dp}{d\eta_v} + \frac{N_a^0 N_a^-}{N_a} + \frac{N_d^0 N_d^+}{N_d}$$
(6.58)

Equation (6.58) is valid for screening in degenerately doped semiconductors under the assumption that the perturbation energy is substantially less than the thermal energy.

### 6.2.2 Nondegenerate Statistics

When the doping of the material is such that the Fermi energy is greater than  $\mathscr{C}_v + 4kT$  and less than  $\mathscr{C}_c - 4kT$ ,  $\eta$  is negative, and  $F_{1/2}(\eta) = F_{-1/2}(\eta)$ . From (6.54), (6.55), and (6.58) the effective screening concentration is

$$n^* = n + p + \frac{N_a^0 N_a^-}{N_a} + \frac{N_d^0 N_d^+}{N_d}$$
(6.59)

where  $N_a^0 = N_a - N_a^-$  and  $N_d^0 = N_d - N_d^+$ . Eliminating the neutral concentrations,

$$n^* = n + p + N_a^- \left(1 - \frac{N_a^-}{N_a}\right) + N_d^+ \left(1 - \frac{N_d^+}{N_d}\right)$$
(6.60)

For nondegenerate *n*- or *p*-type material, (6.60) can be further simplified. In *n*-type material, for example, all the acceptors will usually be ionized, so  $N_a^- = N_a$ . The acceptors are ionized by electrons from the donors, with the remaining electrons from the donors contributing to conduction. Therefore,  $N_d^+ = n + N_a$ . Using these arguments and space charge neutrality, in (6.60) the effective electron screening concentration is

$$n^* = n + \frac{(n + N_a)(N_d - N_a - n)}{N_d}$$
(6.61)

For p-type material, the effective hole screening concentration is

$$p^* = p + \frac{(p + N_d)(N_a - N_d - p)}{N_a}$$
(6.62)

Since  $N_d$  and  $N_a$  are usually constant in a material, (6.61) and (6.62) are useful in examining screening under conditions where *n* or *p* vary.

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# 6.3 COLLISION INTEGRAL

Boltzmann's equation for the time rate of change of the electron distribution function under the influence of internal and applied forces is

$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar} \mathbf{F} \cdot \nabla_k f - \mathbf{v} \cdot \nabla_r f + \frac{\partial f}{\partial t} \Big|_c$$
(5.4)

In Chapter 5 the first and second terms on the right-hand side of this equation were evaluated under the assumption that the third term could be put in the form

$$\frac{\partial f}{\partial t}\Big|_{c} = \frac{-(f - f_{0})}{\tau_{m}} \tag{5.6}$$

That is, we assumed that the time rate of change of the distribution function due to collisions (the collision term) could be described by a momentum relaxation time,  $\tau_m$ . In this section we examine the conditions under which this assumption is valid and show how  $\tau_m$  can be obtained from the scattering potentials derived in Section 6.1. An equation relating the collision term or momentum relaxation time to the basic scattering process is called a *collision integral*. The scattering process itself can be described, quantum mechanically, by a matrix element or, classically, by a differential scattering cross section. We examine these two treatments and develop the relationship between them.

### 6.3.1 Quantum Treatment

The Hamiltonian for an electron undergoing a scattering process is

$$\mathbf{H} = \mathbf{H}_0 + \Delta \mathbf{U} \tag{6.63}$$

where  $H_0$  is the unperturbed energy operator and  $\Delta U$  is one (or more) of the scattering potentials, in operator form, derived in Section 6.1. Since the process evolves in time, Schrödinger's equation is

$$(\mathbf{H}_0 + \Delta \mathbf{U})\psi(t) = i\hbar \frac{\partial \psi(t)}{\partial t}$$
(6.64)

Solutions to (6.64) are obtained by constructing time-dependent wavefunctions from a set of time-independent Bloch wavefunctions,

$$\Psi(t) = \sum_{k} A_{k}(t) \Psi_{k} \exp\left[\frac{(-i\mathscr{E}_{k}t)}{\hbar}\right]$$
(7.13)

where  $\psi_k$  are given by (2.10).

This scattering problem is formally equivalent to the optical transition problem described in Chapter 7. For an electron that is scattered from a

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state with wavevector  $\mathbf{k}$  to one with wavevector  $\mathbf{k}'$ , the scattering rate is

$$S_{kk'} \equiv \frac{|A_k(t)|^2}{t}$$
(6.65)

Using (7.36) this can be written as

$$S_{kk'} = \frac{2\pi}{\hbar} \mid H_{kk'} \mid^2 \delta(\mathscr{E}_k - \mathscr{E}_{k'})$$
(6.66)

where from (7.19) the matrix element is

$$H_{kk'} = \frac{1}{N} \int_{V} \psi_k^* \Delta \mathbf{U} \psi_{k'} \, d\mathbf{r}$$
(6.67)

In (6.67), N is the number of primitive or Wigner–Seitz unit cells and V is the crystal volume.

For an electron to be scattered from an initial state k to one of the (N - 1) states k', the initial state k must be occupied and the final state k' must be unoccupied. Conversely, an electron in one of the occupied (N - 1) states k' can be scattered into the unoccupied state k. Considering these two competing processes and summing over all (N - 1) values of k', the time rate of *increase* of the distribution function due to collisions is

$$\frac{\partial f}{\partial t}\Big|_{c} = N_{s} \sum_{k'}^{N-1} \left[ S_{k'k} f_{k'} (1 - f_{k}) - S_{kk'} f_{k} (1 - f_{k'}) \right]$$
(6.68)

where  $N_s$  is the number of scattering centers and  $f_k$  is the nonequilibrium distribution function at energy  $\mathscr{C}(\mathbf{k})$ . Since the number of unit cells in the crystal, N, is very large, the summation over the (N - 1) values of  $\mathbf{k}'$  can be approximated by an integration over the  $(N - 1) \approx N$  values of  $\mathbf{k}'$  in the Brillouin zone. From (2.30), (1.20), and (1.12), each value of  $\mathbf{k}'$  occupies a reciprocal volume,

$$\Omega_{k'} = \frac{(2\pi)^3}{V} \tag{6.69}$$

The integral approximation of (6.68) is, therefore,

$$\frac{\partial f}{\partial t}\Big|_{c} = \frac{N_{s}V}{(2\pi)^{3}} \int_{\Omega_{K}} \left[ S_{k'k} f_{k'} (1 - f_{k}) - S_{kk'} f_{k} (1 - f_{k'}) \, d\mathbf{k'} \right]$$
(6.70)

When (6.70) is used in (5.4), an integrodifferential form of Boltzmann's equation is obtained which is quite general and valid for arbitrary degeneracy.

It is instructive to examine (6.70) in thermal equilibrium. Under this condition there is no change in the distribution function and the left-hand side of (6.70) must equal zero. For this to be true for any value of k',

$$S_{k'k} = S_{kk'} \frac{f_{0k}(1 - f_{0k'})}{f_{0k'}(1 - f_{0k})}$$
(6.71)

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where the subscript zero denotes the equilibrium Fermi-Dirac distribution function,

$$f_{0k} = \left[1 + \exp\left(\frac{\mathscr{C}_k - \mathscr{C}_f}{kT}\right)\right]^{-1}$$
(6.72)

If the material is nondegenerate,  $\mathscr{C}_k - \mathscr{C}_f \gg kT$ , and (6.71) reduces to

$$S_{k'k} = S_{kk'} \exp\left(\frac{\mathscr{E}_{k'} - \mathscr{E}_k}{kT}\right)$$
(6.73)

From (6.73) it can be seen that  $S_{k'k} = S_{kk'}$  only when  $\mathscr{E}_{k'} = \mathscr{E}_k$  or  $|\mathbf{k}'| = |\mathbf{k}|$ . That is, the scattering rate from a state  $\mathbf{k}$  to  $\mathbf{k}'$  is equal to its inverse only for elastic collisions. It is only under this condition that a universal momentum relaxation time can be defined.

Assuming elastic collisions we will now evaluate the nonequilibrium distribution coefficients for an arbitrary force field. With this we can then obtain the relationship between the momentum relaxation time and the matrix element, or using (6.67) the scattering potential, for a scattering process that conserves energy.

Consider an electron with initial wavevector  $\mathbf{k}$  scattering into a final state  $\mathbf{k}'$  under the influence of an arbitrary force,  $\mathbf{G}$ . This force can include electric, magnetic, and thermal fields. From (5.18) the nonequilibrium distribution function in the relaxation time approximation is

$$f_{k} = f_{0k} + \frac{\partial f_{0k}}{\partial \mathcal{C}_{k}} \frac{\hbar}{m^{*}} \mathbf{k} \cdot \mathbf{G}$$
(6.74)

For a collision at the origin of the reciprocal-space coordinate system in Fig.

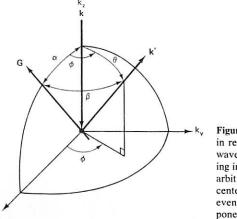


Figure 6.5 Spherical coordinate system in reciprocal space for an electron with wavevector k (along the  $k_z$  axis) scattering into a state with wavevector k' in an arbitrary force field G. The scattering center is at the origin. For simplicity the event is rotated so that G has no  $k_y$  component. Sec. 6.3 Collision Integral

6.5,

$$\mathbf{k} \cdot \mathbf{G} = kG \cos \alpha \tag{6.75}$$

and

$$\mathbf{k}' \cdot \mathbf{G} = kG \cos \beta \tag{6.76}$$

The magnitudes of  $\mathbf{k}$  and  $\mathbf{k}'$  are equal when energy is conserved.

Using (6.74), (6.75), and (6.76), the expression involving distribution functions in the integrand of (6.70) is

$$f_{k'}(1 - f_k) - f_k(1 - f_{k'})$$
$$= \frac{\partial f_0}{\partial \mathcal{E}} \frac{\hbar}{m^*} kG[\cos\beta(1 - \cos\alpha) - \cos\alpha(1 - \cos\beta)] \quad (6.77)$$

Eliminating  $\cos \beta$  with the equation for a spherical triangle (see Fig. 6.5) gives

$$\cos \beta = \cos \alpha \cos \theta + \sin \alpha \sin \theta \cos \phi \qquad (6.78)$$

Equation (6.77) becomes

$$f_{k'}(1 - f_k) - f_k(1 - f_{k'})$$
$$= \frac{\partial f_0}{\partial \mathcal{E}} \frac{\hbar}{m^*} kG[\sin \alpha \sin \theta \cos \phi - \cos \alpha (1 - \cos \theta)] \quad (6.79)$$

Inserting (6.79) into (6.70), the collision term is

$$\frac{\partial f}{\partial t}\Big|_{c} = -\frac{\partial f_{0}}{\partial \mathcal{E}} \frac{\hbar}{m^{*}} G \frac{N_{s}V}{(2\pi)^{3}} \int_{\Omega \kappa} S_{kk'} [\cos \alpha (1 - \cos \theta) - \sin \alpha \sin \theta \cos \phi] k \, d\mathbf{k}' \qquad (6.80)$$

Equation (6.80) can be simplified to give an expression for  $\tau_m$  in the following manner: First, note that the differential volume in k-space is

$$d\mathbf{k} = k^2 \sin \theta \, d\theta \, d\phi \, dk \tag{6.81}$$

Then, integrate  $\phi$  from 0 to  $2\pi$ , which eliminates the  $\phi$ -dependent term. Finally, from (6.74) and (6.75),

$$-\frac{\partial f_0}{\partial \mathcal{E}}\frac{\hbar}{m^*}kG\cos\alpha = -(f-f_0) \tag{6.82}$$

Following these steps, (6.80) becomes

$$\frac{1}{\tau_m} = \frac{N_s V}{(2\pi)^2 k} \int_k \int_0^{\pi} S_{kk'} \sin \theta (1 - \cos \theta) \, d\theta \, k^3 \, dk \tag{6.83}$$

Equation (6.66) for the scattering rate,  $S_{kk'}$ , shows that the integration over

k is zero except at the point where energy is conserved. Using (6.66) and assuming a parabolic band, the relationship between the momentum relaxation time and the matrix element for the scattering process is

$$\frac{1}{\tau_m} = \frac{N_s V m^{*2} v}{2\pi \hbar^4} \int_0^\pi |H_{kk'}|^2 \sin \theta (1 - \cos \theta) \, d\theta \tag{6.84}$$

### 6.3.2 Classical Treatment

The classical derivation of the momentum relaxation time proceeds rather simply. For  $N_s/V$  scattering centers per unit volume with scattering cross section,  $\sigma_m$ , the mean free time between collisions for an electron with velocity, v, is

$$\frac{1}{\tau_m} = \frac{N_s v}{V} \,\sigma_m \tag{6.85}$$

The scattering cross section is determined by setting a scattering center with differential cross section,  $\sigma(\theta)$ , at the origin in Fig. 6.5. The  $\theta$ -dependence allows for different scattering mechanisms. An electron scattered by the center into the solid angle  $(\theta, \phi)$  loses  $(1 - \cos \theta)$  of its initial momentum in the incident direction. Taking into account all possible scattering angles yields

$$\sigma_m = \int_{\Phi=0}^{2\pi} \int_{\theta=0}^{\pi} \sigma(\theta) \sin \theta (1 - \cos \theta) \, d\theta \, d\phi \qquad (6.86)$$

Using (6.85) and (6.86), the momentum relaxation time is

$$\frac{1}{\tau_m} = \frac{2\pi N_s \upsilon}{V} \int_0^\pi \sigma(\theta) \sin \theta (1 - \cos \theta) \, d\theta \tag{6.87}$$

This is the classical collision integral.

Since the quantum and classical integrals have the same angular dependence, a relationship can be obtained between the differential scattering cross section,  $\sigma(\theta)$ , and the matrix element,  $H_{kk'}$ , for a given scattering process. Equating (6.84) and (6.87), we obtain

$$\sigma(\theta) = \left(\frac{Vm^*}{2\pi\hbar^2} \mid H_{kk'} \mid\right)^2 \tag{6.88}$$

### **6.4 MATRIX ELEMENTS**

In principle the calculation of a matrix element for electron scattering from a given scattering potential using

$$H_{kk'} = \frac{1}{N} \int_{V} \psi_k^* \, \Delta \mathbf{V} \, \psi_{k'} \, d\mathbf{r}$$
(6.67)

is relatively straightforward. In detail, however, the procedure is often quite laborious, involving a number of approximations and assumptions. Here, we simply indicate the general procedure and refer the reader to the literature for the detailed treatment.

### 6.4.1 General Procedure

The usual procedure for evaluating a matrix element is first to expand the scattering potential in a Fourier series,

$$\Delta U(\mathbf{r}) = \sum_{g} A_{g} \exp \left( i \mathbf{g} \cdot \mathbf{r} \right)$$
(6.89)

where the Fourier coefficients are

$$A_g = \frac{1}{V} \int_V \Delta U(\mathbf{r}) \exp\left(-i\mathbf{g} \cdot \mathbf{r}\right) d\mathbf{r}$$
(6.90)

For Bloch wavefunctions,

$$\Psi_k(\mathbf{r}) = \exp\left(i\mathbf{k}\cdot\mathbf{r}\right)u_k(\mathbf{r}) \tag{2.10}$$

$$H_{kk'} = \frac{1}{N} \sum_{g} \int_{V} \exp\left(-i\mathbf{k}\cdot\mathbf{r}\right) u_{k}^{*}(\mathbf{r}) A_{g} \exp\left(i\mathbf{g}\cdot\mathbf{r}\right)$$
$$\times \exp\left(i\mathbf{k}'\cdot\mathbf{r}\right) u_{k'}(\mathbf{r}) d\mathbf{r}$$
(6.91)

$$H_{kk'} = \frac{1}{N} \sum_{g} A_g \int_{V} u_k^*(\mathbf{r}) u_{k'}(\mathbf{r}) \exp\left[i(\mathbf{g} + \mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}\right] d\mathbf{r} \qquad (6.92)$$

Since the integral is zero except when

$$\mathbf{g} = \mathbf{k} - \mathbf{k}' \tag{6.93}$$

(6.92) is

$$H_{kk'} = \frac{A_g}{N} \int_V u_k^*(\mathbf{r}) u_{k'}(\mathbf{r}) \, d\mathbf{r}$$
(6.94)

For parabolic bands  $u_k(\mathbf{r}) = u_{k'}(\mathbf{r})$ , and the matrix element is simply the Fourier coefficient that satisfies (6.93)

$$H_{kk'} = A_{k-k'} {(6.95)}$$

where  $A_{k-k'}$  is given by (6.90).

### 6.4.2 Screening Factor

Since the matrix element for ionized impurity scattering is relatively easy to obtain, we will derive it as an example of the procedure. Also, by comparing the screened and unscreened matrix elements for ionized impurity

Inserting the unscreened potential for ionized impurity scattering (6.1) into (6.90) yields

$$A_g = \frac{Zq^2}{4\pi\epsilon(0)V} \int_V \exp\left(-i\mathbf{g}\cdot\mathbf{r}\right) \frac{d\mathbf{r}}{\mathbf{r}}$$
(6.96)

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For the differential volume element

$$d\mathbf{r} = r^2 \sin \theta \ d\theta \ d\phi \ dr \tag{6.97}$$

$$A_{g} = \frac{Zq^{2}}{\epsilon(0)V} \int_{0}^{\infty} r \exp(-igr) dr$$
(6.98)

The integral is evaluated with (3.21) to obtain

$$A_g = \frac{Zq^2}{\epsilon(0)V \mid g \mid^2} \tag{6.99}$$

or from (6.95),

$$H_{kk'} = \frac{Zq^2}{\epsilon(0) V | k - k' |^2}$$
(6.100)

For the screened potential, (6.41),

$$A_{g} = \frac{Zq^{2}}{4\pi\epsilon(0)V} \int_{V} \exp\left(-\frac{\mathbf{r}}{\lambda}\right) \exp\left(-i\mathbf{g}\cdot\mathbf{r}\right) \frac{d\mathbf{r}}{\mathbf{r}}$$
(6.101)

Following the procedures above gives us

$$A_{g} = \frac{Zq^{2}}{\epsilon(0)V(|g|^{2} + 1/\lambda^{2})}$$
(6.102)

or

$$H_{kk'} = \frac{Zq^2}{\epsilon(0)V(|\dot{k} - k'|^2 + 1/\lambda^2)}$$
(6.103)

A comparison of the screened equation (6.103) and the unscreened equation (6.100) indicates that the screening factor for a scattering process in general is

$$\Lambda = \frac{|k - k'|^2}{|k - k'|^2 + 1/\lambda^2}$$
(6.104)

In Table 6.1 we have summarized the scattering potentials and matrix elements for various scattering mechanisms. Screening can be accounted for by multiplying the matrix elements by (6.104).

	IVI	echanisms			
Scattering Mechanisms	Scattering Potential	Matrix Element			
Impurities		- 2			
Ionized	$\frac{Zq^2}{4\pi\epsilon(0)r}$	$\frac{Zq^2}{\epsilon(0)V k-k' ^2}$			
Neutral	$\frac{\hbar^2}{m^*} \left(\frac{r_{\rm B}}{r^5}\right)^{1/2}$	$\frac{2\pi\hbar^2}{m^*V} \left(\frac{20r_{\rm B}}{k}\right)^{1/2}$			
Acoustic phonons		20 X X X X X X X X X X X X X X X X X X X			
Deformation potential	$\mathscr{E}_A \nabla \cdot \mathbf{u}$	$\mathscr{E}_A \left(\frac{\hbar}{2V\rho\omega_s}\right)^{V_2} \left(\mathbf{a}\cdot\mathbf{q}_s\right) \left(n_q + \frac{1}{2} \pm \frac{1}{2}\right)^{V_2}$			
Piezoelectric	$\frac{iqe_{pz}}{\epsilon(0)q_s}\nabla\cdot\mathbf{u}$	$\frac{q e_{pz}}{\epsilon(0)} \left(\frac{\hbar}{2V \rho \omega_s}\right)^{1/2} \left(n_q + \frac{1}{2} \pm \frac{1}{2}\right)^{1/2}$			
Optical phonons					
Deformation potential	$D\delta u$	$D\left(\frac{\hbar}{2V\rho\omega_{\rm LO}}\right)^{1/2}\left(n_q+\frac{1}{2}\pm\frac{1}{2}\right)^{1/2}$			
Polar	$\frac{iqe^*}{\omega\epsilon(\infty)q_s}\delta u$	$\frac{qe^*}{\Omega\epsilon(x)q_s} \left(\frac{\hbar}{2V\rho\omega_{\rm LO}}\right)^{1/2} \left(n_q + \frac{1}{2} \pm \frac{1}{2}\right)^{1/2}$			

TABLE 6.1 Scattering Potentials and Matrix Elements for Various Scattering Mechanisms<sup>a</sup>

<sup>*a*</sup>  $r_{\rm B}$  = Bohr radius;  $n_q$  = phonon occupation number;  $e^* = \Omega \omega_{\rm LO} \epsilon(\infty) \rho^{1/2} [1/\epsilon(\infty) - 1/\epsilon(0)]^{1/2}$ .

### 6.5 RELAXATION TIMES

With the matrix elements listed in Table 6.1, momentum relaxation times can be calculated from (6.84) for the various scattering mechanisms. Assuming isotropic parabolic energy bands, ionized impurity scattering can be described by the Brooks–Herring equation [H. Brooks, *Adv. Electron. Electron Phys.* 7, 158 (1955)],

$$\frac{1}{\tau_{II}(x)} = \frac{2.41Z^2 N_I}{\epsilon_r^2(0)T^{3/2}} g(n^*, T, x) \left(\frac{m}{m^*}\right)^{1/2} x^{-3/2} \operatorname{second}^{-1}$$
(6.105)

where the screening term

$$g(n^*, T, x) = \ln (1 + b) - \frac{b}{1 + b}$$
 (6.106)

. ....

and

$$b = 4.31 \times 10^{13} \, \frac{\epsilon_r(0) T^2}{n^*} \left(\frac{m^*}{m}\right) x \tag{6.107}$$

In these equations  $N_I$  is the total ionized impurity concentration in cm<sup>-3</sup> and  $n^*$  is the effective screening concentration in cm<sup>-3</sup> given by (6.58).

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For neutral impurity scattering, we use Erginsoy's result [C. Erginsoy, *Phys. Rev.* 79, 1013 (1950)],

$$\frac{1}{\tau_{NI}} = 1.22 \times 10^{-7} \epsilon_r(0) N_N \left(\frac{m}{m^*}\right)^2 \text{ second}^{-1}$$
 (6.108)

where  $N_N$  is the total neutral impurity concentration in cm<sup>-3</sup>. Notice that this momentum relaxation time is independent of the carrier energy, x. Usually, neutral impurities have an appreciable effect on carrier scattering only for relatively uncompensated samples at low temperatures.

The momentum relaxation time for deformation potential scattering by acoustic phonons was first calculated by Bardeen and Shockley (J. Bardeen and W. Shockley, *Phys. Rev. 80*, 72 (1950)]. Their result is

$$\frac{1}{\tau_{DA}(x)} = \frac{4.17 \times 10^{19} \mathcal{C}_A^2 T^{3/2}}{C_l} \left(\frac{m^*}{m}\right)^{3/2} x^{1/2} \text{ second}^{-1} \qquad (6.109)$$

for  $\mathcal{E}_A$  in eV and  $C_l$  in dyn/cm<sup>2</sup>.  $C_l$  is the spherically averaged longitudinal elastic constant indicated by (6.111) below.

For materials with no inversion symmetry, the acoustic phonons also scatter carriers by means of a piezoelectric interaction. A momentum relaxation time for this process was first formulated by Meijer and Polder [H. J. G. Meijer and D. Polder, *Physica 19*, 255 (1953)]. With spherical averaging of the elastic and piezoelectric constants over a cubic crystal structure [J. D. Zook, *Phys. Rev. 136*, A849 (1964)], this is given by

$$\frac{1}{\tau_{PA}(x)} = 1.05 \times 10^7 h_{14}^2 \left[ \left( \frac{3}{C_l} + \frac{4}{C_l} \right) \right] T^{1/2} \left( \frac{m^*}{m} \right)^{1/2} x^{-1/2} \text{ second}^{-1}$$
(6.110)

In (6.110)  $h_{14} = e_{14}/\epsilon(0)$  is the piezoelectric constant in V/cm and the average longitudinal and transverse elastic constants are

$$C_l = \frac{1}{5}(3C_{11} + 2C_{12} + 4C_{44}) \tag{6.111}$$

and

$$C_t = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}) \tag{6.112}$$

in dyn/cm<sup>2</sup>. For a hexagonal crystal structure the momentum relaxation time is anisotropic.

For impurities and acoustic phonons the scattering processes are, to a good approximation, elastic. For optical phonons, however, the phonon energy is comparable to the thermal energy of the carriers and the scattering processes are inelastic. Despite this, a momentum relaxation time can still be defined for deformation potential scattering by optical phonons [W. A. Harrison, *Phys. Rev. 104*, 1281 (1956)]. This is given by Sec. 6.5 Relaxation Times

$$\frac{1}{\tau_{\rm DO}(x)} = \frac{2.07 \times 10^{19} \mathscr{C}_A^2 T^{1/2} \theta}{C_l [\exp (\theta/T) - 1]} \left(\frac{m^*}{m}\right)^{3/2} \left[ \left(x + \frac{\theta}{T}\right)^{1/2} + \exp\left(\frac{\theta}{T}\right) \left(x - \frac{\theta}{T}\right)^{1/2} \right] \operatorname{second}^{-1}$$
(6.113)

for  $\mathscr{C}_A$  in eV and  $C_l$  in dyn/cm<sup>2</sup>.  $\theta$  in this equation is the longitudinal optical phonon temperature,

$$\equiv \frac{\hbar\omega_{\rm LO}}{k} \tag{6.114}$$

 $\mathscr{C}_A$  is the acoustic phonon deformation potential constant, which is related to the optical phonon deformation potential constant, D, by

θ

$$\mathscr{E}_A^2 = \frac{C_l D^2}{\rho \omega_{\rm LO}^2} \tag{6.115}$$

For polar scattering of carriers by optical phonons a universal relaxation time can be defined only for temperatures much less than or much greater than the optical phonon temperature. It is thus necessary to use a variational method to solve the Boltzmann equation and determine the carrier scattering. However, Ehrenreich [H. Ehrenreich, J. Appl. Phys. 32, 2155 (1961)] has developed a relaxation time based on a variational calculation for polar scattering which gives the correct solutions to the Boltzmann equation at low and high temperatures. This is given by,

$$\frac{1}{\tau_{\rm PO}(x)} = \frac{1.04 \times 10^{14} \left[\epsilon_r(0) - \epsilon_r(\infty)\right] \theta^{1/2} (\theta/T)^r}{\epsilon_r(0)\epsilon_r(\infty) \left[\exp\left(\theta/T\right) - 1\right]} \left(\frac{m^*}{m}\right)^{1/2} x^{-r} \operatorname{second}^{-1}$$
(6.116)

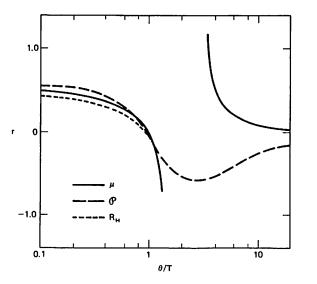
where r varies with  $(\theta/T)$  as shown in Fig. 6.6.

The results of this section for the momentum relaxation times are summarized in Table 6.2 in the form

$$\tau_i(x) = \tau_i x^{r_i} \tag{6.117}$$

These expressions are valid only for scattering in isotropic parabolic energy bands. For scattering in more complex bands, see D. L. Rode, *Semiconductors and Semimetals*, Vol. 10, *Transport Phenomena*, ed. R. K. Willardson and A. C. Beer (New York: Academic Press, 1975) or J. D. Wiley (ibid.). It should also be noted that the momentum relaxation times were derived under the assumption that screening can be neglected for *phonon* scattering. This is usually a good assumption for samples with nondegenerate doping.

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**Figure 6.6** Variation of the parameter r in Equation (6.116) with  $(\theta/T)$  obtained by equating variational solutions for the mobility,  $\mu$ , thermoelectric power,  $\mathcal{P}$ , and Hall coefficient.  $R_H$ , with the corresponding expressions in the relaxation time approximation. [From H. Ehrenreich, General Electric Research Lab. Rep. No. 61-RL-(27626), June 1961.]

TABLE 6.2	Momentum Relaxation Times and Reduced Energy Dependence for
	Materials with Isotropic Parabolic Bands <sup>a</sup>

Scattering Mechanisms	τ <sub>i</sub> (sec)	ri
Impurities		
Ionized	$\frac{0.414\epsilon_r^2(0)T^{3/2}}{Z^2N_f(\text{cm}^{-3})g(n^*,T,x)} \left(\frac{m^*}{m}\right)^{1/2}$	2
Neutral	$\frac{8.16 \times 10^6}{\epsilon_r(0)N_N(\mathrm{cm}^{-3})} \left(\frac{m^*}{m}\right)^2$	0
Acoustic phonons		
Deformation potential	$\frac{2.40 \times 10^{-20} C_l (dyn/cm^2)}{\ell_A^2 (eV) T^{3/2}} \left(\frac{m}{m^*}\right)^{3/2}$	- <u>‡</u>
Piezoelectric	$\frac{9.54 \times 10^{-8}}{h_{14}^2(\text{V/cm})(3/C_1 + 4/C_2)T^{1/2}} \left(\frac{m}{m^*}\right)^{1/2}$	ł
Optical phonons		
Deformation potential	$\frac{4.83 \times 10^{-20} C_l (\text{dyn/cm}^2) [\exp{(\theta/T)} - 1]}{\mathscr{C}_{\lambda}^2 (\text{eV}) T^{1/2} \theta} \left(\frac{m}{m^*}\right)^{3/2}$	≅ -½
Polar	$\frac{9.61 \times 10^{-15} \epsilon_r(0) \epsilon_r(\infty) [\exp(\theta/T) - 1]}{[\epsilon_r(0) - \epsilon_r(\infty)] \theta^{1/2} (\theta/T)'} \left(\frac{m}{m^*}\right)^{1/2}$	$r\left(\frac{\theta}{T}\right)$

"  $N_I$  = concentration of ionized impurities;  $g(n^*, T, x) = \ln (1 + b) - b/(1 + b); b = 4.31$  $\times 10^{13} [\epsilon_r(0)T^2/n^*(cm^{-3})](m^*/m)x; N_N$  = concentration of neutral impurities;  $C_I = \frac{1}{2}(3C_{11})$ 

+  $2C_{12}$  +  $4C_{44}$ ;  $C_{t} = \frac{1}{3}(C_{11} - C_{12} + 3C_{44}); \theta = h\omega_{LO}/k.$ 

### 6.6 COMBINED SCATTERING

In most calculations of transport properties it is necessary to consider several scattering processes at the same time. If these scattering mechanisms are independent of one another, the matrix elements or differential scattering cross sections for each process can be added to obtain the total scattering. In the relaxation time approximation we see from (6.84) or (6.87) that this is equivalent to adding the reciprocal times for each process,

$$\frac{1}{\tau_m(x)} = \sum_i \frac{1}{\tau_i(x)}$$
(6.118)

where the  $\tau_i(x)$  are given by (6.105), (6.108), (6.109), (6.110), (6.113), and/ or (6.116). The desired transport property is then obtained by averaging the appropriate expression involving  $\tau_m(x)$  over the electron distribution. From (5.54) this procedure is

$$\langle \tau_m^s(x)x' \rangle = \frac{2}{3} \frac{\int_0^\infty \tau_m^s(x)(-\partial f_0/\partial x)x'^{-3/2} dx}{\int_0^\infty f_0 x^{1/2} dx}$$
(6.119)

For some combinations of scattering mechanisms it is possible to evaluate (6.119) analytically. The usual procedure is to integrate the numerator by parts and obtain a solution in terms of Fermi-Dirac integrals of order j, which are tabulated in Appendix B. For problems involving ionized impurity scattering this procedure is complicated by the energy or x dependence of the screening term.  $g(n^*, T, x)$ , given by (6.106) and (6.107). Since it is a slowly varying function of x, however, reasonable approximations can be made. The usual procedure is to evaluate  $g(n^*, T, x)$  at a constant energy,  $x = x_m$ , and remove it from the integral. The value of  $x_m$  is determined by the condition that the integrand remaining after the removal of  $g(n^*, T, x_m)$ be a maximum [E. M. Conwell and V. F. Weisskopf, *Phys. Rev.* 77, 388 (1950)]. Typically,  $x_m$  has a value of about 3 or so.

For most combinations of scattering mechanisms it is necessary to evaluate (6.119) numerically. As an example of this, the temperature dependence of the mobility,

$$\mu = \frac{q\langle \tau_m \rangle}{m^*} \tag{5.50}$$

for high-purity *n*-type GaAs is shown in Fig. 6.7. Here the mobility for each relevant scattering mechanism was calculated separately from (5.50), (6.105), (6.108), (6.109), (6.110), (6.116), and (6.119) and then combined to compare with experimental data.

As can be seen, the mobility of this GaAs sample is dominated by ionized impurity scattering at low temperatures and by polar optical phonon

Sec. 6.6

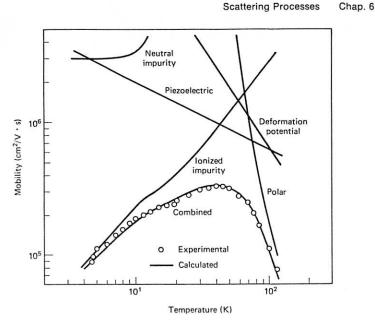


Figure 6.7 Temperature dependence of the mobility for *n*-type GaAs showing the separate and combined scattering processes. [From C. M. Wolfe, G. E. Stillman, and W. T. Lindley, *J. Appl. Phys.* 41, 3088 (1970).]

scattering at high temperatures. Deformation potential optical phonon scattering is not important for  $\Gamma$  conduction bands [H. Ehrenreich and A. W. Overhauser, *Phys. Rev. 104*, 331 (1956)]. This mobility behavior is typical for polar semiconductors. In these calculations the singly ionized  $N_I$  in (6.105) is given by

$$N_I = n + 2N_a (6.120)$$

 $n^*$  in (6.107) by (6.61), and  $N_N$  in (6.108) by

$$N_{N} = N_{d} - N_{a} - n \tag{6.121}$$

 $N_d$  and  $N_a$  were obtained by analyzing the experimental temperature dependence of *n* with (4.90). For *n*-type material this equation is

$$\frac{n(n+N_a)}{N_d-N_a-n} = \frac{N_c}{g_d} \exp\left(\frac{-\Delta \mathcal{E}_d}{kt}\right)$$
(6.122)

The other parameters required in the analysis are typically obtained from other, independent measurements. These are listed for GaAs in Table 6.3 together with the appropriate parameters for other materials for which the analysis above is valid.

TABLE 6.3	Parameters for Calculating the Transport Properties of n-Type
	Semiconductors with Isotropic Parabolic Bands

Combined Scattering

		<u>m*</u>	(0)		θ	EA	$C_l$	$h_{14}^2 \left(\frac{3}{C_l} + \frac{4}{C_l}\right)$ (10 <sup>3</sup> V <sup>2</sup> /dyn)
1	Material	m	€ <sub>r</sub> (0)	€ <i>,</i> (∞)	(K)	(eV)	(10 <sup>12</sup> dyn/cm <sup>2</sup> )	$(10^{2} v^{2}/dyn)$
>	GaN	0.218	9.87	5.80	1044	8.4	2.65	18.32
	GaP	0.13	11.10	9.11	580	13.0	1.66	1.15
>	GaAs	0.067	12.53	10.90	423	6.3	1.44	2.04
	GaSb	0.042	15.69	14.44	346	8.3	1.04	
	InP	0.082	12.38	9.55	497	6.8	1.21	0.137
	InAs	0.025	14.54	11.74	337	5.8	1.0	0.192
	InSb	0.0125	17.64	15.75	274	7.2	0.79	0.409
	ZnS	0.312	8.32	5.13	506	4.9	1.28	6.87
	ZnSe	0.183	9.20	6.20	360	4.2	1.03	0.620
	ZnTe	0.159	9.67	7.28	297	3.5	0.84	0.218
	CdS	0.208	8.58	5.26	428	3.3	0.85	32.5
	CdSe	0.130	9.40	6.10	303	3.7	0.74	16.7
	CdTe	0.096	10.76	7.21	246	4.0	0.70	0.445
	HgSe	0.0265	25.6	12.0	268	4	0.80	0.445
	HgTe	0.0244	20.0	14.0	199	4	0.61	0.445
	PbS		175	17	300	20		
	PbSe		250	24	190	24	0.71	
	PbTe		400	33	160	25		

### PROBLEMS

**6.1.** In a collision with an acoustic phonon, show that an electron with initial velocity  $v_i$  will gain or lose at most only

$$\frac{4u_s}{v_i} - 4\left(\frac{u_s}{V_i}\right)^2$$

of its initial energy, where  $u_s$  is the sound velocity.

**6.2.** An acoustic wave of the form  $A \exp [i(\mathbf{q}\cdot\mathbf{r} - \omega t)]$  propagates through an *n*-type semiconductor with a parabolic band where it produces a variation in the energy of the electrons

$$\mathscr{E} = \mathscr{E}_1 A \exp\left[i(\mathbf{q} \cdot \mathbf{r} - \omega t)\right]$$

Since the force exerted on an electron is  $\mathbf{F} = -\nabla_r \mathcal{E}$ , show that in the relaxation time approximation, a good approximation to the electron distribution is

$$f = f_0 + \frac{\partial f_0}{\partial \mathcal{E}} \frac{i\tau_m \mathbf{v} \cdot \mathbf{q} \mathcal{E}}{1 + i\tau_m \mathbf{v} \cdot \mathbf{q}}$$

Does this distribution provide conduction?

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**6.3.** (a) Evaluate  $r_{\rm H}$  for ionized impurity scattering using the momentum relaxation time determined in the Brooks-Herring approximation.

(b) Plot the temperature variation of  $r_{\rm H}$  using parameters appropriate to GaAs.

- **6.4.** Use the Rutherford scattering cross section to derive the mobility for ionized impurity scattering in the Conwell–Weisskopf approximation.
  - (a) Discuss the validity of the Born approximation for ionized impurity scattering.
  - (b) Discuss the differences between C-W and B-H approximation, particularly in the temperature range where there is carrier freeze-out.

# Optical Properties

When light is incident on a semiconductor, the optical phenomena of absorption, reflection, and transmission are observed. From these optical effects, we obtain much of the information we have concerning the energy band structure and electronic processes in semiconductors. Figure 7.1 shows a hypothetical absorption spectrum as a function of photon energy for a typical semiconductor. As can be seen, a number of processes can contribute to absorption. At high energies photons are absorbed by the transitions of electrons from filled valence band states to empty conduction band states. For energies just below the lowest forbidden energy gap, radiation is absorbed due to the formation of excitons and electron transitions between band and impurity states. The transitions of free carriers within energy bands produce an absorption continuum which increases with decreasing photon energy. Also, the crystalline lattice itself can absorb radiation, with the energy being given off in optical phonons. Finally, at low energies, or long wavelengths, electronic transitions can be observed between impurities and their associated bands.

Many of these processes have important technological applications. For example, intrinsic photodetectors utilize band-to-band absorption, while semiconductor lasers generally operate by means of transitions between impurity and band states. In this chapter we examine these optical processes in detail.