

Chapter 2

Electron Transport

Abstract We introduce basic quantum mechanical concepts of electron wave packet transport, the scattering theory about electron transition from one steady state to another that eventually form a net nonzero charge flow, i.e., current. Boltzmann equation is discussed about carrier transport in terms of drift and diffusion versus ballistic transport. Major scattering processes in semiconductors are introduced and discussed.

2.1 Quantum Mechanical Wave Transport

In semiclassical transport theory the electrons are treated as classical point-like particles during free flights between scattering events. The scattering processes are however treated quantum mechanically. During the free flights, two things must be consistent with each other:

1. A wavepacket representing the point-like electron with well-defined position and momentum;
2. The quantum uncertainty principle.

The semiclassical treatment of the electron transport driven by an external electric field E is normally referred to as the Drude drift model. Here it is assumed that the electron speed v is zero after a collision with a scattering center. The electron will be driven by the external electric field. By the classical Newton mechanics $F = m^*a$, where F is the force asserted on the electron, and a the acceleration, we have

$$-eE = m^* \frac{dv}{dt} \quad (2.1)$$

Let τ be the mean time between two successive collisions, we obtain the average speed v_{average} and thereafter the mobility μ are

$$v_{\text{average}} = \frac{-e\tau}{m^*} E, \quad \mu = \frac{e\tau}{m^*} \quad (2.2)$$

The mean free path $\ell = v_{\text{average}}\tau$. On the one hand, well-defined position and momentum indicate

$$\Delta p \ll p, \quad \Delta x \ll \ell \quad (2.3)$$

while the quantum uncertainty principle states

$$\hbar \approx \Delta p \Delta x \ll p\ell = \frac{p^2}{m^*}\tau \quad (2.4)$$

Since at thermal equilibrium,

$$\frac{p^2}{2m^*} \approx k_B T$$

where k_B is the Boltzmann constant and T the temperature, the validity of the semi-classical approach is insured when

$$\tau \gg \frac{\hbar}{k_B T} \quad (2.5)$$

Otherwise, quantum treatment of transport during the free flights is necessary where the wave nature of electron dynamics is to be fully accounted for.

Quantum mechanically, we denote the solution of a Schrödinger equation as a wave function $\Psi(\mathbf{r}, t)$, which in general is space \mathbf{r} and time t dependent

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H(\mathbf{r}, t)\Psi(\mathbf{r}, t) \quad (2.6)$$

When the Hamiltonian $H(\mathbf{r}, t)$ in the above Schrödinger equation describes an electron in an electron system, $|\Psi(\mathbf{r}, t)|^2 d\mathbf{r}$ represents the probability to find the electron in a space volume $d\mathbf{r}$ centered at \mathbf{r} at time t .

In the previous chapter we have discussed the general features of electron eigen states in semiconductor, which are characterized as Bloch states denoted by wave functions Ψ_{nk} and energies $E_n(\mathbf{k})$. Here n is the energy band index and \mathbf{k} is the wave vector of the Bloch state. For the devices discussed in this book, the magnetic field is negligible so that the electron spin up and down states are degenerate. In other words, each Bloch state actually consists of two states, one spin up and one spin down.

Knowing the electron states in the semiconductor, we then fill these states by the available electrons. At zero temperature, starting from the electron state of the lowest energy we fill each electron state by two electrons (Pauli exclusion principle). For intrinsic bulk semiconductor, all electron states up to the top of the valence band are completely filled, and the electron states from the bottom of the conduction band are totally empty. Same situation happens for insulators. Actually the only difference between intrinsic semiconductors and insulators is in their energy bandgaps (energy separations between the valence band top and the conduction band bottom). Insulators have much larger energy bandgaps than semiconductors. The filling of the electron states in metals are rather different: the conduction bands of metals are

partially filled by electrons. The different occupation features of energy bands of semiconductors and metals are responsible for the different electric conductances of the materials. We will discuss it shortly.

At finite temperature T , the occupation of electron state with eigen value E_i (for Bloch state, $i = n\mathbf{k}$) is given by the Fermi Dirac distribution

$$f(E_i, E_f) = \frac{1}{e^{(E_i - E_f)/k_B T} + 1} \quad (2.7)$$

where E_f is called Fermi level which is determined by

$$N = \sum_i \frac{1}{e^{(E_i - E_f)/k_B T} + 1} \quad (2.8)$$

where N is the total number of electrons. Note that an energy state can contain either 0 or 1 electron. The mean number of electrons in the energy state is therefore numerically equal to the probability of its being occupied.

The spatial distribution of an electron occupying state denoted by $\Psi_i(\mathbf{r}, t)$ and E_i is $|\Psi_i(\mathbf{r}, t)|^2 f(E_i, E_f)$, and the spatial distribution $n(\mathbf{r}, t)$ of the total electrons is

$$n(\mathbf{r}, t) = \sum_i |\Psi_i(\mathbf{r}, t)|^2 f(E_i, E_f) \quad (2.9)$$

Note that in the above equation, the time-dependence is explicit. At steady state, $\Psi_i(\mathbf{r}, t) = e^{-E_i t/\hbar} \Psi_i(\mathbf{r})$ and the carrier distribution n is time-independent. We will return to this issue from time to time when we study electronic devices.

The motion of the electron is described by its probability flow density

$$\mathbf{j}(\mathbf{r}, t) = \frac{\hbar}{2im_0} [\Psi^*(\mathbf{r}, t) \nabla \Psi(\mathbf{r}, t) - \Psi(\mathbf{r}, t) \nabla \Psi^*(\mathbf{r}, t)] \quad (2.10)$$

In the absence of a potential energy, the Hamiltonian of the electron consists of only $-\hbar^2 \nabla^2 / 2m_0$ and the solution of the corresponding Schrödinger equation is the plane wave form $\Psi(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}}$ with a flow density

$$\mathbf{j} = \frac{\hbar \mathbf{k}}{m_0} \quad (2.11)$$

by inserting $\Psi(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}}$ into Eq. (2.10).

It is easy to show that the probability flow density \mathbf{j} satisfies the continuity equation

$$\frac{\partial(\Psi^* \Psi)}{\partial t} = -\nabla \cdot \mathbf{j} \quad (2.12)$$

Let us have a look about the probability flow density of a steady-state Bloch electron in the semiconductor. Inserting the Bloch wave function

$$\Psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} e^{i\mathbf{k} \cdot \mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}, t)$$

into Eq. (2.10)

$$\mathbf{j}_{nk}(\mathbf{r}) = \frac{\hbar \mathbf{k}}{Nm_0} u_{nk}^* u_{nk} + \frac{\hbar}{2im_0} (u_{nk}^* \nabla u_{nk} - u_{nk} \nabla u_{nk}^*) \quad (2.13)$$

where N is the number of unit cells contained in the semiconductor.

We recall that the periodic Bloch function $u_{nk}(\mathbf{r}, t)$ is periodic with respect to unit cell, it is also normalized within one unit cell. The probability flow density of the Bloch electron averaged in the semiconductor thus becomes

$$\langle \mathbf{j}_{nk}(\mathbf{r}) \rangle = \int \frac{\hbar \mathbf{k}}{Nm_0} u_{nk}^* u_{nk} d\mathbf{r} + \int \frac{\hbar}{2im_0} (u_{nk}^* \nabla u_{nk} - u_{nk} \nabla u_{nk}^*) d\mathbf{r} \quad (2.14)$$

Since

$$\int_{\text{cell}} u_{nk}^* \nabla u_{nk} d\mathbf{r} = 0 \quad (2.15)$$

we have

$$\langle \mathbf{j}_{nk}(\mathbf{r}) \rangle = \frac{\hbar \mathbf{k}}{m_0} \quad (2.16)$$

This is very much alike the probability flow density of a free electron Eq. (2.11). It indicates that a Bloch electron $\Psi_{nk}(\mathbf{r}, t)$ can be viewed as a plane wave with a wave vector \mathbf{k} .

At equilibrium, the occupation of Bloch state Ψ_{nk} is determined by its energy $E_n(\mathbf{k})$. In other words, Ψ_{nk} and Ψ_{n-k} are equally occupied, since $E_n(\mathbf{k}) = E_n(-\mathbf{k})$, i.e., Eq. (1.41). Since the two Bloch states have the same probability flow density with opposite directions, there is no net electron flow at equilibrium.

We have thus far discussed the probability flow density of a Bloch electron, i.e., an eigen function of the electron Hamiltonian. In practice, the electron under investigation is injected into the device through contacts which is not initially an eigen state of the electron Hamiltonian in the device. Let us denote the initial state of injecting electron as $\psi(\mathbf{r}, 0)$ at $t = 0$. The motion of the electron state is governed by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H\Psi(\mathbf{r}, t) \quad (2.17)$$

Discretizing the time t by step δt so that $t = n\delta t$, where n is a positive integer. The wave function of the electron becomes $\Psi(\mathbf{r}, n\delta t)$ which is further denoted as $\Psi^n(\mathbf{r})$, and the above time-dependent Schrödinger equation can be written as

$$i\hbar \frac{\Psi^{n+1}(\mathbf{r}) - \Psi^n(\mathbf{r})}{\delta t} = H\Psi^n(\mathbf{r}) \rightarrow \Psi^{n+1}(\mathbf{r}) = \left(1 - \frac{i\delta t}{\hbar} H\right) \Psi^n(\mathbf{r}) \quad (2.18)$$

This equation has an intuitive form such that a future wave function Ψ^{n+1} is given explicitly in terms of its preceding wave function Ψ^n , hence it is known as the explicit forward-time-centered-space (FTCS) scheme [1]. However this solution is

unstable due to boundless growth of errors through successive time integration. Alternatively we can try the implicit form

$$\Psi^n(\mathbf{r}) = \left(1 + \frac{i\delta t}{\hbar} H\right) \Psi^{n+1}(\mathbf{r}) \quad (2.19)$$

and though this form is stable, it is fairly inaccurate. Thus Goldberg, Schey, and Schwartz have employed the Cayley form [2]

$$\left(1 + \frac{i\delta t}{2\hbar} H\right) \Psi^{n+1}(\mathbf{r}) = \left(1 - \frac{i\delta t}{2\hbar} H\right) \Psi^n(\mathbf{r}) \quad (2.20)$$

It was indicated [2] that unitarity is the characteristics of the original Schrödinger equation which ensures that the normalization of the wave functions does not change in time. When H is Hermitian, $e^{\pm i\delta t H/\hbar}$ are clearly unitary, while their first-order approximations $1 \pm i\delta t H/\hbar$ are not unitary. On the other hand, the Cayley form Eq. (2.20) is unitary, which has a further desirable property of being precise to order δt^2 .

The value of δt in Eq. (2.20) is determined in such a way that $\delta t E \leq \hbar$ in order to convert the Schrödinger equation (2.17) into the Cayley form of Eq. (2.20).

In the Goldberg scheme, the initial wave packet is described by a single-momentum Gaussian wave packet [2]

$$\left(\frac{\sigma^2}{\pi}\right)^{3/4} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_0) - |\mathbf{r} - \mathbf{r}_0|^2 / 2\sigma^2} \quad (2.21)$$

centered at \mathbf{r}_0 , where \mathbf{k} is the momentum and σ describes the spatial extension of the wave packet. As an example, let us study the wave packet transport of one conduction-band electron with $m_x^* = 0.1905$, $m_y^* = 0.1905$, and $m_z^* = 0.9163$, in a Si quantum wire embedded in SiO_2 with a cross section $(-L_x : L_x) \times (-L_y : L_y)$ extended along the z axis. In the following numerical simulations, $L_x = L_y = 2.7$ nm, $L_z = (-500 : 500)$ nm. We assume that the potential barrier provided by the surrounding SiO_2 is infinitely high. Furthermore, we introduce a negative point charge at the center of the quantum wire. The initial Gaussian wave packet can be expressed as

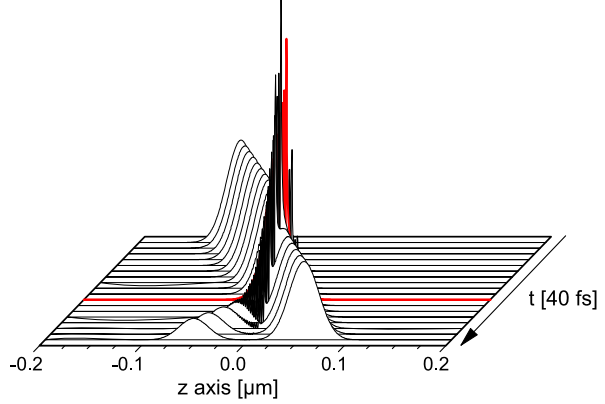
$$\psi_{i,k}(\mathbf{r}, 0) = \psi_i(x, y) \left(\frac{\sigma^2}{\pi}\right)^{1/4} e^{ik(z-z_0) - (z-z_0)^2 / 2\sigma^2} \quad (2.22)$$

where $\psi_i(x, y)$ is the i th eigen function in the xy plane. Let $z_0 = -100$ nm, $\sigma = 10$ nm, and

$$\psi_i(x, y) = \sin\left[\frac{\pi(x + L_x)}{2L_x}\right] \sin\left[\frac{\pi(y + L_y)}{2L_y}\right] \quad (2.23)$$

which is the ground state in the xy plane. Denote $E_k = \hbar^2 k^2 / 2m_z^*$ as the kinetic energy of the electron along the z axis, it is just straightforward to calculate the

Fig. 2.1 Wave packet transport $a(z, t)$ initially centered at $z = -0.1 \mu\text{m}$. $E_k = 150 \text{ meV}$. The red curve is the wave packet profile when the wave packet center reaches $z = 0$



wave packet transport $\psi(\mathbf{r}, t)$ as a function of E_k by Eq. (2.20), the flow density $\mathbf{j}(\mathbf{r}, t)$ by Eq. (2.10). Physically, the current flow is nonzero only along the z axis, so that we present the wave packet transport in the form of

$$a(z, t) = \iint |\psi(\mathbf{r}, t)|^2 dx dy \quad (2.24)$$

Figure 2.1 shows the temporal development of a Gaussian wave packet initially centered at $z = -0.1 \mu\text{m}$ with a kinetic energy $E_k = 150 \text{ meV}$ along the z axis. It is easy to estimate that the speed of such a wave packet is $2.4 \times 10^5 \text{ m/s}$ (effective mass $m_z^* = 0.9163$) and the time to move from $z = -0.1 \mu\text{m}$ to $z = 0$ is 0.417 ps , as marked by the red profile in Fig. 2.1. Here it is observed that the wave packet splits into two by the negative point charge, one is reflected back (moves along the $-z$ axis) and the other tunnels through the potential barrier induced by the negative point charge then transports further along the z axis.

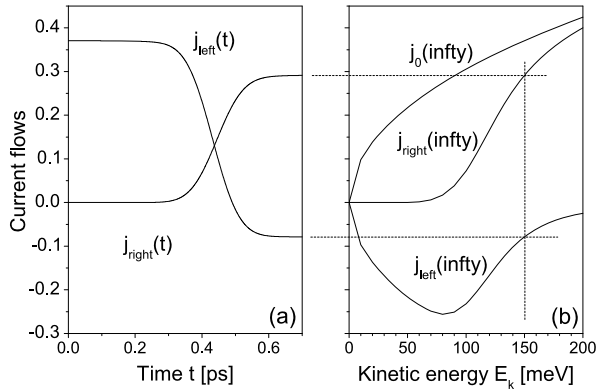
In order to see the temporal development of the wave packet more clearly, we split the current flow into two parts, one for $z < 0$ and the other $z \geq 0$

$$\begin{aligned} j_{\text{left}}(t) &= \int_{-\infty}^0 \left[\iint \mathbf{j}(\mathbf{r}, t) dx dy \right] dz \\ j_{\text{right}}(t) &= \int_0^{\infty} \left[\iint \mathbf{j}(\mathbf{r}, t) dx dy \right] dz \end{aligned} \quad (2.25)$$

Figure 2.2(a) shows the temporal developments of the above two current flows when $E_k = 150 \text{ meV}$. Here we see that after the wave packet reaches the point charge, the tunneling part starts to emerge on the right side of the point charge, thus a gradual increase of $j_{\text{right}}(t)$ (> 0 , i.e., along the z axis), the reflected part move along the $-z$ axis, thus $j_{\text{left}}(t) < 0$.

If we put two electrodes at $z = \pm\infty$, two currents, $j_{\text{left}}(\infty)$ and $j_{\text{right}}(\infty)$, will be eventually detected when $t \rightarrow \infty$, which are shown in Fig. 2.2(b). For the sake of comparison, the transport of the wave packet through a perfect Si quantum wire

Fig. 2.2 (a) Current flows $j_{\text{left}}(t)$ and $j_{\text{right}}(t)$ as functions of time t . $E_k = 150$ meV. (b) $j_{\text{left}}(\infty)$ and $j_{\text{right}}(\infty)$ as functions of E_k . $j_0(\infty)$ denotes the current flow through a perfect Si quantum wire



(without the point charge at the quantum wire center), $j_0(\infty)$, is also presented which is exactly the relationship of Eq. (2.16) as expected. Figure 2.2(b) shows that the wave packet is easily scattered when its kinetic energy is small. When the kinetic energy is larger than 200 meV, the wave packet overcomes the point charge so that the scattering becomes negligible.

The wave packet transport is extremely important in nano-scale electronic and photonic devices. See more in Chaps. 4 and 5.

2.2 Scattering Theory

By the above section we understand that at equilibrium, the electrons remain in their initial states in the semiconductor and there will be no net carrier flow. External forces are therefore needed in order to obtain any responses from the electrons. Before we formulate the electron transport theory as well as discuss all other properties of semiconductor materials and devices, we repeat here the basic quantum mechanical description about the response of electrons under external perturbation.

We shall use the quantum theory in the following to discuss various transition processes of electron. We first formulate the quantum perturbation theory in its simplest form. The electron is described by the Hamiltonian H_0

$$\begin{aligned}
 i\hbar \frac{\partial \Psi_i(\mathbf{r}, t)}{\partial t} &= H_0 \Psi_i(\mathbf{r}, t) \\
 H_0 \Psi_i(\mathbf{r}) &= E_i \Psi_i(\mathbf{r}) \\
 \Psi_i(\mathbf{r}, t) &= e^{-i E_i t / \hbar} \Psi_i(\mathbf{r})
 \end{aligned} \tag{2.26}$$

At $t = 0$ a perturbation $V' e^{-i\omega t}$ is switched on, where V' is time independent. The wave function $\Psi(\mathbf{r}, t)$ of the new Schrödinger equation

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = (H_0 + V' e^{-i\omega t}) \Psi(\mathbf{r}, t) \tag{2.27}$$

is expanded in the basis of $\{\Psi_i, E_i\}$ in the form of

$$\Psi(\mathbf{r}, t) = \sum_i a_i(t) \Psi_i(\mathbf{r}) e^{-iE_i t/\hbar} \quad (2.28)$$

so that

$$i\hbar \frac{da_m(t)}{dt} = \sum_i \langle \Psi_m(\mathbf{r}) | V' | \Psi_i(\mathbf{r}) \rangle e^{i(E_m - E_i - \hbar\omega)t/\hbar} a_i(t) \quad (2.29)$$

Suppose that before $t = 0$, the electron under investigation occupies state Ψ_n , i.e., $a_n(t < 0) = 1$ and $a_i(t < 0) = 0$ if $i \neq n$. By the first-order perturbation theory,

$$i\hbar \frac{da_m(t)}{dt} = \langle \Psi_m(\mathbf{r}) | V' | \Psi_n(\mathbf{r}) \rangle e^{i(E_m - E_n - \hbar\omega)t/\hbar} \quad (2.30)$$

It must be emphasized here that the above equation is actually valid for a very short time duration of $[t, t + dt]$. After dt , the occupations of all the electron states will all be modified and eventually we need to work with Eq. (2.29) along the time axis, which will be done in the next section. However, Eq. (2.30) itself is very rich in physics if being treated carefully. The most important aspect to be taken into account for is the fact that during the transition from Ψ_n to Ψ_m under the influence of $V' e^{-i\omega t}$, the occupation $a_n(t)$ of the initial state Ψ_n will be gradually dissipated.

Let

$$\langle \Psi_m | V' | \Psi_n \rangle = V'_{mn}$$

We introduce the dissipation process phenomenologically by the concept of a lifetime, \hbar/Γ_n , of the electron occupying state Ψ_n . In other words, due to the transitions from Ψ_n to Ψ_m , the occupation a_n gradually decreases. Hence, we can simulate that the total wave function of the initial state Ψ_n is

$$\Psi_n(\mathbf{r}) e^{iE_n t/\hbar - \Gamma_n t/\hbar}$$

Equation (2.30) is now replaced by

$$i\hbar \frac{da_m(t)}{dt} = V'_{mn} e^{i(E_m - E_n - \hbar\omega)t/\hbar - \Gamma_n t/\hbar} \quad (2.31)$$

The transition probability is calculated by integrating from 0 to t

$$a_m(t) = \frac{1}{i\hbar} \int_0^t V'_{mn} e^{i(E_m - E_n - \hbar\omega)t'/\hbar - \Gamma_n t'/\hbar} dt' = \frac{V'_{mn} [1 - e^{i(E_m - E_n - \hbar\omega)t/\hbar - \Gamma_n t/\hbar}]}{E_m - E_n - \hbar\omega + i\Gamma_n} \quad (2.32)$$

Let $t \rightarrow \infty$,

$$a_m(\infty) = \frac{V'_{mn}}{E_m - E_n - \hbar\omega + i\Gamma_n} \quad (2.33)$$

so that

$$|a_m(\infty)|^2 = \frac{|V'_{mn}|^2}{(E_m - E_n - \hbar\omega)^2 + \Gamma_n^2} \quad (2.34)$$

And the averaged transition probability per unit time, i.e., the transition rate, is obtained by dividing $|a_m(\infty)|^2$ by lifetime \hbar/Γ_n of occupation of state Ψ_n

$$p_m \equiv \frac{|a_m(\infty)|^2}{\hbar/\Gamma_n} = \frac{|V'_{mn}|^2}{\hbar} \frac{\Gamma_n}{(E_m - E_n - \hbar\omega)^2 + \Gamma_n^2} \quad (2.35)$$

In the following, we try to derive the scattering theory in a rigorous way which will be the starting point of the principles of almost all semiconductor nanostructured devices to be discussed in this book.

By purely and formally writing

$$H = H_0 + V' \quad (2.36)$$

where H_0 represents the Hamiltonian operator of the electron at equilibrium, V' is the interaction of the electron with an external field. By the Bloch theorem, the eigen solution of H_0 is

$$\begin{aligned} i\hbar \frac{\partial \Psi_{nk}(\mathbf{r}, t)}{\partial t} &= H_0 \Psi_{nk}(\mathbf{r}, t) \\ \Psi_{nk}(\mathbf{r}, t) &= e^{-iE_{nk}t/\hbar} \Psi_{nk}(\mathbf{r}) \\ H_0 \Psi_{nk}(\mathbf{r}) &= E_{nk} \Psi_{nk}(\mathbf{r}, t) \end{aligned} \quad (2.37)$$

where n is the band index and \mathbf{k} the wave vector. In the following we use short notations to simply mathematical expressions: \mathbf{k} represents quantum numbers $n\mathbf{k}$ for Bloch state, and $|\mathbf{k}\rangle = \Psi_{nk}(\mathbf{r}, t) = e^{-iE_{nk}t/\hbar} \Psi_{nk}(\mathbf{r})$. And between two states \mathbf{k} and \mathbf{q} , $\langle \mathbf{q} | \mathbf{k} \rangle = \delta_{\mathbf{q}, \mathbf{k}}$, i.e., the wave functions are orthogonal. Note that $\delta_{\mathbf{q}, \mathbf{k}} = 0$ if $\mathbf{q} \neq \mathbf{k}$, and $\delta_{\mathbf{q}, \mathbf{k}} = 1$ if $\mathbf{q} = \mathbf{k}$.

Assume that the electron occupies state $|\mathbf{k}\rangle$ before we switch on interaction V' . We like to solve the equation of

$$(H_0 + V')|\Psi\rangle = E_{\mathbf{k}}|\Psi\rangle \quad (2.38)$$

i.e., $|\Psi\rangle$ is a state of Hamiltonian $H_0 + V'$. The above equation can be re-formatted as $(E_{\mathbf{k}} - H_0)|\Psi\rangle = V'|\Psi\rangle$, which is equivalent to

$$(E_{\mathbf{k}} - H_0)|\Psi\rangle = (E_{\mathbf{k}} - H_0)|\mathbf{k}\rangle + V'|\Psi\rangle$$

since $(E_{\mathbf{k}} - H_0)|\mathbf{k}\rangle = 0$. We obtain the following equation by dividing the above expression by $(E_{\mathbf{k}} - H_0)$

$$|\Psi\rangle = |\mathbf{k}\rangle + \frac{1}{E_{\mathbf{k}} - H_0} V'|\Psi\rangle \quad (2.39)$$

We obtain the formal formula of scattering wave function by adding a correction $i\Gamma$

$$|\Psi\rangle = |\mathbf{k}\rangle + \frac{1}{E_{\mathbf{k}} - H_0 + i\Gamma} V' |\Psi\rangle = |\mathbf{k}\rangle + G_{\mathbf{k}} V' |\Psi\rangle \quad (2.40)$$

which is known as the Lippmann-Schwinger equation. We will discuss Γ more in the next section. In the above equation,

$$G_{\mathbf{k}} = \frac{1}{E_{\mathbf{k}} - H_0 + i\Gamma} = \sum_{\mathbf{q}} \frac{|\mathbf{q}\rangle \langle \mathbf{q}|}{E_{\mathbf{k}} - E_{\mathbf{q}} + i\Gamma} \quad (2.41)$$

In the last equality, a representation of unity as a sum over eigenstates of H_0 is inserted to make the expression more explicitly.

We can write the solution of Eq. (2.40) as

$$|\Psi\rangle = \frac{1}{1 - G_{\mathbf{k}} V'} |\mathbf{k}\rangle \quad (2.42)$$

and expand it

$$|\Psi\rangle = |\mathbf{k}\rangle + G_{\mathbf{k}} V' |\mathbf{k}\rangle + G_{\mathbf{k}} V' G_{\mathbf{k}} V' |\mathbf{k}\rangle + G_{\mathbf{k}} V' G_{\mathbf{k}} V' G_{\mathbf{k}} V' |\mathbf{k}\rangle + \dots \quad (2.43)$$

The n th approximation, also known as the n th Born approximation, to the scattering state $|\Psi\rangle$ consists of terminating the above expansion after n terms.

We define a transition matrix $T_{\mathbf{k}}$ as

$$\begin{aligned} T_{\mathbf{k}} &= V' + V' G_{\mathbf{k}} V' + V' G_{\mathbf{k}} V' G_{\mathbf{k}} V' + V' G_{\mathbf{k}} V' G_{\mathbf{k}} V' G_{\mathbf{k}} V' + \dots \\ &= V' + V' \frac{1}{E_{\mathbf{k}} - H_0 + i\Gamma} V' + \dots \end{aligned} \quad (2.44)$$

i.e., $V' |\Psi\rangle = T_{\mathbf{k}} |\mathbf{k}\rangle$, so that the scattering state can be written

$$|\Psi\rangle = |\mathbf{k}\rangle + G_{\mathbf{k}} T_{\mathbf{k}} |\mathbf{k}\rangle \quad (2.45)$$

The probability that the electron initially at state $|\mathbf{k}\rangle$ ends up at state $|\mathbf{q}\rangle$ is

$$\begin{aligned} \langle \mathbf{q} | \Psi \rangle &= \langle \mathbf{q} | \mathbf{k} \rangle + \frac{1}{E_{\mathbf{k}} - E_{\mathbf{q}} + i\Gamma} \left(\langle \mathbf{q} | V' | \mathbf{k} \rangle + \langle \mathbf{q} | V' \frac{1}{E_{\mathbf{k}} - H_0 + i\Gamma} V' | \mathbf{k} \rangle + \dots \right) \\ &= \delta_{\mathbf{q}, \mathbf{k}} + \frac{1}{E_{\mathbf{k}} - E_{\mathbf{q}} + i\Gamma} \left(\langle \mathbf{q} | V' | \mathbf{k} \rangle + \langle \mathbf{q} | V' \frac{1}{E_{\mathbf{k}} - H_0 + i\Gamma} V' | \mathbf{k} \rangle + \dots \right) \end{aligned} \quad (2.46)$$

We have thus far introduced the formal scattering theory about the probability of an electron at initial state $|\mathbf{k}\rangle$ being scattered to state $|\mathbf{q}\rangle$ due to an external perturbation V' . Now we apply the theory to calculate transition amplitudes between the relevant unperturbed eigenstates due to the appearance of the external perturbation V' which is switched on at $t = 0$.

Let H_0 be time-independent and all solutions of the eigenvalue problem $H_0|\mathbf{k}\rangle = E_k|\mathbf{k}\rangle$ are known, it is straightforward to construct the solution of the time-dependent Schrödinger equation

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = H_0 |\Psi(t)\rangle \quad (2.47)$$

which coincides at $t = 0$ with a given initial state $|\Psi(0)\rangle$. Under these circumstances, the state

$$|\Psi(t)\rangle = e^{-iH_0t/\hbar} |\Psi(0)\rangle = \sum_{\mathbf{k}} e^{-iE_k t/\hbar} |\mathbf{k}\rangle \langle \mathbf{k} | \Psi(0) \rangle \quad (2.48)$$

represents the general solution of Eq. (2.47).

When the external perturbation V' is switched on at $t = 0$, the Hamiltonian becomes $H_0 + V'$ and the Schrödinger equation becomes

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = (H_0 + V') |\Psi(t)\rangle \quad (2.49)$$

The above expression is normally referred to as the Schrödinger equation in the Schrödinger picture. We transform the above equation into the so-called interaction picture by a time-dependent unitary operator

$$|\hat{\Psi}(t)\rangle = e^{iH_0t/\hbar} |\Psi(t)\rangle \quad (2.50)$$

In the interaction picture, the Schrödinger equation becomes

$$i\hbar \frac{\partial |\hat{\Psi}(t)\rangle}{\partial t} = \hat{V}'(t) |\hat{\Psi}(t)\rangle \quad (2.51)$$

where the new interaction operator is given by

$$\hat{V}'(t) = e^{iH_0t/\hbar} V' e^{-iH_0t/\hbar} \quad (2.52)$$

Next we introduce the time development operator $\hat{T}(t)$ such that

$$|\hat{\Psi}(t)\rangle = \hat{T}(t) |\hat{\Psi}(0)\rangle \quad (2.53)$$

Insert the above expression into the Schrödinger equation in the interaction picture, i.e., Eq. (2.51), we can see that the time development operator satisfies the integral equation

$$\hat{T}(t) = 1 - \frac{i}{\hbar} \int_0^t \hat{V}'(t') \hat{T}(t') dt' \quad (2.54)$$

A direct calculation of the above time development operator from eigenstate $|\mathbf{k}\rangle$ to $|\mathbf{q}\rangle$ is

$$\langle \mathbf{q} | \hat{T}(t) | \mathbf{k} \rangle = \delta_{\mathbf{q},\mathbf{k}} - \frac{i}{\hbar} \int_0^t \langle \mathbf{q} | \hat{V}'(t') \hat{T}(t') | \mathbf{k} \rangle dt'$$

$$\begin{aligned}
&= \delta_{\mathbf{q}, \mathbf{k}} - \frac{i}{\hbar} \sum_{\mathbf{k}'} \int_0^t \langle \mathbf{q} | \hat{V}'(t') | \mathbf{k}' \rangle \langle \mathbf{k}' | \hat{T}(t') | \mathbf{k} \rangle dt' \\
&= \delta_{\mathbf{q}, \mathbf{k}} - \frac{i}{\hbar} \sum_{\mathbf{k}'} \int_0^t e^{i(E_{\mathbf{q}} - E_{\mathbf{k}'})t' / \hbar} \langle \mathbf{q} | V'(t') | \mathbf{k}' \rangle \langle \mathbf{k}' | \hat{T}(t') | \mathbf{k} \rangle dt'
\end{aligned} \tag{2.55}$$

On the other hand, when V' is small, Eq. (2.54) can be solved by a power series in terms of \hat{V}' such that the zero-order solution

$$\hat{T}^{(0)}(t) = 1 \tag{2.56}$$

which is the solution when $\hat{V}'(t') = 0$. The first-order solution is

$$\hat{T}^{(1)}(t) = 1 - \frac{i}{\hbar} \int_0^t \hat{V}'(t') \hat{T}^{(0)}(t') dt' = 1 - \frac{i}{\hbar} \int_0^t \hat{V}'(t') dt' \tag{2.57}$$

Iterating the mathematical process we obtain a formal solution to Eq. (2.54)

$$\hat{T}(t) = 1 - \frac{i}{\hbar} \int_0^t \hat{V}'(t') dt' - \frac{1}{\hbar^2} \int_0^t \hat{V}'(t') \left[\int_0^{t'} \hat{V}'(t'') dt'' \right] dt' + \dots \tag{2.58}$$

When $\mathbf{k} \neq \mathbf{q}$, the transition amplitude in the first-order perturbation theory is then given by the simple and much-used formula

$$\langle \mathbf{q} | \hat{T}^{(1)}(t) | \mathbf{k} \rangle = -\frac{i}{\hbar} \int_0^t e^{i(E_{\mathbf{q}} - E_{\mathbf{k}})t' / \hbar} \langle \mathbf{q} | V'(t') | \mathbf{k} \rangle dt' \tag{2.59}$$

Notice that $t = 0$ is a time preceding the onset of the perturbation V' .

If V' does not depend on the time, or

$$V'(t) = V_0^* e^{i\omega t} + V_0 e^{-i\omega t}$$

where V_0 and ω are time-independent, the time integration of Eq. (2.59) is trivial. We first focus on the first case, i.e., V' is time-independent, while the second case will be studied in the next section.

Starting with an initial state $|\mathbf{k}\rangle$ at $t = 0$, Eq. (2.59) shows that after a time interval t , the electron will evolve from its initial state $|\mathbf{k}\rangle$ into state $|\mathbf{q}\rangle$ due to perturbation V' switched on at $t = 0$. In other words, the probability that the electron will stay in its initial state will be decreased. Let us now study the probability that the electron dwells in its initial state. Back to Eq. (2.55) and note that V' is weak and time-independent,

$$\langle \mathbf{q} | \hat{T}(t) | \mathbf{k} \rangle = -\frac{i}{\hbar} \langle \mathbf{q} | V' | \mathbf{k} \rangle \int_0^t e^{i(E_{\mathbf{q}} - E_{\mathbf{k}})t' / \hbar} \langle \mathbf{k} | \hat{T}(t') | \mathbf{k} \rangle dt' \tag{2.60}$$

for $\mathbf{q} \neq \mathbf{k}$. Here the transitions via intermediate states $\mathbf{k}' \neq \mathbf{k}$ are neglected since under the first-order perturbation assumption, the possibility of a two-step process, i.e., from \mathbf{k} to \mathbf{k}' ($\mathbf{k}' \neq \mathbf{k}$), then from \mathbf{k}' to \mathbf{q} ($\mathbf{q} \neq \mathbf{k}$), is expected to be very small.

By Eq. (2.55), the equation of motion for $\langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle$ is, rigorously,

$$\frac{\partial}{\partial t} \langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle = -\frac{i}{\hbar} \sum_{\mathbf{q} \neq \mathbf{k}} e^{i(E_{\mathbf{k}} - E_{\mathbf{q}})t/\hbar} \langle \mathbf{k} | V' | \mathbf{q} \rangle \langle \mathbf{q} | \hat{T}(t) | \mathbf{k} \rangle - \frac{i}{\hbar} \langle \mathbf{k} | V' | \mathbf{k} \rangle \langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle \quad (2.61)$$

If Eq. (2.60) is substituted into (2.61), we obtain a differential-integral equation for the probability amplitude that the electron will dwell in the initial state $|\mathbf{k}\rangle$ at time t after switching on V' at time 0

$$\begin{aligned} \frac{\partial}{\partial t} \langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle = & -\frac{1}{\hbar^2} \sum_{\mathbf{q} \neq \mathbf{k}} |\langle \mathbf{q} | V' | \mathbf{k} \rangle|^2 \int_0^t \langle \mathbf{k} | \hat{T}(t') | \mathbf{k} \rangle e^{i(E_{\mathbf{q}} - E_{\mathbf{k}})(t' - t)/\hbar} dt' \\ & - \frac{i}{\hbar} \langle \mathbf{k} | V' | \mathbf{k} \rangle \langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle \end{aligned} \quad (2.62)$$

The solution of this equation demands care. We are interested in a long time which implies rapid oscillations of the exponential factor in the integrand as a function of the final state energy $E_{\mathbf{q}}$. The slowly varying amplitude $\langle \mathbf{k} | \hat{T}(t') | \mathbf{k} \rangle$ can therefore be removed from the t' integrand. The remaining integral can be evaluated

$$\int_0^t e^{i(E_{\mathbf{q}} - E_{\mathbf{k}})(t' - t)/\hbar} dt' = \frac{\hbar[1 - e^{-i(E_{\mathbf{q}} - E_{\mathbf{k}})t/\hbar}]}{i(E_{\mathbf{q}} - E_{\mathbf{k}})} \quad (2.63)$$

which oscillates between 0 and $-i\hbar/(E_{\mathbf{q}} - E_{\mathbf{k}})$ as a function of t . Moreover, it becomes singular when $E_{\mathbf{q}} = E_{\mathbf{k}}$. Such a result is not physical. One critical factor we missed so far is that the transition process from initial state $|\mathbf{k}\rangle$ to other state $|\mathbf{q}\rangle$ will diminish gradually the probability that the electron will stay at its initial state $|\mathbf{k}\rangle$. This is normally referred to as the lifetime of state $|\mathbf{k}\rangle$ under perturbation V' . In other words, $|\mathbf{k}\rangle$, which is an eigen state of Hamiltonian H_0 , is no long an eigen state of Hamiltonian $H_0 + V'$.

We thus introduce a lifetime related parameter $\Gamma_{\mathbf{k}}$ to initial state $|\mathbf{k}\rangle$, such that the eigen value is now $E_{\mathbf{k}} + i\Gamma_{\mathbf{k}}$. In other words, we now express the total wave function of state $|\mathbf{k}\rangle$ as

$$e^{-i(E_{\mathbf{k}} + i\Gamma_{\mathbf{k}})t/\hbar} \Psi_{\mathbf{k}}(\mathbf{r}) \quad (2.64)$$

in the presence of V' , see Eq. (2.37). $\Gamma_{\mathbf{k}}$ will be obtained self-consistently shortly. The self-consistency is more clear in Sect. 3.7 when we discuss the excitation of an exciton in a quantum dot.

Integration (2.63) now becomes

$$\int_0^t e^{i(E_q - E_k - i\Gamma_k)(t' - t)/\hbar} dt' = \frac{\hbar[1 - e^{-i(E_q - E_k - i\Gamma_k)t/\hbar}]}{i(E_q - E_k - i\Gamma_k)} \\ \Rightarrow \frac{\hbar}{i(E_q - E_k - i\Gamma_k)} \quad (2.65)$$

when $t \gg \Gamma_k/\hbar$. The resulting differential equation is

$$\frac{\partial}{\partial t} \langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle = \left(\frac{i}{\hbar} \sum_{q \neq k} \frac{|\langle \mathbf{q} | V' | \mathbf{k} \rangle|^2}{E_q - E_k - i\Gamma_k} - \frac{i}{\hbar} \langle \mathbf{k} | V' | \mathbf{k} \rangle \right) \langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle \quad (2.66)$$

and the solution is

$$\langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle = \exp \left[\left(\frac{i}{\hbar} \sum_{q \neq k} \frac{|\langle \mathbf{q} | V' | \mathbf{k} \rangle|^2}{E_q - E_k - i\Gamma_k} - \frac{i}{\hbar} \langle \mathbf{k} | V' | \mathbf{k} \rangle \right) t \right] \quad (2.67)$$

since $\langle \mathbf{k} | \hat{T}(0) | \mathbf{k} \rangle = 1$.

Just like (2.64), the above expression describes the exponential decay of the electron occupation in the initial state $|\mathbf{k}\rangle$. Therefore,

$$\langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle = \exp \left(-\frac{\Gamma_k}{\hbar} t - \frac{i\Delta E_k}{\hbar} t \right) \quad (2.68)$$

where

$$\Gamma_k = \sum_{q \neq k} |\langle \mathbf{q} | V' | \mathbf{k} \rangle|^2 \frac{\Gamma_k}{(E_k - E_q)^2 + \Gamma_k^2} \quad (2.69)$$

normally referred to as the relaxation energy of state $|\mathbf{k}\rangle$ under the presence of V' , describes how long the electron will stay in its initial state $|\mathbf{k}\rangle$. \hbar/Γ_k is therefore denoted as the lifetime. And the eigen value of state $|\mathbf{k}\rangle$ is shifted, up to second order in V' , by

$$\Delta E_k = \langle \mathbf{k} | V' | \mathbf{k} \rangle + \sum_{q \neq k} |\langle \mathbf{q} | V' | \mathbf{k} \rangle|^2 \frac{E_k - E_q}{(E_k - E_q)^2 + \Gamma_k^2} \quad (2.70)$$

Equation (2.69) shows that Γ_k is proportional to V' , which is natural. Without V' , the electron will stay at its initial state forever. Switching on perturbation V' makes $|\mathbf{k}\rangle$ no longer an eigen state of the new Hamiltonian $H_0 + V'$ so that the probability of finding the electron at $|\mathbf{k}\rangle$ will decrease.

When perturbation $\langle \mathbf{q} | V' | \mathbf{k} \rangle$ is very small, Γ_k will also be very small. In this case, we retrieve common textbook expressions about the relaxation energy Γ_k and energy shift ΔE_k

$$\Gamma_k = \pi \sum_{q \neq k} |\langle q | V' | k \rangle|^2 \delta(E_k - E_q) \quad (2.71)$$

$$\Delta E_k = \langle k | V' | k \rangle + \sum_{q \neq k} \frac{|\langle q | V' | k \rangle|^2}{E_k - E_q}$$

since

$$\lim_{\Gamma \rightarrow 0} \frac{\Gamma}{E^2 + \Gamma^2} = \pi \delta(E) \quad (2.72)$$

We now understand the fundamental constrain about the validity of the above expressions: Γ_k must be very small, which, however, is not always guaranteed by a small $\langle q | V' | k \rangle$. We will discuss in more detail in the next section.

When Eq. (2.68) is substituted back into Eq. (2.60), the integration can be carried out and we obtain

$$\langle q | \hat{T}(t) | k \rangle = \langle q | V' | k \rangle \frac{1 - e^{-\Gamma_k t / \hbar} e^{i(E_q - E_k - \Delta E_k)t / \hbar}}{E_q - E_k - \Delta E_k + i\Gamma_k} \quad (2.73)$$

for $t \geq 0$, and hence, the probability that the electron has evolved from its initial state $|k\rangle$ into state $|q\rangle$ is

$$P_{q \leftarrow k}(t) = |\langle q | \hat{T}(t) | k \rangle|^2$$

$$= |\langle q | V' | k \rangle|^2 \frac{1 - 2e^{-\Gamma_k t / \hbar} \cos[(E_q - E_k - \Delta E_k)t / \hbar] + e^{-2\Gamma_k t / \hbar}}{(E_q - E_k - \Delta E_k)^2 + \Gamma_k^2} \quad (2.74)$$

After a time that is very long compared with the lifetime \hbar/Γ_k that the electron stays in eigenstate $|k\rangle$, i.e., $t \rightarrow \infty$, the probability that the electron will be found in state $|q\rangle$ is

$$P_{q \leftarrow k}(\infty) = \frac{|\langle q | V' | k \rangle|^2}{(E_q - E_k - \Delta E_k)^2 + \Gamma_k^2} \quad (2.75)$$

exhibiting the typical bell-shaped resonance behavior with a peak at $E_q = E_k + \Delta E_k$ and a width Γ_k . And the transition rate, i.e., the transition probability per unit time, is obtained by dividing $P_{q \leftarrow k}(\infty)$ by lifetime \hbar/Γ_k

$$P_{q \leftarrow k} = \frac{|\langle q | V' | k \rangle|^2}{\hbar} \frac{\Gamma_k}{(E_q - E_k - \Delta E_k)^2 + \Gamma_k^2} \quad (2.76)$$

This is almost the same as we obtained before, see Eq. (2.35), where the lifetime was introduced phenomenologically. Note that in deriving Eq. (2.35), the effect of V' on the eigenvalue of state $|k\rangle$, i.e., ΔE_k of Eq. (2.70), was neglected.

Let us have a close look at Γ_k . By Eq. (2.71), and when $\langle \mathbf{q} | V' | \mathbf{k} \rangle$ is constant in a small energy range ΔE in the neighborhood of E_q ,

$$\begin{aligned}\Gamma_k &= \pi \sum_{\mathbf{q} \neq \mathbf{k}} |\langle \mathbf{q} | V' | \mathbf{k} \rangle|^2 \delta(E_q - E_k) \\ &\approx \pi |\langle \mathbf{q} | V' | \mathbf{k} \rangle|^2 \int_{\mathbf{q} \neq \mathbf{k}} \delta(E_q - E_k) N_{\text{DOS}}(E_q) dE_q \\ &= \pi |\langle \mathbf{q}_k | V' | \mathbf{k} \rangle|^2 N_{\text{DOS}}(E_{q_k})\end{aligned}\quad (2.77)$$

$N_{\text{DOS}}(E_q)$ is the density of states. Here $|\mathbf{q}_k\rangle$ is such a representative state that its eigenvalue equals E_k , $N_{\text{DOS}}(E_{q_k})$ is the density of these states. Notice that $|\mathbf{q}_k\rangle \neq |\mathbf{k}\rangle$!

2.3 Time-Dependent Perturbation

We now discuss the scattering processes involving energy dissipation. The processes include both the absorption and emission of energy by the electron to and from its surrounding environment.

We consider an external perturbation in the form of

$$V'(t) = 2V' \cos(\omega t) = V' e^{i\omega t} + V' e^{-i\omega t} \quad (2.78)$$

where V' and ω are time-independent. Rather importantly, V' and ω are physical quantities so that they are real.

By Eq. (2.55), and for $\mathbf{q} \neq \mathbf{k}$,

$$\langle \mathbf{q} | \hat{T}(t) | \mathbf{k} \rangle = -\frac{i}{\hbar} \langle \mathbf{q} | V' | \mathbf{k} \rangle \int_0^t [e^{i(E_q - E_k - \hbar\omega)t'/\hbar} + e^{i(E_q - E_k + \hbar\omega)t'/\hbar}] \langle \mathbf{k} | \hat{T}(t') | \mathbf{k} \rangle dt' \quad (2.79)$$

And the probability that the electron remains in its initial state,

$$\begin{aligned}\frac{\partial}{\partial t} \langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle &= -\frac{i}{\hbar} \sum_{\mathbf{q} \neq \mathbf{k}} [e^{i(E_k - E_q - \hbar\omega)t/\hbar} + e^{i(E_k - E_q + \hbar\omega)t/\hbar}] \langle \mathbf{k} | V' | \mathbf{q} \rangle \langle \mathbf{q} | \hat{T}(t) | \mathbf{k} \rangle \\ &\quad - \frac{2i}{\hbar} \cos(\omega t) \langle \mathbf{k} | V' | \mathbf{k} \rangle \langle \mathbf{k} | \hat{T}(t) | \mathbf{k} \rangle\end{aligned}\quad (2.80)$$

By inserting Eq. (2.79) into the above equation and following the same considerations when solving Eq. (2.62), we expect to have

$$\int_0^t e^{i(E_q - E_k \pm \hbar\omega)(t'-t)/\hbar} dt' \implies \frac{\hbar}{i(E_q - E_k - i\Gamma_k \pm \hbar\omega)} \quad (2.81)$$

which will be most significant when $E_q - E_k \pm \hbar\omega = 0$. The physics is straightforward that the electron, initially occupying state $|\mathbf{k}\rangle$, will transit to another state $|\mathbf{q}\rangle$

after absorbing a quasi particle $\hbar\omega$ of the perturbation field described by Eq. (2.78), when $E_q - E_k - \hbar\omega = 0$, whereas for $E_q - E_k + \hbar\omega = 0$, the electron will emit $\hbar\omega$ while transiting from $|k\rangle$ to $|q\rangle$. The probabilities of other transition processes are weak. There is another term

$$\int_0^t e^{i(E_q - E_k)(t' - t)/\hbar} \cos[\omega(t' + t)] dt' \rightarrow 0 \quad (2.82)$$

since (1) we now study the case of $\omega \neq 0$ so that $E_q \neq E_k$ when expression (2.81) is significant, and (2) $\cos[\omega(t' + t)]$ oscillates rapidly.

Furthermore, in practical systems and applications, the effective range of $\hbar\omega$ is at least in the order of eV (photodetections and light-emitting devices in the visible optical range) so that $1/\omega$ is less than 10^{-12} s, while the time scale of most first-order perturbation processes is in the range of 10^{-15} . In other words, we consider the time duration of $\omega t \rightarrow 0$ so that $\cos(\omega t) = 1$ in Eq. (2.80). Thus

$$\frac{\partial}{\partial t} \langle k | \hat{T}(t) | k \rangle = - \left(\frac{i}{\hbar} \sum_{q \neq k} \frac{|\langle q | V' | k \rangle|^2}{E_q - E_k \pm \hbar\omega - i\Gamma_k} - \frac{2i}{\hbar} \langle k | V' | k \rangle \right) \langle k | \hat{T}(t) | k \rangle \quad (2.83)$$

which leads to the solution of

$$\langle k | \hat{T}(t) | k \rangle = \exp \left(-\frac{\Gamma_k}{\hbar} t - \frac{i\Delta E_k}{\hbar} t \right) \quad (2.84)$$

exactly the same as Eq. (2.68) but different parameters

$$\begin{aligned} \Gamma_k &= \sum_{q \neq k} |\langle q | V' | k \rangle|^2 \frac{\Gamma_k}{(E_k - E_q \pm \hbar\omega)^2 + \Gamma_k^2} \\ \Delta E_k &= \langle k | V' | k \rangle + \sum_{q \neq k} |\langle q | V' | k \rangle|^2 \frac{E_k - E_q \pm \hbar\omega}{(E_k - E_q \pm \hbar\omega)^2 + \Gamma_k^2} \end{aligned} \quad (2.85)$$

It is easy to see that Eqs. (2.69) and (2.70) are retrieved when $\omega \rightarrow 0$. Note that when $\omega = 0$, the external perturbation expression of Eq. (2.78) is $2V'$, while it is V' for Eqs. (2.69) and (2.70).

By Eq. (2.79),

$$\langle q | \hat{T}(t) | k \rangle = \langle q | V' | k \rangle \frac{1 - e^{i(E_q - E_k - \Delta E_k \pm \hbar\omega + i\Gamma_k)t/\hbar}}{E_q - E_k - \Delta E_k \pm \hbar\omega + i\Gamma_k} \quad (2.86)$$

so that when $t \rightarrow \infty$,

$$\langle q | \hat{T}(\infty) | k \rangle = \frac{\langle q | V' | k \rangle}{E_q - E_k - \Delta E_k \pm \hbar\omega + i\Gamma_k} \quad (2.87)$$

Finally we obtain the total transition probability

$$P_{q \leftarrow k} = |\langle q | \hat{T}(\infty) | k \rangle|^2 = \left| \frac{\langle q | V' | k \rangle}{E_q - E_k - \Delta E_k \pm \hbar\omega + i\Gamma_k} \right|^2 \quad (2.88)$$

and the transition rate $p_{q \leftarrow k} = P_{q \leftarrow k} / (\hbar / \Gamma_k)$

$$p_{q \leftarrow k} = \frac{|\langle q | V' | k \rangle|^2}{\hbar} \frac{\Gamma_k}{(E_q - E_k - \Delta E_k \pm \hbar\omega)^2 + \Gamma_k^2} \quad (2.89)$$

Equations (2.85) and (2.89) will be extensively used in this book. The “−” sign in “±” in the above equation is normally referred as the absorption of a quasi particle $\hbar\omega$, and the “+” sign as the emission of $\hbar\omega$.

2.4 Acceleration Theorems

We now take a close look at the properties of electrons transporting in a semiconductor crystal. As we learned before, the state of an electron in a periodic crystal is described the Bloch theorem. By substituting the Bloch solution of

$$\Psi_{nk}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk}(\mathbf{r}) \quad (2.90)$$

into the Hamiltonian

$$H_0 \Psi(\mathbf{r}) = \left[\frac{-\hbar^2 \nabla^2}{2m_0} + V(\mathbf{r}) \right] \Psi(\mathbf{r}) = E \Psi(\mathbf{r}) \quad (2.91)$$

for an electron in the periodic lattice potential

$$V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r}) \quad (2.92)$$

where \mathbf{R} is any lattice vector, we find that $u_{nk}(\mathbf{r})$ is determined by the following eigenvalue equation

$$\left[\frac{\hbar^2}{2m_0} \left(\frac{1}{i} \nabla + \mathbf{k} \right)^2 + V(\mathbf{r}) \right] u_{nk}(\mathbf{r}) = E_{nk} u_{nk}(\mathbf{r}) \quad (2.93)$$

with boundary condition

$$u_{nk}(\mathbf{r}) = u_{nk}(\mathbf{r} + \mathbf{R}) \quad (2.94)$$

For the sake of the following discussion, we define

$$H_k \equiv \frac{\hbar^2}{2m_0} \left(\frac{1}{i} \nabla + \mathbf{k} \right)^2 + V(\mathbf{r}) \quad (2.95)$$

Because of the periodic boundary condition we can regard Eq. (2.93) as an eigenvalue problem restricted to a single cell of the crystal.

We expand the energy dispersion relation $E_{n\mathbf{k}+\mathbf{q}}$ of the Bloch electron around \mathbf{k}

$$E_{n\mathbf{k}+\mathbf{q}} = E_{n\mathbf{k}} + \sum_i \frac{\partial E_{n\mathbf{k}}}{\partial k_i} q_i + \frac{1}{2} \sum_{ij} \frac{\partial^2 E_{n\mathbf{k}}}{\partial k_i \partial k_j} q_i q_j + O(q^3) \quad (2.96)$$

On the other hand, since $E_{n\mathbf{k}+\mathbf{q}}$ is the eigenvalue of $H_{\mathbf{k}+\mathbf{q}}$, we write

$$\begin{aligned} H_{\mathbf{k}+\mathbf{q}} &= \frac{\hbar^2}{2m_0} \left(\frac{1}{i} \nabla + \mathbf{k} + \mathbf{q} \right)^2 + V(\mathbf{r}) \\ &= H_{\mathbf{k}} + \frac{\hbar^2}{m_0} \mathbf{q} \cdot \left(\frac{1}{i} \nabla + \mathbf{k} \right) + \frac{\hbar^2 q^2}{2m_0} \\ &= H_{\mathbf{k}} + V' + \frac{\hbar^2 q^2}{2m_0} \end{aligned} \quad (2.97)$$

where

$$V' = \frac{\hbar^2}{m_0} \mathbf{q} \cdot \left(\frac{1}{i} \nabla + \mathbf{k} \right) \quad (2.98)$$

By the first-order perturbation theory, i.e., Eq. (2.70), we find that the energy correction due to \mathbf{q} in the Hamiltonian Eq. (2.97) is

$$\langle u_{n\mathbf{k}} | V' | u_{n\mathbf{k}} \rangle = \int u_{n\mathbf{k}}^* \frac{\hbar^2}{m_0} \mathbf{q} \cdot \left(\frac{1}{i} \nabla + \mathbf{k} \right) u_{n\mathbf{k}} d\mathbf{r} \quad (2.99)$$

Here we have only kept the term linear in \mathbf{q} , while the q^2 -term in Eq. (2.97) is related to the effective mass (see Chap. 1). We expect that the above term is equivalent to the second term on the right side of Eq. (2.96), i.e.,

$$\sum_i \frac{\partial E_{n\mathbf{k}}}{\partial k_i} q_i = \int u_{n\mathbf{k}}^* \frac{\hbar^2}{m_0} \mathbf{q} \cdot \left(\frac{1}{i} \nabla + \mathbf{k} \right) u_{n\mathbf{k}} d\mathbf{r} \quad (2.100)$$

It is easy to see that the above equation can be re-formatted as

$$\frac{\partial E_{n\mathbf{k}}}{\partial \mathbf{k}} = \frac{\hbar^2}{m_0} \int u_{n\mathbf{k}}^* \left(\frac{1}{i} \nabla + \mathbf{k} \right) u_{n\mathbf{k}} d\mathbf{r} \quad (2.101)$$

Expressing the above equation in terms of the Bloch functions $\Psi_{n\mathbf{k}}(\mathbf{r})$, we have

$$\frac{1}{\hbar} \frac{\partial E_{n\mathbf{k}}}{\partial \mathbf{k}} = - \int \Psi_{n\mathbf{k}}^* \frac{i\hbar \nabla}{m_0} \Psi_{n\mathbf{k}} d\mathbf{r} \quad (2.102)$$

Since $-i\hbar \nabla / m_0$ is the velocity operator

$$\mathbf{v} = \frac{\mathbf{p}}{m_0} = \frac{-i\hbar \nabla}{m_0}$$

it is thus established by Eq. (2.102),

$$\mathbf{v}_{nk} = \frac{1}{\hbar} \frac{\partial E_{nk}}{\partial \mathbf{k}} \quad (2.103)$$

is the mean velocity of an electron in Bloch state $\Psi_{nk}(\mathbf{r})$. This is the first acceleration theorem about the electron in a Bloch state. It indicates that an electron in a Bloch state has a non-vanishing mean velocity, the electron moves forever without degradation of its mean velocity, in spite of the interaction of the electron with the fixed lattice of ions.

We now introduce the second acceleration theorem which states that in a steady applied electric field, \mathbf{E} , the acceleration of an electron in a periodic lattice $V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r})$ is described by

$$\hbar \dot{\mathbf{k}} = -e\mathbf{E} \quad (2.104)$$

We write the total Hamiltonian of the electron as $H = H_0 + V'(\mathbf{r})$, where

$$H_0 = \frac{\mathbf{p}^2}{2m_0} + V(\mathbf{r}), \quad V'(\mathbf{r}) = -\mathbf{F} \cdot \mathbf{r} \quad (2.105)$$

m_0 is the free electron mass, H_0 is the original Hamiltonian of the electron in the lattice for which we have the Bloch solution

$$H_0 \Psi_{nk}(\mathbf{r}) = E_{nk} \Psi_{nk}(\mathbf{r}), \quad \Psi_{nk}(\mathbf{r}) = \frac{1}{\sqrt{N}} e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk}(\mathbf{r})$$

where N is the number of unit cells. $\mathbf{F} = -e\mathbf{E}$ is the force on an electron due to the applied electric field \mathbf{E} which induces $V'(\mathbf{r})$ the extra potential energy in the above equation. Note that $\mathbf{E}(\mathbf{r}) = -\nabla U(\mathbf{r})$ so that $U(\mathbf{r}) = -\mathbf{E} \cdot \mathbf{r}$ when \mathbf{E} is constant. Here $U(\mathbf{r})$ is the electric potential. The potential energy $V'(\mathbf{r})$ of an electron in an electric potential $U(\mathbf{r})$ is $-eU(\mathbf{r})$, resulting in the expression of $V'(\mathbf{r})$ in Eqs. (2.105).

Since

$$\begin{aligned} \nabla_{\mathbf{k}} \Psi_{nk}(\mathbf{r}) &= i\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk}(\mathbf{r}) + e^{i\mathbf{k} \cdot \mathbf{r}} \nabla_{\mathbf{k}} u_{nk}(\mathbf{r}) \\ &= i\mathbf{r} \Psi_{nk}(\mathbf{r}) + e^{i\mathbf{k} \cdot \mathbf{r}} \nabla_{\mathbf{k}} [e^{-i\mathbf{k} \cdot \mathbf{r}} \Psi_{nk}(\mathbf{r})] \end{aligned} \quad (2.106)$$

Multiple the above expression by $i\mathbf{F}$,

$$i\mathbf{F} \cdot \nabla_{\mathbf{k}} \Psi_{nk}(\mathbf{r}) = -\mathbf{F} \cdot \mathbf{r} \Psi_{nk}(\mathbf{r}) + i e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{F} \cdot \nabla_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{r}} \Psi_{nk}(\mathbf{r}) \quad (2.107)$$

i.e.,

$$i\mathbf{F} \cdot \nabla_{\mathbf{k}} = -\mathbf{F} \cdot \mathbf{r} + i e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{F} \cdot \nabla_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{r}} \quad (2.108)$$

by which we rewrite the total Hamiltonian of the electron as

$$H = H_0 + H_F + i\mathbf{F} \cdot \nabla_{\mathbf{k}} \quad (2.109)$$

where

$$H_F = -i e^{i\mathbf{k}\cdot\mathbf{r}} \mathbf{F} \cdot \nabla_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \quad (2.110)$$

We first have a look at H_F by calculating the transition rate from an initial Bloch state $|n\mathbf{k}\rangle$ to another Bloch state $|m\mathbf{q}\rangle$ using the perturbation theory in Sect. 2.2. By Eq. (2.76), we first calculate the transition matrix

$$\begin{aligned} A_{mqnk} &= \langle m\mathbf{q} | H_F | n\mathbf{k} \rangle = \langle m\mathbf{q} | -i e^{i\mathbf{k}\cdot\mathbf{r}} \mathbf{F} \cdot \nabla_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} | n\mathbf{k} \rangle \\ &= -\frac{i}{N} \int e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}} u_{m\mathbf{q}}^*(\mathbf{r}) \mathbf{F} \cdot \nabla_{\mathbf{k}} u_{n\mathbf{k}}(\mathbf{r}) d\mathbf{r} \end{aligned} \quad (2.111)$$

Since $u_{n\mathbf{k}}(\mathbf{r})$ is periodic with respect to unit cells, $\nabla_{\mathbf{k}} u_{n\mathbf{k}}(\mathbf{r})$ is also periodic. The integration over \mathbf{r} in the above equation can therefore be separated into an integration over \mathbf{r} within one unit cell and a summation over all unit cells involved in the semiconductor

$$A_{mqnk} = -\frac{i}{N} \sum_{\ell} e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{R}_{\ell}} \int_{\text{cell}} u_{m\mathbf{q}}^*(\mathbf{R}_{\ell} + \mathbf{r}) \mathbf{F} \cdot \nabla_{\mathbf{k}} u_{n\mathbf{k}}(\mathbf{R}_{\ell} + \mathbf{r}) d\mathbf{r} \quad (2.112)$$

where \mathbf{R}_{ℓ} is the lattice vector of unit cell ℓ . A few further mathematical manipulations lead to

$$\begin{aligned} A_{mqnk} &= -\frac{i}{N} \sum_{\ell} e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{R}_{\ell}} \mathbf{F} \cdot \nabla_{\mathbf{k}} \left[\int_{\text{cell}} u_{m\mathbf{q}}^*(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) d\mathbf{r} \right] \\ &= -\frac{i}{N} \mathbf{F} \cdot \nabla_{\mathbf{k}} \left[\int_{\text{cell}} u_{m\mathbf{q}}^*(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) d\mathbf{r} \right] \sum_{\ell} e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{R}_{\ell}} \\ &= -i \mathbf{F} \cdot \nabla_{\mathbf{k}} \left[\int_{\text{cell}} u_{m\mathbf{q}}^*(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) d\mathbf{r} \right] \delta_{\mathbf{q},\mathbf{k}} \end{aligned} \quad (2.113)$$

In other words, H_F does not mix electron states of different \mathbf{k} . Furthermore, it is easy to see that

$$\int_{\text{cell}} u_{n\mathbf{k}}^*(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) d\mathbf{r} = 1$$

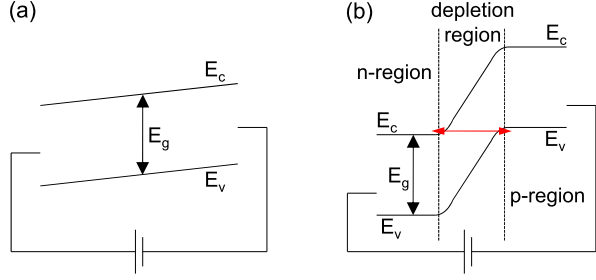
so that A_{mqnk} is nonzero only when $m \neq n$, which indicates that H_F mixes only states with the same \mathbf{k} but from different bands. In other words, H_F induces inter-band mixing.

Note that

$$\int_{\text{cell}} u_{m\mathbf{k}}^*(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) d\mathbf{r}$$

is \mathbf{k} dependent when $m \neq n$. See optical properties of semiconductor materials in late chapters.

Fig. 2.3 (a) Schematic band structure of bulk semiconductor under a weak electric field. (b) Electric-field-induced interband transitions in the depletion region of a $p-n$ junction



By Eqs. (2.76), (2.77), the transition of an electron from its initial valence band state (v) to a final conduction band state (c) induced by H_F

$$p_{ck \leftarrow vk} = \frac{|A_{ckvk}|^2}{\hbar} \frac{\Gamma_{vk}}{(E_{ck} - E_{vk} - \Delta E_{vk})^2 + \Gamma_{vk}^2} \quad (2.114)$$

$$\Gamma_{vk} \approx \pi \int |A_{ckvk}|^2 \delta(E_{ck} - E_{vk}) N_{\text{DOS}}(E_{ck}) dE_{ck}$$

Since the conduction band is separated from the valence band by the energy bandgap, $E_{ck} - E_{vk} \neq 0$, $\Gamma_{vk} \rightarrow 0$ and thus $p_{ck \leftarrow vk} = 0$.

The above conclusion is only valid for bulk semiconductor under weak electric field, see Fig. 2.3(a). Things will be totally different when the applied field is very strong. For example, the electric field can induce interband transitions in the depletion region of a pn junction, see Fig. 2.3(b).

For semiconductor bulk materials, we can therefore neglect H_F and define a set of functions $\xi_k(\mathbf{r}, t)$ as solutions to the time-dependent Schrödinger equation of our electron in electric field \mathbf{E}

$$i\hbar \frac{\partial \xi_k(\mathbf{r}, t)}{\partial t} = (H_0 + i\mathbf{F} \cdot \nabla_k) \xi_k(\mathbf{r}, t) \quad (2.115)$$

We do a perturbation analysis by assuming a solution with $\xi_k(\mathbf{r}, t)$ confined to one band, say band n , with a zero-order eigen energy E_{nk}

$$\xi_{nk}(\mathbf{r}, t) = e^{-iE_{nk}t/\hbar} \tilde{\xi}_{nk}(\mathbf{r}) \quad (2.116)$$

differentiate it with respect to t then multiply with $i\hbar$

$$i\hbar \frac{\partial \xi_{nk}(\mathbf{r}, t)}{\partial t} = \left(E_{nk} + i\hbar \frac{\partial \mathbf{k}}{\partial t} \cdot \nabla_k \right) \xi_{nk}(\mathbf{r}, t) \quad (2.117)$$

Comparing Eq. (2.115) with Eq. (2.117) we see

$$\hbar \frac{\partial \mathbf{k}}{\partial t} = \hbar \dot{\mathbf{k}} = \mathbf{F} \quad (2.118)$$

which is the second acceleration theorem. It is just what can be expected in classical mechanics for a particle of charge $-e$ and momentum $\hbar \mathbf{k}$.

We note that the above discussion is performed in the absence of magnetic fields. It is more difficult to treat rigorously the motion of a lattice electron in a magnetic field. For electrons in non-degenerate bands and not-too-strong magnetic fields the result of the detailed calculations is that the equation of motion may be generalized to

$$\mathbf{F} = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \quad (2.119)$$

where \mathbf{E} and \mathbf{B} are electric and magnetic fields.

We have discussed the energy band structure of the electrons in pure and bulk semiconductor in Chap. 1 and understand that at zero temperature (no thermal excitation. In reality, the temperature is not important in terms of thermal excitation between valence band and conduction since under almost all device function temperature, $k_B T$ is far less than the energy bandgap.) and in darkness (no optical excitation) the energy bands up to the valence band are completely filled while the energy bands from the conduction band are totally empty. An energy bandgap exists between the valence band and the conduction band. A consequence of the acceleration theorems is that semiconductor in its pure and bulk form (in darkness) is not conducting, for two major reasons. First, the interband transition induced by an electric field is negligibly small, see Eqs. (2.114) and Fig. 2.3(a). The change of the electron in the valence band from one Bloch state to another, Eq. (2.118), is actually suppressed by the Pauli exclusion principle since all Bloch states in the valence band are occupied. As discussed in Sect. 2.1, a complete occupied band does not contribute any net carrier transport current.

Metals, on the other hand, are totally different. The conduction band of a metal is partially filled. Electrons, especially those close to the Fermi level, can gain momentum from the electric field by Eq. (2.118) then transit to other unoccupied Bloch states above the Fermi level, resulting in a conducting carrier transport current.

2.5 Impurities and Fermi Level of Doped Semiconductor

By Sect. 2.4 we know that pure semiconductors have rarely been used for device applications by themselves. Semiconductors become useful when one uses the concept of doping to alter, in a controllable manner, the density of carriers that can carry current.

To increase the free carrier density, impurities known as dopants are introduced. The dopants are chosen from the periodic table so that they either have an extra electron in their outer shell compared to the host semiconductor, or have one less electron. The resulting dopant is called a donor or acceptor. The impurities of key interest in semiconductors are the point ones which create a local disturbance in the crystal structure. The effect of this crystal disturbance can be of two kinds:

1. The disturbance may create a potential profile which differs from the periodic lattice potential only over one or a few unit cells. This potential is deep and localized and the impurity is called a deep-level impurity.

2. The disturbance may create a long range potential disturbance which may extend over tens or more unit cells. Such impurities are called shallow-level impurities.

If a slice of semiconductor (take silicon for example) is placed in a furnace with a dense vapor of an impurity (e.g., boron), then it is found that the impurity atoms will tend to diffuse into the solid slice. The movement of the impurity atoms is described by Fick's law, which gives the relationship between the concentration $c(x)$, at a spatial position x , with the flux of impurities (number crossing unit area per unit time) $F(x)$ by

$$F(x) = -D \frac{\partial c(x)}{\partial x} \quad (2.120)$$

D is the diffusion coefficient which typically varies with temperature as

$$D = D_0 \exp\left(-\frac{eV_a}{k_B T}\right) \quad (2.121)$$

The significance of V_a is that it represents an energy that is required to displace a crystal atom by the impurity atom. For boron in silicon this energy appears to be close to 5 eV so that, even though $D_0 \sim 10^8 \text{ m}^2/\text{h}$, it still takes around ten hours for boron to diffuse a few micrometers into silicon at 1100 °C [3].

It is common to deposit the impurities for a short interval, then “turn off” the supply and continue the diffusion process to drive in the impurities.

By using oxide masking the process of diffusion can be carried out in selected areas. Silicon dioxide will prevent many standard impurities from diffusing into the semiconductor beneath. Thus SiO_2 masking can determine areas for diffusion. However, the diffusion proceeds in general as far laterally under the oxide as it goes down into the semiconductor.

When impurities are inserted into a layer of semiconductor by diffusion, the profile (the change of impurity density with depth) is limited to a Gaussian or error function. It is difficult to make extremely abrupt changes of concentrations. A proton-enhanced diffusion method fires energetic H^+ ions into the semiconductor which damages the crystal lattice. It is found that this damage is closely confined to a well-defined plane below the surface of the material and that the depth of this plane can be controlled by the proton energy. In silicon, one needs about 100 keV for a depth of 1 μm and proportional accelerating voltages for other depths. The damage to the lattice permits impurities already present in the material to diffuse at lower temperatures than is usual (i.e., 800 °C for Si rather than above 1000 °C). Impurities can be moved into relatively well-defined regions with negligible diffusion of the conventional type occurring. More abrupt changes of concentration can be achieved and other types of profiling may be possible. The damage done to the crystal lattice by the proton beam has to be annealed out by heating for a short time-but not too long enough to cause significant diffusion.

Ion implantation, depicted schematically in Fig. 2.4, is a technique (in a high-vacuum system) closely linked to proton-enhanced diffusion but here the impurities are fired into the semiconductor in the form of a stream of ionized atoms- an ion

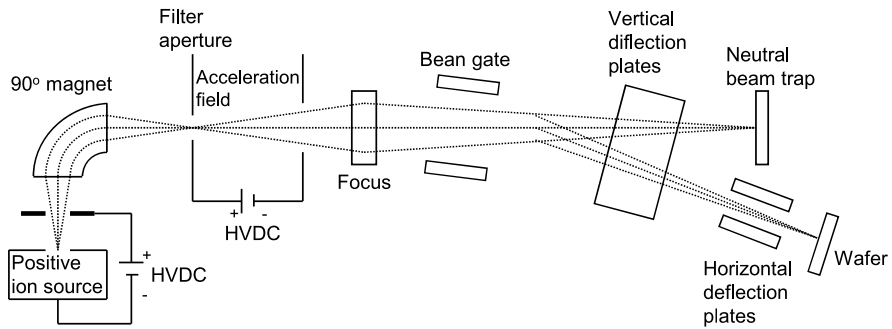


Fig. 2.4 Principle of an ion implanter

beam. This is formed by first creating a gas discharge which contains the required impurity atoms. In the discharge the atoms are stripped of their valence electrons (ionized), then drawn off from the gas discharge by suitable apertures and focusing electrodes to form an ion beam. If a gas which contains the desired impurity atoms cannot be found, one uses some inert gas in the discharge. The energetic ions in this gas can then knock out, or sputter, the required impurity atoms from some solid material which does contain them. The sputtered ions can be drawn off along with other ions. The required impurity ions are selected by passing the beam through a magnetic field which gives different curvatures in the trajectory of particles with different charge/mass ratios. The selected impurities can then pass through an aperture or slit to be focused and accelerated into the semiconductor material.

The ions, when implanted, cease to be ions and become impurity atoms but they are by no means necessarily correctly placed in substitutional sites. They usually have created considerable damage to the crystal structure on their way into the crystal. To activate the impurities in the desired substitutional sites and to reduce the damage one anneals the crystal at certain temperatures. At these temperatures, negligible diffusion of the impurity atoms occurs, but the dislocations of the atoms and the interstitial impurities can re-adjust under the action of thermal agitation. Annealing, like diffusion, may take several hours to achieve the desired result. In summary, impurities can in principle be implanted at required depth by different acceleration potentials. Special impurity profiles, especially shallow and sharp ones, can be made and are likely to find commercial use in the manufacture of specialized devices.

Associated with the impurities are new electronic states that are called impurity levels. The impurity levels can be produced in the regions of allowed bands (i.e., conduction or valence band) in which case their effects are minimal. However, the new levels could be produced in the bandgap region (the so-called bandgap levels) in which case they can greatly alter the electronic and optical properties of the semiconductors.

The wave functions of bandgap levels are no longer in the Bloch form. In general, the impurity level can be expressed in terms of the Bloch states. The deep level is highly localized so that its wave function is made up of a large number of Bloch

states. The wave function of a shallow long range impurity is extended in the real space and is made up of only a few Bloch states arising from the bandedge states.

Normally, the deep level impurities are to be avoided as much as possible in semiconductors, since an electron in such a level is “trapped” near the impurity. This trapped electron cannot participate in current flow very easily. However, in the case of indirect bandgap material, deep level impurities are often purposely introduced to increase the optical response of the material.

We are now concerned with the theory of the shallow donor and acceptor states associated with impurities in semiconductors. The ionization energies of these impurities are of the order of 40 meV in silicon, 10 meV in germanium and 6 meV in GaAs. Such energies are much less than the energy bandgap; thus it is reasonable to expect the impurity states to be formed from one-particle states of the appropriate band.

We treat a simplified model of a substitutional impurity in the semiconductor with a single spherical energy band by applying the envelope function theory, see Sect. 1.8. Let us be more specific that we substitute a Ga atom in GaAs by a Si atom. The single-particle Hamiltonian of the electron in such a system can be written as $H_0 + V'$, where H_0 is the single-particle Hamiltonian in perfect GaAs, and the modification V' of the lattice potential due to the substitution is

$$V'(\mathbf{r}) = \frac{Z_{\text{Si}}}{4\pi\epsilon_0|\mathbf{r} - \mathbf{R}_\ell|} - \frac{Z_{\text{Ga}}}{4\pi\epsilon_0|\mathbf{r} - \mathbf{R}_\ell|} = \frac{1}{4\pi\epsilon_0|\mathbf{r} - \mathbf{R}_\ell|} \quad (2.122)$$

where $Z_{\text{Si}} = 4$ and $Z_{\text{Ga}} = 3$ are the numbers of valence electrons in Si and Ga atoms, respectively. Here we assume that the substitutional Si atom locates at unit cell \mathbf{R}_ℓ . The above equation is written down when neglecting other valence electrons in the system. The correction to the above expression due to the valence electrons is normally approached by introducing a relative dielectric constant ϵ_r so that

$$V'(\mathbf{r}) = \frac{1}{4\pi\epsilon_0\epsilon_r|\mathbf{r} - \mathbf{R}_\ell|} \quad (2.123)$$

By Eqs. (1.139) and (1.144),

$$V'_{n'nji} = \left\langle a_{n'}(\mathbf{r} - \mathbf{R}_j) \left| \frac{1}{4\pi\epsilon_0\epsilon_r|\mathbf{r} - \mathbf{R}_\ell|} \right| a_n(\mathbf{r} - \mathbf{R}_i) \right\rangle \quad (2.124)$$

Since V' is most prominent in the proximity of $\mathbf{r} = \mathbf{R}_\ell$ while the Wannier function $a_n(\mathbf{r} - \mathbf{R}_i)$ is localized at unit cell \mathbf{R}_i , $V'_{n'nji}$ is significant only when $\mathbf{R}_j = \mathbf{R}_i = \mathbf{R}_\ell$. Furthermore, the integration of the Wannier functions at the same unit cell is nonzero when the Wannier functions are from the same energy band. Finally,

$$V'_{n'nji} \approx \frac{1}{4\pi\epsilon_0\epsilon_r|\mathbf{r} - \mathbf{R}_\ell|} \delta_{n'n} \delta_{ji,\ell} \quad (2.125)$$

Thus, by Eq. (1.152), we have the Schrödinger equation for the envelope function

$$[E_n(-i\nabla) - E]\psi_n(\mathbf{r}) + \frac{1}{4\pi\epsilon_0\epsilon_r|\mathbf{r}|}\psi_n(\mathbf{r}) = 0 \quad (2.126)$$

Consider a spherical conduction band

$$E_{ck} = E_c + \frac{\hbar^2 k^2}{2m^*}, \quad E_c(-i\nabla) = E_c - \frac{\hbar^2 \nabla^2}{2m^*} \quad (2.127)$$

Equation (2.126) becomes

$$\left(-\frac{\hbar^2 \nabla^2}{2m^*} - \frac{e^2}{4\pi\epsilon_0\epsilon_r r} \right) \psi(\mathbf{r}) = (E - E_c) \psi(\mathbf{r}) \quad (2.128)$$

This is just a hydrogen-like Schrödinger equation (1.8), and a series of energy levels are produced,

$$E = E_c - E_b^n = E_c - \frac{13.6}{n^2\epsilon_r^2} \frac{m^*}{m_0} \text{ eV} \quad (2.129)$$

where $n = 1, 2, \dots$. For silicon with ellipsoidal energy surface, the effective mass in the above equation is to be replaced by

$$\frac{3}{m^*} = \frac{2}{m_t^*} + \frac{1}{m_\ell^*} \quad (2.130)$$

where m_ℓ and m_t are longitudinal and transverse effective masses.

According to this simple picture of the donor impurity, the donor energy levels depend only upon the host crystal and not on the nature of the dopant. This is actually due to the fact that Eqs. (2.125), (2.126) are derived under the condition that V' does not vary much within one unit cell. This is only true for shallow impurities. More accurate theories for the donor levels must include the short-range correction within one unit cell related to the dopant impurity atom for a better agreement with the experiments.

Table 2.1 lists E_b^1 of shallow impurities (donors and acceptors) in common semiconductors. E_b^1 ($n = 1$) is normally referred to as the ionization or binding energy of the impurity. Here we observe that the impurity states are hydrogen-like, and loosely bound, largely because the dielectric constant of the semiconductor is high (about 10 for commonly used semiconductors). The small effective mass of carriers in the semiconductor further reduces the binding energy.

We now discuss the distribution of the extra electrons (missing electrons or holes) from donor (acceptor) impurities. As usual, the following assumptions are made:

1. Electrons *in one state* cannot be distinguished from one another.
2. Each state can be occupied by not more than two electrons with opposite spin, i.e., the Pauli exclusion principle.
3. Each impurity state can be occupied by just one electron. Here we only consider the donor impurities. Similar analysis can be made for the acceptor impurities.

Consider that we have n_j electrons in a state e_j whose density of states is g_j ($j = 1, 2, \dots$), the total number of distinguishable distributions W of these electrons

Table 2.1 Shallow impurity energy levels E_b^1 [meV] in semiconductors

Material	Donor	E_b^1	Acceptor	E_b^1
GaAs	Si	5.8	C	26
	Ge	6.0	Be	28
	S	6.0	Mg	28
	Sn	6.0	Si	35
Si	Li	33	B	45
	Sb	39	Al	67
	P	45	Ga	72
	As	54	In	160
Ge	Li	9.3	B	10
	Sb	9.6	Al	10
	P	12.0	Ga	11
	As	13.0	In	11

is

$$W = \prod_j \frac{g_j}{n_j!(g_j - n_j)!} \quad (2.131)$$

Now consider that the system contains N_D donors, whose energy state is e_D , of which N_{DX} are occupied by one electron each. It is reminded here that a donor can be occupied by only one electron. For these donors, we must know if they are correlated or not in order to calculate the number of distinguishable distributions. There are three different situations concerning the impurity correlation:

1. The density of impurities in the system is so low that the electron wave functions of the impurity state e_D are well localized around the donors and the overlappings of the wave functions at different donor sites are negligible.
2. The density of impurities is increased so that wave functions of e_D at different donor sites overlap with each other, forming impurity band.
3. The impurity band is widened due to the increase of the impurity concentration and eventually it merges with the conduction band (Mott transition).

Statistically however, the last two situations are equivalent. In other words, we only need to know whether or not the wave functions of the impurity electrons are localized. If the wave functions are localized, we can distinguish the electron at donor site i from the one at j , even their state energies are the same. But if the wave functions become delocalized, there is then no way to distinguish the electron at donor i from the one at j because the electrons are identical and they are in the same energy state.

First, let us assume that the electron wave functions of the N_D impurities in the system overlap with each other. Among N_D impurities, N_{DX} of them are neutral (they are occupied by electrons). The corresponding number of distinguishable

states, W_e , is

$$W_e = g_D^{N_{DX}} \frac{N_D!}{N_{DX}!(N_D - N_{DX})!} \quad (2.132)$$

Here we add a subscript index e to the number of states indicating that the corresponding impurity electron wave functions are “extended”.

The total number of distinguishable distributions of the system is given by

$$W_t = W_i W_e \quad (2.133)$$

By adopting the method of Lagrange undetermined multipliers and introducing the donor state, e_D , the sum

$$\Sigma = \ln W_t + \alpha \left(n - N_{DX} - \sum_j n_j \right) + \beta \left(U - N_{DX} e_D - \sum_j n_j e_j \right) \quad (2.134)$$

has the following restrains to fulfill

$$0 = \frac{d\Sigma}{dN_{DX}} = \frac{d\Sigma}{dn_j} \quad (2.135)$$

where n is the total number of electrons and U the total energy of the system, $j = 1, 2, \dots$.

It is easy to derive that

$$\alpha = -\frac{E_f}{k_B T}, \quad \beta = \frac{1}{k_B T} \quad (2.136)$$

where E_f is the Fermi level. From the restrains of Eq. (2.135) the Fermi distribution function for the band electrons is obtained:

$$n_j = \frac{g_j}{\exp\left(\frac{e_j - E_f}{k_B T}\right) + 1} \quad (2.137)$$

It must be emphasized that the differentiation, $d(\ln N!)/dN$, which appears in Eq. (2.135), is approximated as

$$\frac{d(\ln N!)}{dN} \approx \ln N \quad (2.138)$$

in order to obtain Eq. (2.137). And Eq. (2.138) is valid only when N is a very large number where statistical analysis is meaningful.

It is usually always valid by saying that N_D and N_{DX} are large number so that Eq. (2.138) remains true, it should be however very cautious to use Eq. (2.137), because these results depend very much on another condition: that the wave functions of those electrons to neutralize impurities (impurity electrons) overlap with each other.

If the wave functions of the impurity electrons are localized and do not overlap with each other, and if there are n_m electrons at impurity site m , $m = 1, 2, \dots, N_D$, the numbers of states of the neutral impurities and of the whole system become

$$W_\ell = \prod_m g_D^{n_m}, \quad W_t = W_i W_\ell \quad (2.139)$$

where the subscript index ℓ indicating “localized”. For each impurity, n_m can be either 0 or 1, as mentioned earlier. Σ , which is defined in Eq. (2.134), now becomes

$$\Sigma = \ln W_t + \alpha \left(n - \sum_m n_m - \sum_j n_j \right) + \beta \left(U - \sum_m n_m e_D - \sum_j n_j e_j \right) \quad (2.140)$$

Since n_j are still large numbers, Eq. (2.140) still has the following restrains to fulfill

$$0 = \frac{d\Sigma}{dn_j} \quad (2.141)$$

so that Eq. (2.137) is obtained again. However, for n_m we can only calculate the change of Σ following the change in n_m from 0 to 1 and from 1 to 0:

$$\Delta \Sigma_{0 \rightarrow 1} = -\frac{E_f - e_D}{k_B T}, \quad \Delta \Sigma_{1 \rightarrow 0} = \frac{E_f - e_D}{k_B T} \quad (2.142)$$

Here the statistics tells us that if E_f is higher than e_D , it is better to occupy the impurity state, from $n_m = 0$ to $n_m = 1$, while for E_f lower than e_D , it is better to empty the impurity state, from $n_m = 1$ to $n_m = 0$ in order to minimize Σ .

We thus see that if the wave functions of the impurity electrons are localized and well separated from each other spatially, the Fermi level of the system is completely determined by the band electrons n_j , Eq. (2.137). The occupation of the impurity states depends then on the relative positions of the Fermi level E_f and the impurity state energy e_D . For shallow impurities, we can determine the critical impurity concentration, N_D^c where the wave functions of the impurity electrons begin to overlap with each other. By the hydrogen-like model, the effective Bohr radius of the shallow impurity state is

$$a = \frac{\epsilon_r}{m^*/m_0} a_0 \quad (2.143)$$

where $a_0 = 0.529 \text{ \AA}$ is the Bohr radius. On the other hand, the averaged distance between two adjacent impurity atoms is

$$a_D = \frac{1}{N_D^{1/3}} \quad (2.144)$$

For n -type GaAs, $\epsilon_r = 13.1$ and $m^* = 0.067m_0$, so that $a = 10.34 \text{ nm}$. It is easy to obtain the critical impurity concentration, $N_D^c = 9.05 \times 10^{17} \text{ cm}^{-3}$ when $a = a_D$.

For n -type Si, $\epsilon_r = 11.9$, $m^* = 0.43m_0$, so that $a = 1.46$ nm and $N_D^c = 3.28 \times 10^{20} \text{ cm}^{-3}$.

The treatment in the above consideration is of course over simplified. For example, the hydrogen-like model may not apply to the n -type Si because the resulting impurity Bohr radius is comparable with its lattice constant (0.543 nm).

2.6 Boltzmann Equation

Carrier transport can be characterized in terms of either classical or quantum physics, while for most cases, the generalized classical approach described by the Boltzmann transport equation is adequate enough.

In the formalism of the Boltzmann transport equations, the electron system is described by the distribution function $f_n(\mathbf{r}, \mathbf{k}, t)$, which gives the occupation probability of a state characterized by a band index n , the \mathbf{k} vector and the space vector \mathbf{r} . To calculate the distribution function $f_n(\mathbf{r}, \mathbf{k}, t)$ in given external fields, we examine its temporal behavior. We consider a group of electrons in the volume element $d\mathbf{r}d\mathbf{k}$ in the phase space. The total differential-quotient is caused by the scattering of electrons from one state to the other and vice versa,

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \dot{\mathbf{k}} \cdot \nabla_{\mathbf{k}} f + \dot{\mathbf{r}} \cdot \nabla_{\mathbf{r}} f = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} \quad (2.145)$$

In the steady state the local differential quotient is zero and we are left with the usual form of the Boltzmann transport equation for the electron system which allows the distribution function to be calculated for given external fields and known scattering mechanisms:

$$\dot{\mathbf{k}} \cdot \nabla_{\mathbf{k}} f + \dot{\mathbf{r}} \cdot \nabla_{\mathbf{r}} f = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} \quad (2.146)$$

On the left side of Eq. (2.146),

$$\dot{\mathbf{k}} = -\frac{e\mathbf{E}}{\hbar} \quad (2.147)$$

is the external force by the acceleration theorem, here we only consider the transport under the influence of an electric field \mathbf{E} . And

$$\dot{\mathbf{r}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} E_{n\mathbf{k}} \quad (2.148)$$

is the group velocity of the Bloch electron, where $E_{n\mathbf{k}}$ is the energy dispersion of the system under consideration.

If the scattering is induced by a quasi-particle, e.g., the phonon state, it is generally assumed that the quasi-particle system sets up an equilibrium state so quickly that we can ignore disturbances in the quasi-particle system. In this approximation

the form of the collision term on the right of Eq. (2.146) can be written in the simpler form

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int \frac{2d\mathbf{q}}{(2\pi)^3} \{P_{\mathbf{q},\mathbf{k}}[1 - f(\mathbf{k})]f(\mathbf{q}) - P_{\mathbf{k},\mathbf{q}}[1 - f(\mathbf{q})]f(\mathbf{k})\} \quad (2.149)$$

where $P_{\mathbf{k},\mathbf{q}}$ is the probability of scattering from state \mathbf{k} to \mathbf{q} , see Eq. (2.88), and we have applied the Pauli exclusion principle.

Furthermore, physically collisions cannot change f_0 which implies that

$$\int \frac{2d\mathbf{q}}{(2\pi)^3} \{P_{\mathbf{q},\mathbf{k}}[1 - f_0(\mathbf{k})]f_0(\mathbf{q}) - P_{\mathbf{k},\mathbf{q}}[1 - f_0(\mathbf{q})]f_0(\mathbf{k})\} = 0 \quad (2.150)$$

It follows that

$$P_{\mathbf{q},\mathbf{k}}[1 - f_0(\mathbf{k})]f_0(\mathbf{q}) = P_{\mathbf{k},\mathbf{q}}[1 - f_0(\mathbf{q})]f_0(\mathbf{k}) \quad (2.151)$$

i.e.,

$$P_{\mathbf{q},\mathbf{k}}e^{-E_{\mathbf{k}}/k_B T} = P_{\mathbf{k},\mathbf{q}}e^{-E_{\mathbf{q}}/k_B T} \quad (2.152)$$

For elastic scattering processes, e.g., alloy and impurity scatterings, so is the acoustic phonon scattering because of the negligible acoustic phonon energy, the electron does not lose or gain energy,

$$P_{\mathbf{k},\mathbf{q}} = P_{\mathbf{q},\mathbf{k}} \quad (2.153)$$

Therefore Eq. (2.149) becomes much simplified:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int \frac{2d\mathbf{q}}{(2\pi)^3} P_{\mathbf{q},\mathbf{k}}[f(\mathbf{q}) - f(\mathbf{k})] \quad (2.154)$$

Equation (2.154) looks quite odd at the first sight. At equilibrium, the principle of detailed balance says

$$P_{\mathbf{q},\mathbf{k}}[f_0(\mathbf{q}) - f_0(\mathbf{k})] = 0 \quad (2.155)$$

which means that $f_0(\mathbf{q}) = f_0(\mathbf{k})$ if $P_{\mathbf{k},\mathbf{q}} \neq 0$. However, we know that there is a factor of $\delta[E_{\mathbf{k}} - E_{\mathbf{q}}]$ in $P_{\mathbf{k},\mathbf{q}}$ (energy conservation) and $f_0(\mathbf{k}) = f_0(E_{\mathbf{k}})$. Therefore, Eq. (2.155) and thus Eq. (2.154) are perfectly alright.

For the optical phonon scattering, $P_{\mathbf{k},\mathbf{q}}$ and $P_{\mathbf{q},\mathbf{k}}$ are two different processes, one is the phonon-absorption while the other emits a phonon:

$$P_{\mathbf{k},\mathbf{q}} = A N_{\text{op}} \delta(E_{\mathbf{k}} - E_{\mathbf{q}} - \hbar\omega_0)$$

for emitting a phonon when transiting from state \mathbf{k} to \mathbf{q} , where A is a constant, N_{op} is the phonon density of states, $\hbar\omega_0$ is the phonon energy, and

$$P_{\mathbf{q},\mathbf{k}} = A(N_{\text{op}} + 1)\delta(E_{\mathbf{q}} - E_{\mathbf{k}} + \hbar\omega_0)$$

to absorb a phonon from state \mathbf{q} to \mathbf{k} .

Denoting s as the phonon wave vector and $P_- = AN_{\text{op}}$ and $P_+ = A(N_{\text{op}} + 1)$, Eq. (2.149) in full detail is now given by

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int \frac{2ds}{(2\pi)^3} \{ P_- [1 - f(\mathbf{k} - s)] f(\mathbf{k}) + P_+ [1 - f(\mathbf{k} + s)] f(\mathbf{k}) - P_- [1 - f(\mathbf{k})] f(\mathbf{k} + s) - P_+ [1 - f(\mathbf{k})] f(\mathbf{k} - s) \} \quad (2.156)$$

Therefore Eqs. (2.154)–(2.155) are derived again if we treat P_- and P_+ as two different scattering processes and Eq. (2.154) remains valid. Other inelastic processes can be treated similarly.

By Eq. (2.154) we then see that if there are several principal scattering mechanisms which are independent from each other, we can write

$$P_{\mathbf{k},\mathbf{q}} = \sum_i P_{i,\mathbf{k},\mathbf{q}} \quad (2.157)$$

If we are only interested in the linear response to the external force, the collision integral Eq. (2.149) can be approached by the relaxation-time approximation

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{f - f_0}{\tau} \quad (2.158)$$

where τ is the relaxation time and f_0 is the distribution function at equilibrium. It is easy to see that if Eq. (2.157) holds true, we obtain the well-known Mathiessen rule:

$$\frac{1}{\tau} = \sum_i \frac{1}{\tau_i} \quad (2.159)$$

where τ_i is the relaxation time corresponding to scattering process $P_{i,\mathbf{k},\mathbf{q}}$.

For weak external fields, the distribution function can be approximated by

$$f(\mathbf{k}) \approx f_0(\mathbf{k}) + f_1(\mathbf{k}) \quad (2.160)$$

where $f_0(\mathbf{k}) \gg f_1(\mathbf{k})$. By substituting the above equation into Eq. (2.154) together with Eq. (2.158) we obtain the relaxation-time expression:

$$-\frac{f(\mathbf{k}) - f_0(\mathbf{k})}{\tau} = \int P_{\mathbf{q},\mathbf{k}} [f_1(\mathbf{q}) - f_1(\mathbf{k})] \frac{2d\mathbf{q}}{(2\pi)^3} \quad (2.161)$$

As a first-order approximation we can neglect $f_1(\mathbf{q})$ in the right side of the above equation to obtain the usual relaxation-time expression:

$$\frac{1}{\tau(\mathbf{k})} = \int P_{\mathbf{q},\mathbf{k}} \frac{2d\mathbf{q}}{(2\pi)^3} \quad (2.162)$$

Equation (2.162) is the usual definition of the total scattering rate.

2.7 Drift, Diffusion and Ballistic Transport

At a phenomenological level, electron transport is described by

$$j_i(\mathbf{r}) = -e \left[n(\mathbf{r}) v_{d,i} - \sum_j D_{ij} \frac{\partial n(\mathbf{r})}{\partial x_j} \right] \quad (2.163)$$

where $i, j = x, y, z$, $n(\mathbf{r})$ and \mathbf{j} are carrier density and current density, respectively, D_{ij} is the diffusion coefficient tensor. v_d is the drift velocity induced by an electric field.

For an dc electric field \mathbf{E} ,

$$\nabla_{\mathbf{r}} f = 0, \quad \frac{\partial f}{\partial t} = 0 \quad (2.164)$$

the Boltzmann transport equation becomes

$$-\frac{e\mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f_0 = -\frac{f - f_0}{\tau} \quad (2.165)$$

together Eq. (1.40), we obtain

$$f = f_0 + \frac{e\mathbf{E} \cdot \nabla_{\mathbf{k}} f_0}{\hbar} \tau \quad (2.166)$$

The drift velocity is given as

$$\mathbf{v}_d \equiv \frac{1}{n} \int \mathbf{v}_{\mathbf{k}} f \frac{2d\mathbf{k}}{(2\pi)^3} = \frac{1}{n} \int \mathbf{v}_{\mathbf{k}} \frac{e\mathbf{E} \cdot \nabla_{\mathbf{k}} f_0}{\hbar} \tau \frac{2d\mathbf{k}}{(2\pi)^3} \quad (2.167)$$

where

$$\int \mathbf{v}_{\mathbf{k}} f_0 \frac{2d\mathbf{k}}{(2\pi)^3} = 0$$

since the group velocity of the system is zero at equilibrium. And

$$n = \int f_0 \frac{2d\mathbf{k}}{(2\pi)^3}$$

is the carrier concentration.

We can also formulate the drift velocity into the concept of carrier mobility such

$$\mathbf{v}_{d,i} = \sum_j \mu_{ij} E_j \quad (2.168)$$

where $\mathbf{E} = (E_x, E_y, E_z)$ is the electric field.

$$\mathbf{v}_d = \frac{1}{n} \int \mathbf{v}_{nk} \frac{e \mathbf{E} \cdot \nabla_{\mathbf{k}} E_{nk}}{\hbar} \frac{\partial f_0}{\partial E_{nk}} \tau \frac{2d\mathbf{k}}{(2\pi)^3} = \frac{1}{n} \int \mathbf{v}_{nk} e \mathbf{E} \cdot \mathbf{v}_{nk} \frac{\partial f_0}{\partial E_{nk}} \tau \frac{2d\mathbf{k}}{(2\pi)^3} \quad (2.169)$$

see Eq. (1.40) about the expression of the group velocity \mathbf{v}_{nk} of Bloch state $n\mathbf{k}$. More explicitly,

$$v_{d,x} = \frac{e}{n} \int (v_{nk,x}^2 E_x + v_{nk,x} v_{nk,y} E_y + v_{nk,x} v_{nk,z} E_z) \frac{\partial f_0}{\partial E_{nk}} \tau \frac{2d\mathbf{k}}{(2\pi)^3} \quad (2.170)$$

Similar expressions can be written down for $v_{d,y}$ and $v_{d,z}$.

For common semiconductors, the integration over $v_{nk,i} v_{nk,j}$ is zero when $i \neq j$ (symmetry consideration). Thus,

$$v_{d,i} = \frac{e E_i}{n} \int v_{nk,i}^2 \frac{\partial f_0}{\partial E_{nk}} \tau \frac{2d\mathbf{k}}{(2\pi)^3} \quad (2.171)$$

Comparing with Eq. (2.168), we obtain the expression for calculating the mobility

$$\mu_i = \frac{e}{n} \int v_{nk,i}^2 \frac{\partial f_0}{\partial E_{nk}} \tau \frac{2d\mathbf{k}}{(2\pi)^3} \quad (2.172)$$

For weak electric-fields, D and μ are electric field independent and verify the Einstein relation

$$D = \frac{\mu k_B T}{e} \quad (2.173)$$

At high electric fields, the Einstein relation fails and the diffusion coefficient becomes $D_{ij}(E)$.

Let us consider a material having a geometry of length L and a cross-section $w \times w$, see Fig. 2.5(a). When L and w are far larger than the mean free path ℓ , it is known by the Ohm's law that the resistance of such a material is

$$R = \frac{L}{w^2} \rho \quad (2.174)$$

where ρ is the resistivity. The electron transport is characterized as drift-diffusion. Denote n as the density of the electrons in the electron system, the current density j and the conductivity σ are

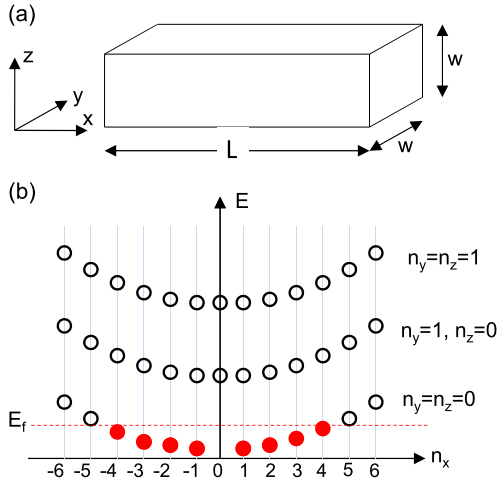
$$j = -nev_{\text{average}} = \frac{ne^2\tau}{m^*} E, \quad \sigma = \frac{ne^2\tau}{m^*} \quad (2.175)$$

from which we can easily obtain the relationship between ρ and σ .

Now we reduce the dimension of the material so that both L and w become much smaller than ℓ . In this case, the electron will not experience any scattering and its transport is just a free flight. The situation is known as ballistic transport. Assume

Fig. 2.5 Electron transport.

(a) Geometric structure.

(b) Energy band diagram, where E_f denotes the Fermi level below which the states (solid dots) are occupied and above it the states (hollow) are empty

$L \gg w$ and the external electric field applies along the x axis. Consider the electron states within the material

$$k_x = \frac{n_x \pi}{L}, \quad k_y = \frac{n_y \pi}{w}, \quad k_z = \frac{n_z \pi}{w} \quad (2.176)$$

where n_x , n_y and n_z are integers. And the energy of the state is

$$E = \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2 \pi^2}{2m^*} \left(\frac{n_x^2}{L^2} + \frac{n_y^2}{w^2} + \frac{n_z^2}{w^2} \right) \quad (2.177)$$

which is plotted schematically in Fig. 2.5(b). Fill the system with electrons up to the Fermi level E_f . For simplicity we consider only the single band of $n_y = n_z = 0$. The time that an electron with charge $-e$ across length L at a speed of v is L/v , resulting in a current of

$$\frac{e}{L/v} = \frac{ev}{L} \quad (2.178)$$

The total current of all electrons is

$$I_{\text{left} \rightarrow \text{right}} = \sum_{\text{occupied } n_x > 0} \frac{2ev}{L} = \frac{2e}{L} \sum_{\text{occupied } n_x > 0} \frac{\hbar k_x}{m^*} = \frac{2\pi e \hbar}{m^* L^2} \sum_{\text{occupied } n_x > 0} n_x \quad (2.179)$$

In the above equation, a factor of “2” is introduced to account for the spin degeneracy.

Since L is relatively large so that we can convert the sum into integration by inserting $\delta n_x = dn_x = 1$

$$I_{\text{left} \rightarrow \text{right}} = \frac{2\pi e \hbar}{m^* L^2} \int_{\text{occupied}} n_x dn_x \quad (2.180)$$

Because of Eq. (2.177),

$$n_x dn_x = \frac{m^*}{\hbar^2 (\pi/L)^2} dE \quad (2.181)$$

so that

$$I_{\text{left} \rightarrow \text{right}} = \frac{2e}{h} \int_{\text{occupied}} dE \quad (2.182)$$

where $h = 2\pi\hbar$.

The current from the right to the left can be similarly obtained. To induce a net nonzero current along the x direction, an external bias V is applied, which causes a potential energy change eV . Assume that the left end is grounded and the right end is biased V , the potential energy at the right end becomes $-eV$, and the net current

$$I_{\text{total}} = \frac{2e}{h} \left(\int dE_{\text{left} \rightarrow \text{right}} - \int dE_{\text{right} \rightarrow \text{left}} \right) = \frac{2e}{h} [E_f - (E_f - eV)] = \frac{2e^2}{h} V \quad (2.183)$$

where E_f is the Fermi level. The resistance of the ballistic transport is

$$R_{\text{ballistic}} = \frac{h}{2e^2} = 12.5 \text{ k}\Omega \quad (2.184)$$

which is a constant.

2.8 Carrier Scatterings

Finally we discuss three type of scattering mechanisms in the rest of this chapter, namely, the phonon scattering where the electron interacts with the lattice; two electrons interact with each other; and, an electron is scattered by an external force, e.g., a photon, or an impurity.

2.8.1 Phonon Scattering

When an ion in a compound semiconductor lattice structure, or an atom in an elemental semiconductor, is displaced by an amount of \mathbf{Q} from its lattice position \mathbf{R} ,

$$\mathbf{Q} = \sum_{\mathbf{q}} \sqrt{\frac{\hbar}{2\rho V \omega_{\mathbf{q}}}} (a_{\mathbf{q}} + a_{-\mathbf{q}}^{\dagger}) e^{i\mathbf{q} \cdot \mathbf{r}} \boldsymbol{\Xi} \quad (2.185)$$

a deformation potential is induced

$$H' = \epsilon \frac{\partial \mathbf{Q}}{\partial \mathbf{r}} = \sum_{\ell j, \mathbf{q}} \sqrt{\frac{\hbar}{2\rho V \omega_{\mathbf{q}}}} (a_{\mathbf{q}} + a_{-\mathbf{q}}^{\dagger}) e^{i\mathbf{q} \cdot \mathbf{r}} \epsilon_{\ell j} q_{\ell} \boldsymbol{\Xi}_j \quad (2.186)$$

where ρ is the material density, ω_q is the frequency of the ion displacement and \mathbf{q} is the wave vector, $\boldsymbol{\Xi}$ is the polarization of the ion displacement, ϵ is a tensor describing the shift of the electron band per unit deformation. a_q^+ is the creation operator of such a collective lattice displacement, which is called the phonon. a_q is the corresponding annihilation operator.

We consider a state which consists of one electron and the phonon background in the form of

$$\psi(\mathbf{k})\Phi(N_q)$$

where $\psi(\mathbf{k})$ is the electron Bloch function and $\Phi(N_q)$ is the phonon state of \mathbf{q} , N_q is the phonon density.

To calculate the transition probability from electron state \mathbf{k} to state \mathbf{k}' , we need to perform the integration

$$\frac{1}{N} u_{\mathbf{k}'}^* u_{\mathbf{k}} e^{i(\mathbf{k}-\mathbf{k}'\pm\mathbf{q})\cdot\mathbf{r}}$$

over the space, where N is the number of the unit cells. The integration can be divided into a sum over the lattice vector \mathbf{R} and an integration in the unit cell because $u_{\mathbf{k}}$ is translationally symmetric:

$$\sum_{\mathbf{R}} \frac{1}{N} e^{i(\mathbf{k}-\mathbf{k}'\pm\mathbf{q})\cdot\mathbf{R}} = \begin{cases} 1 & \text{if } \mathbf{k} - \mathbf{k}' \pm \mathbf{q} = \mathbf{G} \\ 0 & \text{otherwise} \end{cases} \quad (2.187)$$

$$p(\mathbf{k}, \mathbf{k}') = \int_{\text{cell}} u_{\mathbf{k}'}^* u_{\mathbf{k}} d\mathbf{r}$$

where \mathbf{G} is the reciprocal lattice. The terms corresponding to $\mathbf{G} = 0$ are called “normal” (“N”) terms, others are the “umklapp” (“U”) terms. $p(\mathbf{k}, \mathbf{k}')$ is the so-called overlap integral.

Since

$$a_q \Phi(N_q) = N_q \Phi(N_q - 1), \quad a_q^+ \Phi(N_q) = (N_q + 1) \Phi(N_q + 1) \quad (2.188)$$

which correspond to the emission and absorption of a phonon, the transition probability per unit time of one electron from \mathbf{k} to state \mathbf{k}' is

$$P_{\mathbf{k}, \mathbf{k}'} = \frac{\pi p^2(\mathbf{k}, \mathbf{k}')}{\rho V \omega_q} \left(\frac{N_q + 1}{N_q} \right) |\epsilon_{lj} q_l \Xi_j|^2 \frac{\gamma}{[\Omega \pm \omega_q]^2 + \gamma^2/4} \quad (2.189)$$

Here $\hbar\Omega = E(\mathbf{k}') - E(\mathbf{k})$. The upper and lower symbols refer to the phonon emission and absorption, respectively.

Let us discuss the multiple quantum well system grown along the z -direction. The system is based on a semiconductor material with lattice constant a . The thickness of the quantum well is ma , where m is the monolayer number of the well. The period of the system is Na . It is easy to see then $(N - m)a$ is the barrier thickness. Here we concentrate on a lattice-matched heterostructure. The electron-phonon interaction is

a very complicated quantity, which depends strongly on the electron energy as well as sample structure [4, 5]. Generally speaking, in a system whose lattice structure is defined as \mathbf{R}_j , the electron-phonon interaction Hamiltonian, H' , can be written as

$$H' = \sum_j \mathbf{Q}_j \cdot \nabla V(\mathbf{r} - \mathbf{R}_j) \quad (2.190)$$

where \mathbf{Q}_j is the displacement of the atom placed at lattice site \mathbf{R}_j , \mathbf{r} is the electron position, and V is the lattice potential. Let us consider the following phonon mode whose wave vector is \mathbf{q} . The imaginary part of \mathbf{q}

$$\text{Im}(\mathbf{q}) = \begin{cases} k_1 \mathbf{z}_0 & \text{when } z > 0 \\ -k_1 \mathbf{z}_0 & \text{otherwise} \end{cases} \quad (2.191)$$

where \mathbf{z}_0 is the unit vector in the z direction. Such a phonon mode is localized along the z direction but is extended in the xy plane. Using the periodic boundary condition in the region of $(-Na/2, Na/2)$, where N is the number of the lattice sites in one period (we assume that Na is considerably larger than the well width ma so that the boundary conditions do not affect the phonon in the well), the lattice displacement can be expressed by

$$\mathbf{Q}_j = A \sqrt{\frac{N(1 - e^{-k_1 a})}{2 - 2e^{-Nk_1 a/2}}} e^{i\mathbf{q} \cdot \mathbf{R}_j} \quad (2.192)$$

where A is a constant containing factors like the phonon polarization and normalization in the xy plane.

$$\sqrt{\frac{N(1 - e^{-k_1 a})}{2 - 2e^{-Nk_1 a/2}}}$$

is the normalization factor in the z direction. It is easy to see that

$$\sqrt{\frac{N(1 - e^{-k_1 a})}{2 - 2e^{-Nk_1 a/2}}} = 1 \quad (2.193)$$

when $k_1 = 0$, and Eq. (2.192) becomes the normal expression for the extended phonon.

The initial and final electronic states are expressed similarly

$$\psi_i = u \sqrt{\frac{ak_2}{1 - e^{-Nk_2 a}}} e^{i\mathbf{k}_i \cdot \mathbf{r}}, \quad \psi_f = u \sqrt{\frac{ak_3}{1 - e^{-Nk_3 a}}} e^{i\mathbf{k}_f \cdot \mathbf{r}} \quad (2.194)$$

where u is the Bloch function which is unit-cell periodic, and \mathbf{k}_i and \mathbf{k}_f are wave vectors of the initial and final electronic states,

$$\text{Im}(\mathbf{k}_i) = k_2 \mathbf{z}_0, \quad \text{Im}(\mathbf{k}_f) = k_3 \mathbf{z}_0$$

when $z > 0$; and for $z < 0$,

$$\text{Im}(\mathbf{k}_i) = -k_2 z_0, \quad \text{Im}(\mathbf{k}_f) = -k_3 z_0$$

The difference between the normalization factors in Eqs. (2.192), (2.194) is due to the fact that the lattice vector \mathbf{R}_i is discrete while the electronic coordinate \mathbf{r} is continuous. The transition probability between states is

$$P = \langle \psi_i | H' | \psi_f \rangle = \sqrt{\frac{Na^2 k_2 k_3 (1 - e^{-2k_1 a})}{8(1 - e^{-Nk_1 a/2})(1 - e^{-Nk_2 a})(1 - e^{-Nk_3 a})}} \times \sum_j e^{i\mathbf{q} \cdot \mathbf{R}_j} \int_{\text{cell},j} e^{j(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{r}} |u|^2 \mathbf{A} \cdot \nabla V(\mathbf{r} - \mathbf{R}_j) d\mathbf{r} \quad (2.195)$$

For most applications, the doping levels in the electrodes of normal GaAs/AlGaAs systems are about $5 \times 10^{17} \text{ cm}^{-3}$, the corresponding Fermi level is about 25 meV. The doping level in the quantum well, e.g., in a double barrier resonant tunneling diode, is kept as low as possible so that the tunneling or other quantum processes will not be interfered by impurity scattering. The wave length at the Fermi level ($5 \times 10^{17} \text{ cm}^{-3}$ doping) is considerably large ($> 500 \text{ \AA}$) in a GaAs/AlGaAs system) compared with the lattice constant, e.g., 2.87 \AA for an (001) GaAs. For those electronic states whose energies are lower than the Fermi level (these are the states of interest because of the Fermi distribution factor), the wave lengths are even larger. Therefore, $\exp[i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{r}]$ can be replaced by $\exp[i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{R}_j]$. Since

$$\int_{\text{cell},j} |u|^2 \mathbf{A} \cdot \nabla V(\mathbf{r} - \mathbf{R}_j) d\mathbf{r} = A \quad (2.196)$$

is the same for every unit cell, Eq. (2.195) becomes

$$P = A \sqrt{\frac{Na^2 k_2 k_3 (1 - e^{-2k_1 a})}{8(1 - e^{-Nk_1 a/2})(1 - e^{-Nk_2 a})(1 - e^{-Nk_3 a})}} \sum_j e^{i(\mathbf{q} + \mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{R}_j} \quad (2.197)$$

Due to the translational symmetry in the xy plane, the above equation is actually one-dimensional. Since

$$\sum_{n=-N/2}^{N/2} e^{in\alpha - |n\beta|} = \frac{2\beta}{\alpha^2 + \beta^2} \quad (2.198)$$

and let \mathbf{q} , \mathbf{k}_i and \mathbf{k}_f be real components of the wave vectors of the phonon, the initial and the final electronic states, respectively, in the z direction, we finally come

to a rather simple expression for the electron-phonon interaction:

$$P = A \sqrt{\frac{Nk_2k_3(1 - e^{-2k_1a})}{(1 - e^{-Nk_1a/2})(1 - e^{-Nk_2a})(1 - e^{-Nk_3a})}} \times \frac{|k_1 + k_2 - k_3|}{(\mathbf{q} + \mathbf{k}_i - \mathbf{k}_f)^2 + (k_1 + k_2 - k_3)^2} \quad (2.199)$$

When $k_1 = k_2 = k_3 = 0$,

$$\frac{|k_1 + k_2 - k_3|}{Na[(\mathbf{q} + \mathbf{k}_i - \mathbf{k}_f)^2 + (k_1 + k_2 - k_3)^2]} = \delta(\mathbf{q} + \mathbf{k}_i - \mathbf{k}_f) \quad (2.200)$$

so that Eq. (2.199) becomes

$$P = A\delta(\mathbf{q} + \mathbf{k}_i - \mathbf{k}_f) \quad (2.201)$$

which is exactly the expression of electron-phonon interaction for extended electron and phonon states [6].

Let us now discuss the following two cases. First we assume that there is one localized state involved.

By localization we mean the extension of the state $ma = 2/k$ is much smaller than Na . For the quantum well of the usual GaAs/AlGaAs double barrier resonant tunneling system, m is about 20 so that ma is about 50 \AA . We have mentioned early that when the doping level in the electrodes is about $5 \times 10^{17} \text{ cm}^{-3}$, the corresponding Fermi level is about 25 meV and $1/k$ (either k_i or k_f) is longer than 500 \AA . On the other hand, the most active phonons are the optical ones whose wave vector q is very small. Therefore $(\mathbf{q} + \mathbf{k}_i - \mathbf{k}_f)$ can be neglected when particles are localized.

Let $k_1 = 2/ma$ and $k_2 = k_3 = 0$. (It can be shown that the following conclusions remain intact if the values of k_1 , k_2 and k_3 are interchanged.) Since

$$1 - e^{-Nka} = Nka$$

when k is small, Eq. (2.199) becomes

$$P = \frac{A}{ak} \sqrt{\frac{1 - e^{-2ka}}{2N(1 - e^{-Nka/2})}} \quad (2.202)$$

where we have dropped off the subscripts from k . When $k = 2/ma$,

$$1 - e^{-2ka} \approx \frac{4}{m}$$

for large m and

$$1 - e^{-Nka/2} = 1 - e^{-N/m} \approx 1$$

when N/m is much larger than 1. Hence we obtain

$$P \propto A \sqrt{\frac{m}{N}} \quad (2.203)$$

The k 's are not exactly the same as $2/ma$, they depend on the state energy. When considering the electronic state, k decreases when the state energy increases (the state with higher energy penetrates more into the barrier region). Together with other constant from mathematical operation, the relation of proportionality (\propto) instead of equality ($=$) is used in Eq. (2.203) and later in Eqs. (2.205), (2.206).

It is concluded from Eq. (2.203) that when one state (either the phonon, or the initial or the final electronic state) is localized, the electron-phonon interaction is reduced when the extension of the localization, ma , is reduced. It was shown that the electron-phonon interaction is also reduced when one of the electronic states is evanescent [7]. The evanescent state is different from the localized one. It is only bounded at one end while the other end is free.

When the state becomes de-localized, i.e., when m becomes much large and is comparable with N , $(\mathbf{q} + \mathbf{k}_i - \mathbf{k}_f)$ cannot be neglected. By simple mathematical manipulation it is easy to see

$$P \propto A \quad (2.204)$$

Now we consider the situation when two or three states are localized. By similar mathematics as we used to discuss the case when one state is localized, we obtain for the case when two states are localized

$$P \propto \begin{cases} A & \text{for } |k_1 + k_2 - k_3| \neq 0 \\ A \frac{N}{m} & \text{otherwise} \end{cases} \quad (2.205)$$

For the case that all of the three states are localized, we obtain

$$P \propto \begin{cases} A (\frac{N}{m})^{1/2} & \text{for } |k_1 + k_2 - k_3| \neq 0 \\ A (\frac{N}{m})^{3/2} & \text{otherwise} \end{cases} \quad (2.206)$$

Quite different from the case when there is only one state localized, Eqs. (2.205), (2.206) show that the electron-phonon interaction is enhanced when more than one interacting states become localized. The strength of the electron-phonon interaction also increases when the extension of the localization is reduced.

The reader is reminded that the localization defined here is only along the z direction. The effect of two or three dimensional localization on the electron-phonon interaction can be discussed in a similar way. Such an effect could be very important for the novel quantum wire and quantum dot system. It can be expected from the above one-dimensional localization discussions that the dependence of the electron-phonon interaction on the localization extension can be much stronger.

2.8.2 Carrier-Carrier Interaction

Two main contributions to the carrier-carrier scattering can be easily identified:

- the individual carrier-carrier interaction via the screened Coulombic potential in the form of

$$V' = \frac{e^2}{4\pi\epsilon r} e^{-\beta r} \quad (2.207)$$

which accounts for two-body short-range interaction;

- the electron-plasmon interaction, which accounts for the collective long-range behavior of the electron gas.

Screened Carrier-Carrier Interaction The scattering probability of two electrons from state $(\mathbf{k}_1, \mathbf{k}_2)$ to $(\mathbf{k}_3, \mathbf{k}_4)$ is

$$\frac{|V'|^2}{\hbar^2} \frac{\gamma}{\Omega^2 + \gamma^2/4} \quad (2.208)$$

where

$$\hbar\Omega = E(\mathbf{k}_1) + E(\mathbf{k}_2) - E(\mathbf{k}_3) - E(\mathbf{k}_4) \quad (2.209)$$

The transition matrix element is

$$|V'|^2 = \frac{e^2}{\epsilon} \frac{\delta_{\mathbf{k}_1+\mathbf{k}_2, \mathbf{k}_3+\mathbf{k}_4}}{|\mathbf{k}_1 - \mathbf{k}_3|^2 + \beta^2} \quad (2.210)$$

The overlap integral is omitted here.

Electron-Plasmon Interaction The squared matrix element is calculated

$$\begin{aligned} |V'|^2 &= \frac{e^2 \hbar^3 (2\mathbf{k} \cdot \mathbf{q} + q^2)^2}{8\epsilon\omega_q q^2 m^2} \\ &\times \left[\frac{N_q \gamma}{(\Omega^+ - \omega_q)^2 + \gamma^2/4} + \frac{(N_q + 1)\gamma}{(\Omega^- + \omega_q)^2 + \gamma^2/4} \right] \end{aligned} \quad (2.211)$$

where

$$\hbar\Omega^+ = E(\mathbf{k} + \mathbf{q}) - E(\mathbf{k})$$

$$\hbar\Omega^- = E(\mathbf{k} - \mathbf{q}) - E(\mathbf{k})$$

\mathbf{q} is the wave vector of the plasmon, N_q is the equilibrium distribution population of the plasmon, ω_q is the plasmon frequency.

In the above equation, it is clear to see the term when an electron at state \mathbf{k} absorbs/emits a plasmon of state \mathbf{q} with an energy exchange $\hbar\omega_q$ and a wave vector change \mathbf{q} .

2.8.3 Impurity Scattering

- Conwell and Weisskopf approach (CW)

$$V'(r) = \begin{cases} \frac{Ze^2}{4\pi\epsilon r} & r < b \\ 0 & r > b \end{cases} \quad (2.212)$$

where $b = (3/4\pi n_i)^{1/3}$ is the mean distance between impurities, n_i the impurity concentration. Z is the number of charge units of the impurity.

- Brooks and Herring approach (BH):

$$V'(r) = \frac{Ze^2}{4\pi\epsilon r} e^{-\beta r} \quad (2.213)$$

where β^{-1} is the screening length, ϵ the dielectric constant. The scattering probability of BH approach is

$$P_{\mathbf{k},\mathbf{k}'} = \frac{2\pi Z^2 n_i e^4 p^2(\mathbf{k}, \mathbf{k}')}{\hbar \epsilon^2 (\beta^2 + |\mathbf{k} - \mathbf{k}'|^2)^2} \cdot \frac{\gamma}{[E(\mathbf{k}') - E(\mathbf{k})]^2 / \hbar^2 + \gamma^2 / 4} \quad (2.214)$$

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Physical Models of Semiconductor Quantum Devices

Fu, Y.

2014, XI, 408 p., Hardcover

ISBN: 978-94-007-7173-4