$$\mathbf{v}_g = \frac{\hbar \mathbf{k}_0}{m^*} \tag{1.76}$$

which looks like momentum divided by mass. But for nonparabolic bands described by eq. (1.43), the group velocity is

$$\mathbf{v}_g = \frac{\hbar \mathbf{k}_0}{m^*[1+2\alpha E(k)]} \tag{1.77}$$

In the semiclassical view of electron transport, the electron wave packet is treated as a particle; the uncertainty in the momentum is assumed to be small so that the electron's energy is sharply defined, and the uncertainty in the electron's position is assumed to be small in comparison to the distance over which applied and built-in potentials vary significantly. The motion of the center of this wave packet is described by eq. (1.75), which looks like the classical relation between force and momentum. The velocity of the electron [eq. (1.14)] corresponds to the velocity of a classical particle only for spherical, parabolic bands. This semiclassical treatment of carrier dynamics is the basis for each of the following chapters, but collisions involve rapidly varying potentials and must be treated quantum mechanically.

1.5 SCATTERING OF ELECTRONS BY THE RANDOM POTENTIAL, $U_S(\mathbf{r}, t)$

Bloch waves move through the lattice unimpeded by the crystal potential. Occasionally, however, the electron encounters a perturbation caused when a lattice vibration moves an atom or by impurities or defects which may be present. When an electron encounters such a perturbation it scatters — and scattering "knocks" an electron wave packet centered at k_0 to k_0'. Frequent scattering tends to "wash out" the interference effects due to the carrier's wave nature. Scattering plays a dominant role in transport, and it is important that we know $S(k_0, k_0')$, the *transition rate* from k_0 to k_0'. We now derive an expression for $S(k_0, k_0')$ in terms of $U_S(z,t)$, the perturbing potential.

The wave equation [eq. (1.1)] is written as

$$\left[H_0 + U_S(z,t)\right] \Psi(z,t) = i\hbar \frac{\partial \Psi(z,t)}{\partial t} \tag{1.78}$$

where H_0 is the Hamiltonian operator for the unperturbed problem (the problem without the scattering potential). We assume that the unperturbed problem,

$$H_0 \psi_k = E(k) \psi_k \tag{1.79}$$

$$\Psi_k^0(z,t) = \psi_k(z)\, e^{-iE(k)t/\hbar} \tag{1.80}$$

has been solved. These solutions form a complete, orthonormal set so we can express the solution to the perturbed problem as linear combinations of them:

$$\Psi(z,t) = \sum_k c_k(t)\, \Psi_k^0(z,t) = \sum_k c_k(t)\, \psi_k(z)\, e^{-iE(k)t/\hbar} \tag{1.81}$$

Now consider the situation sketched in Fig. 1.12 — an electron wave packet centered at k_0 enters, interacts with $U_S(z,t)$, and emerges centered at k_0'. At $t = 0$ we have

$$\begin{aligned} c_{k_0}(t=0) &= 1 \\ c_k(t=0) &= 0 \qquad (k \neq k_0) \end{aligned} \tag{1.82}$$

After the scattering event, the probability of finding the electron with wave vector k_0' is

$$P(k = k_0') = \lim_{t\to\infty} |\, c_{k_0'}(t)|^2 \tag{1.83}$$

so the transition rate from k_0 to k_0' is

$$S(k_0, k_0') = \lim_{t\to\infty} \frac{|\, c_{k_0'}(t)|^2}{t} \tag{1.84}$$

(To allow $t \to \infty$ in these expressions, without another collision occurring, collisions must be infrequent.)

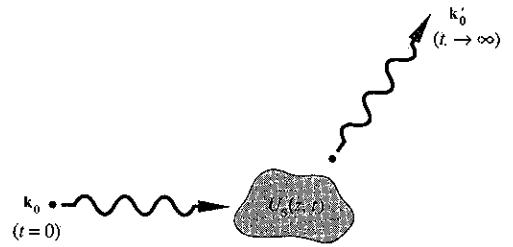

Fig. 1.12 Scattering of a wave packet centered at $k = k_0$ to one centered at $k = k_0'$.

To find c_k, we insert eq. (1.81) in eq. (1.78) and obtain

$$U_S(z,t)\sum_k c_k(t)\,\psi_k\,e^{-iE(k)t/\hbar} = i\hbar\sum_k \frac{\partial c_k}{\partial t}\,\psi_k\,e^{-iE(k)t/\hbar} \tag{1.85}$$

Next, we multiply both sides by $\psi^*_{k'_0}\,e^{iE(k'_0)t/\hbar}$, integrate, and make use of the orthogonality of eigenfunctions, to find

$$i\hbar\frac{\partial c_{k'_0}}{\partial t} = \sum_k H_{k'_0k}\,c_k(t)\,e^{i[E(k'_0)-E(k)]t/\hbar} \tag{1.86}$$

where

$$H_{k'_0k}(t) \equiv \int_{-\infty}^{+\infty} \psi^*_{k'_0}(z)\,U_S(z,t)\,\psi_k(z)\,dz \tag{1.87}$$

is the *matrix element* of the scattering potential between states k'_0 and k.

Since we assume that the scattering is weak, $c_{k_0} \simeq 1$ for all time, and the other c_k's are always small. With this approximation, the *Born approximation*, the sum in eq. (1.86) can be approximated by one term as

$$i\hbar\frac{\partial c_{k'_0}}{\partial t} = H_{k'_0k_0}\,e^{i[E(k'_0)-E(k_0)]t/\hbar}$$

which can be integrated to find

$$c_{k'_0}(t) = \frac{1}{i\hbar}\int_0^t H_{k'_0k_0}\,e^{i[E(k'_0)-E(k_0)]t/\hbar}dt + c_{k'_0}(0) \tag{1.88}$$

Because the final state k'_0 was empty at $t = 0$, $c_{k'_0}(0) = 0$.

Let's specify the time-dependent matrix element as

$$H_{k'_0,k_0}(t) = H^{a,e}_{k'_0k_0}(\omega)\,e^{\mp i\omega t} \tag{1.89}$$

which may represent one Fourier component of a more general potential. (The significance of the "a" and "e" superscripts which apply the minus and plus signs,

respectively, will be explained shortly.) With eq. (1.89) for the matrix element, eq. (1.88) can be integrated as

$$c_{k'_0} = \frac{1}{i\hbar}H(\omega)^{a,e}_{k'_0k_0}\,\frac{e^{i[E(k'_0)-E(k_0)\mp\hbar\omega]t/\hbar}}{i[E(k'_0)-E(k_0)\mp\hbar\omega]/\hbar} - 1 \tag{1.90}$$

When we define

$$\Lambda = [E(k'_0)-E(k_0)\mp\hbar\omega]/\hbar \tag{1.91}$$

then eq. (1.90) can be written as

$$c_{k'_0}(t) = \frac{1}{i\hbar}H^{a,e}_{k'_0k_0}\,e^{i\Lambda t/2}\,\frac{\sin(\Lambda t/2)}{\Lambda t/2}\,t \tag{1.92}$$

Now, according to eq. (1.84), we find the transition rate as

$$S(k_0,k'_0) = \lim_{t\to\infty}\frac{|H^{a,e}_{k'_0k_0}|^2}{t\hbar^2}\left[\frac{\sin(\Lambda t/2)}{\Lambda t/2}\right]^2 t^2 \tag{1.93}$$

For large t, the function in brackets is very sharply peaked near the origin and looks like a δ-function. The strength of the δ-function is determined from the area under the curve as

$$\int_{-\infty}^{\infty}\left[\frac{\sin(\Lambda t/2)}{\Lambda t/2}\right]^2 d\Lambda = \frac{2\pi\hbar}{t} \tag{1.94}$$

so we can replace the quantity in brackets in eq. (1.93) by $2\pi\delta(\Lambda)/t$ to find

$$S(k_0,k'_0) = \frac{2\pi}{\hbar}|H^a_{k'_0k_0}|^2\,\delta[E(k'_0)-E(k_0)-\hbar\omega] + \frac{2\pi}{\hbar}|H^e_{k'_0k_0}|^2\,\delta[E(k'_0)-E(k_0)+\hbar\omega] \tag{1.95}$$

The δ-function in eq. (1.95) simply states conservation of energy and applies when scattering is weak, so that time can approach infinity in eq. (1.93). For frequent scattering, there is an uncertainty in the final energy given by eq. (1.12) that is known as

collisional broadening. The first term in eq. (1.95) contributes when $E(k_0') = E(k_0) + \hbar\omega$; an energy of $\hbar\omega$ has been absorbed. The second contributes when $E(k_0') = E(k_0) - \hbar\omega$; an energy of $\hbar\omega$ has been emitted.

Equation (1.95) is the basic result of scattering theory that we will apply to carriers in semiconductors. The result is known as *Fermi's golden rule*. To apply the golden rule, the scattering potential must be identified so that the matrix element can be evaluated. For electrons in semiconductors, the wave functions for the unperturbed problem are Bloch waves. When the matrix element [eq. (1.87)] is evaluated for Bloch waves, one finds (Ref. [1.5])

$$H_{k'k} = I(k,k')\, U_S(k-k') \tag{1.96}$$

where

$$I(k,k') \equiv \int_{-\infty}^{+\infty} u_k^*(z)\, u_k(z)\, dz \tag{1.97}$$

is called the *overlap integral* and

$$U_S(k-k') = \int_{-\infty}^{+\infty} e^{-ik'x}\, U_S(z,t)\, e^{+ikz}\, dz \tag{1.98}$$

For a parabolic band, $I(k,k') \approx 1$ (Ref. [1.5]) and

$$\boxed{H_{k'k} \approx \int_{-\infty}^{\infty} e^{-ik'x}\, U_S(z,t)\, e^{ikz}\, dz} \tag{1.99}$$

which is just what we would have obtained from eq. (1.87) using plane waves rather than Bloch waves. When we evaluate scattering rates in Chapter 2, we'll assume that the energy bands are parabolic and employ eq. (1.99).

1.5.1 Examples

To illustrate how the golden rule is applied to scattering problems, we consider two simple, but illustrative, examples. Short-range scattering potentials might be approximated by a δ-function potential:

$$U_S(z) = A_0\, \delta(z) \tag{1.100}$$

From eq. (1.99) we find

$$H_{k'k} = A_0 \tag{1.101}$$

and from eq. (1.95), the transition rate becomes

$$S(k,k') = \frac{2\pi}{\hbar} A_0^2\, \delta[E(k') - E(k)] \tag{1.102}$$

This time-independent scattering potential elastically scatters electrons with a transition rate that is proportional to the squared magnitude of the scattering potential. The δ-function potential is an approximate description of ionized impurity scattering when it is strongly screened by free carriers.

As a second example, consider the scattering potential,

$$U_S(z,t) = A_\beta\, e^{\pm(i\beta z - \omega t)} \tag{1.103}$$

which may represent one Fourier component of a more general potential. For plane waves confined to a normalization length, $-L/2 \le z \le L/2$,

$$\psi(z) = \frac{1}{\sqrt{L}}\, e^{ikz} \tag{1.104}$$

and the matrix element becomes

$$H_{k'k} = \int_{-L/2}^{L/2} \frac{A_\beta}{L}\, e^{i(k-k'\pm\beta)z}\, dz \tag{1.105}$$

If the normalization length is long, the oscillating, exponential factor ensures that no net contribution to the integral will result unless $k' = k \pm \beta$, so

$$H_{k'k} = A_\beta\, \delta(k - k' \pm \beta) \tag{1.106}$$

For this scattering potential, the transition rate is

$$S(k,k') = \frac{2\pi}{\hbar} A_\beta^2\, \delta(k' - k \mp \beta)\, \delta[E(k') - E(k) \mp \hbar\omega] \tag{1.107}$$

which is, again, proportional to the squared magnitude of the perturbing potential. To satisfy the first δ-function,

$$\hbar k' = \hbar k \pm \hbar \beta \tag{1.108}$$

which we interpret as a statement of conservation of momentum. The scattered electron has either absorbed or emitted momentum. [The momentum-conserving δ-function was absent in eq. (1.102) because the δ-function scattering potential contained Fourier components with all momenta.] Similarly, the second δ-function in eq. (1.107) states that

$$E(k') = E(k) \pm \hbar \omega \tag{1.109}$$

which is a statement of conservation of energy. For time-dependent scattering potentials such as eq. (1.103), carriers either absorb or emit energy. This scattering potential is a good description of the perturbing potential due to lattice vibrations (phonons).

1.6 LATTICE VIBRATIONS (PHONONS)

Because much of the scattering in semiconductors is due to lattice vibrations, it is important that we understand their basic properties. If an atom is displaced from its equilibrium position, the bonding forces tend to push it back, so it oscillates about its

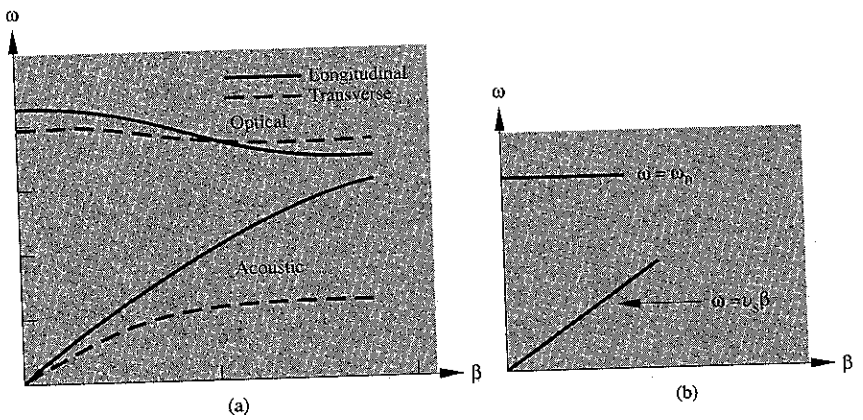

Fig. 1.13 (a) Typical dispersion relations for elastic waves propagating along a high-symmetry direction in cubic semiconductors; (b) simplified dispersion relations useful when only longitudinal lattice vibrations near the center of the Brillouin zone are considered. After Datta (Ref. [1.1]).

equilibrium site. Since lattice waves propagate in a periodic medium, they have properties much like those of Bloch waves. Figure 1.13a shows a typical dispersion relation, ω versus β, observed for elastic waves in cubic semiconductors such as silicon and gallium arsenide. (We label the wave vector $\boldsymbol{\beta}$ rather than $\mathbf{k}$ to distinguish elastic waves from electron waves.) Six types of elastic waves exist — three *acoustic* modes, and three *optical* modes. Acoustic modes are like sound waves in that adjacent atoms are displaced in the same direction — only the magnitude of the displacement varies from atom to atom. Of the three acoustic modes, one is longitudinal (LA) and two are transverse (TA). For longitudinal waves, atoms are displaced in the direction of propagation; the two transverse modes, in which atoms are displaced in a transverse direction, are degenerate in cubic Si and GaAs.

In Chapter 2 we shall establish that the scattering of electrons within a valley is due to lattice vibrations with wave vectors very near the origin of the Brillouin zone. For small $\boldsymbol{\beta}$, the dispersion relation for acoustic modes can be approximated by

$$\omega(\boldsymbol{\beta}) = \upsilon_s |\boldsymbol{\beta}| \tag{1.110}$$

where υ_s is the sound velocity.

Optical modes differ from acoustic modes in that adjacent atoms are displaced out of phase. (The term "optical" arises because such vibrations can interact strongly with light.) As shown in Fig. 1.13a, the dispersion relation for optical modes displays relatively little variation with wave vector. When electrons are scattered by optical phonons and remain within the same valley, only small wave vectors are involved and the dispersion relation can be approximated as

$$\omega(\boldsymbol{\beta}) = \omega_0 \tag{1.111}$$

where ω_0 is a constant. Figure 1.13b shows a simplified dispersion relation for acoustic and optical modes that is often used for scattering calculations.

Lattice vibrations are much like the vibrations of a harmonic oscillator, so the energy of each normal mode must be quantized according to

$$E(\beta) = \hbar \omega(\beta) \left(N_\beta + \frac{1}{2}\right) \tag{1.112}$$

The quantum of energy is viewed as a particle called a *phonon*, and the number of phonons is given by the Bose-Einstein factor as

$$N_\beta = \frac{1}{e^{\hbar \omega(\beta)/k_B T_L} - 1} \tag{1.113}$$

For

$$\hbar\omega(\beta) << k_B T_L$$

eq. (1.113) reduces to

$$N_\beta \approx \frac{k_B T_L}{\hbar\omega(\beta)} \tag{1.114}$$

which is known as *equipartition* and is usually valid for acoustic phonons — except at very low temperatures. Equation (1.114) is easy to understand; $k_B T_L$ is the thermal energy and $\hbar\omega(\beta)$ is the energy of the phonon at β, so eq. (1.114) just tells us how many phonons are needed to account for the thermal energy. In Chapter 2, we shall describe how phonons, both acoustic and optical, scatter carriers.

1.7 SUMMARY

A simple approach for treating carrier motion within conventional devices has been outlined. This semiclassical approach treats carriers as particles whose dynamics, between collisions, are governed by eqs. (1.14) and (1.75), which are analogous to Newton's laws. Carrier scattering, however, is treated by quantum mechanics using Fermi's golden rule. The semiclassical approach is applicable when the applied and built-in potentials vary slowly on the scale of an electron's wavelength. Room-temperature, thermal average electrons have a wavelength of about 120 Å in Si and about 240 Å in GaAs, so the semiclassical approach may be questioned in ultrasmall devices. Many devices contain quantum wells, and the carriers within such wells clearly display their wave nature. Nevertheless, the semiclassical treatment adequately describes the performance of most conventional devices (by which we mean those not specifically designed to exploit the wave nature of carriers). Our focus in this text is on the semiclassical transport of carriers, but we shall, from time to time, consider the transport of carriers confined in quantum wells.

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PROBLEMS

1.1 Consider the effect of a perturbing potential that is constant in both space and time,

$$U_S(z, t) = U_0$$

and answer the following questions.

(a) Obtain an expression for the transition rate, $S(k, k')$.

(b) Interpret your answer to part (a). What does your result imply about the motion of electrons through regions of uniform potential?