

Figure 1. Slab of GaAs with a bias voltage applied through ohmic contacts. If the bias voltage exceeds a critical value, negative differential mobility occurs in the device

Poisson's equation, i.e. using x for position and t for time,

$$\frac{\partial n}{\partial t} - \frac{\partial}{\partial x} (nv(F)) = 0, \quad (1)$$

$$\frac{\partial F}{\partial x} = -\frac{e}{\epsilon} (n - n_0), \quad (2)$$

where diffusion is neglected. Here, n is the number density of the electrons

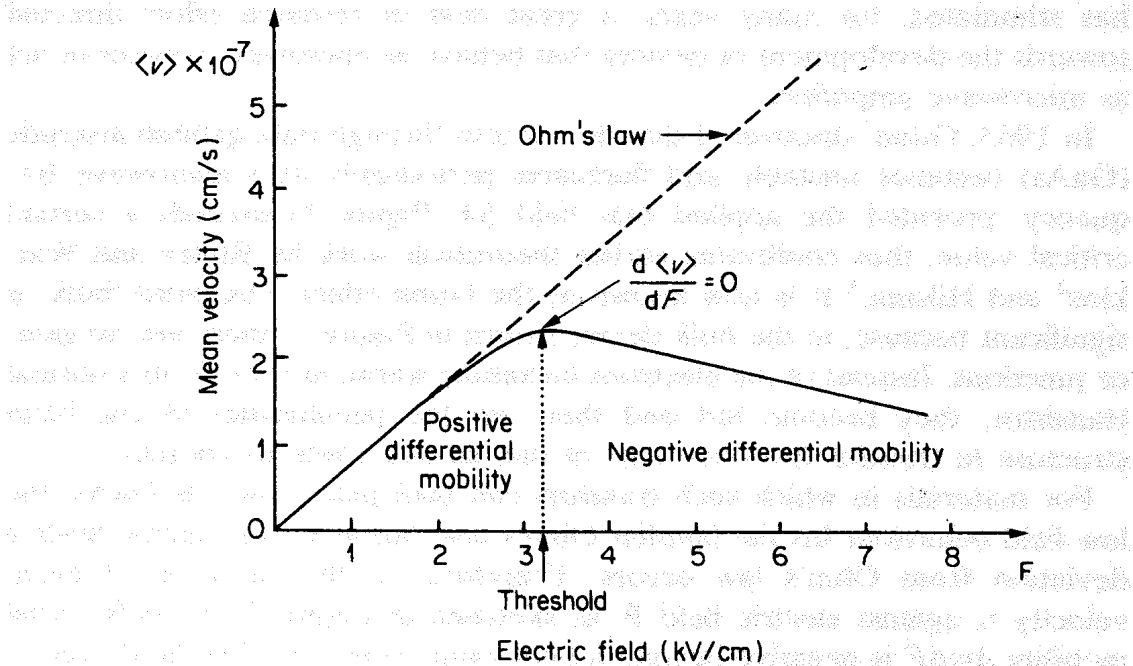


Figure 2. Sketch of the velocity-field characteristic of bulk GaAs. A threshold electric field ~ 3 kV/cm separates positive and negative differential mobility regimes. The deviation from Ohm's law is clearly evident

inside a semiconductor, $v(F)$ is the electron velocity, n_0 is the equilibrium density, F is the applied electric field, e is the electronic charge, and $\epsilon = \kappa_0 \epsilon_\infty$, where κ_0 is the permittivity of free space and ϵ_∞ is the high-frequency dielectric constant. Now suppose that a fluctuation in the electron density occurs that drives n_0 to $n = n_0 + n_1(x, t)$. In such an event the equilibrium values of velocity and electric field (v_0 and F_0) are driven to the new values $v = v_0 + v_1(x, t)$, $F = F_0 + F_1(x, t)$ so that

$$\frac{\partial n_1}{\partial t} - n_0 \frac{\partial v_1}{\partial x} - v_0 \frac{\partial n_1}{\partial x} = 0, \quad (3)$$

$$\frac{\partial F_1}{\partial x} = -\frac{e}{\epsilon} n_1, \quad (4)$$

$\partial v_1 / \partial x$ is $(\partial v / \partial F)_{F_0} \partial F_1 / \partial x$, however, which means that equations (3) and (4) reduce to

$$\left[\frac{\partial}{\partial t} - v_0 \frac{\partial}{\partial x} + \frac{n_0 e}{\epsilon} \left(\frac{\partial v}{\partial F} \right)_{F_0} \right] n_1 = 0 \quad (5)$$

where the quantity $(\partial v / \partial F)_{F_0}$, the gradient of the velocity-field characteristic, is called the differential mobility μ_0 . Note that it is not the same as v/F that is the more usually discussed mobility. If all the fluctuating quantities vary as $e^{i(kx - \omega t)}$, where k is a wave number and ω is an angular frequency, then the dispersion equation of the system is

$$\omega + kv_0 = -i \left(\frac{n_0 e}{\epsilon} \right) \mu_0 \quad (6)$$

From equation (6) it is seen that all fluctuations must vary as $\exp[(-n_0 e / \epsilon) \mu_0 t]$. If, for any electric field, $\mu_0 < 0$ then the differential mobility is negative and the space charge n will grow. This is what is meant by instability. For real k the oscillation frequency is kv_0 and the rise or decay constant is $\text{Im}(\omega)$. If the lower limit of k is $\sim 2\pi/L$, where L is the length of the sample, then the oscillation frequency is $f \sim v_0/L$. Typically L is $\sim 10 \mu\text{m}$ and v_0 is between 10^7 and 2×10^7 cm/s. These figures imply that $f \sim 10\text{--}20$ GHz.

The critical field at which the Gunn effect begins in GaAs is a little over 3 kV/cm. This means, for devices as thin as $\sim 10 \mu\text{m}$, that the applied voltage need only be ~ 3 V. This is obviously a great advantage implying, as it does, the possibility of making hand-held microwave devices.

The transferred electron mechanism in GaAs can be used to make amplifiers and oscillators, but probably the most dramatic development is the use of the GaAs microwave generator to make miniature radar systems.⁴ As can be seen from the rough calculations given earlier, these require, as a power source, only a simple torch battery. They are used to make burglar

alarms, small portable radar torches for ground surveillance (giving ranges of ~ 25 to 625 m), navigation beacons, and hand-held speed torches for use by traffic police.

At the heart of all these devices lies the transferred electron effect and it is the computer simulation of this mechanism that this chapter deals with. The effect involves the movement of electrons that receive so much energy from the applied electric field that they become hot, in the sense that they have an energy far in excess of the thermal energy. It is necessary, therefore, to study the motion of electrons in an applied electric field and to study the mechanisms that can scatter them. This is a difficult task, especially if the conventional transport equations are solved. However, since a computer has to be used anyway it turns out that a simulation, using Monte Carlo techniques, has a number of advantages.

2. THE MONTE CARLO METHOD

The application of simulation techniques in theoretical physics and engineering serves two main purposes. The first is circumventing the difficulty of providing useful solutions to important non-linear equations such as the Boltzmann transport equation. Analytical solutions to these equations often involve drastic approximations and provide unrealistic results. The second purpose is to provide deeper insight into the physical mechanisms that such equations describe.

One simulation technique that has proved immensely powerful in electron transport theory is the Monte Carlo method.⁵⁻⁸ This chapter is devoted to a description of that method and is illustrated by an application to the study of electron transport in non-degenerate semiconductors such as GaAs with electron densities of $\sim 10^{21} \text{ m}^{-3}$.

Many parameters of a physical system are governed by probability distributions. Therefore, if a mathematically random distribution is used to interrogate such distributions we can, in principle, generate the physical values of these parameters. This is, broadly speaking, the Monte Carlo method. In practice, of course, the physical distributions may be quite complex and difficult to manipulate even with a computer. The manipulations can be simplified by 'mapping' the complex distributions on to a simple pseudo-random distribution; the most convenient pseudo-random distribution is the uniform distribution, which is readily available on most computer systems.

In general, if $p(\phi)$ and $p(r)$ are the respective probability densities, associated with ϕ in the physical distribution and r in the pseudo-random distribution, then

$$\int_0^\phi p(\phi') d\phi' = \int_0^r p(r') dr' \quad (7)$$

In a uniform distribution $p(r) \neq 1$ so that (7) becomes

$$r = \int_0^{\phi} p(\phi') d\phi' \quad (8)$$

Hence, provided that this integral can be evaluated in a simple closed analytical form, inversion will yield a random value for the physical variable ϕ in terms of the uniformly distributed random number r . A simple example of this technique is the generation of the random flight times of a classical particle in a gas for the case when Γ , the total scattering rate, is constant. The probability of this particle travelling unimpeded for a time t and then being scattered at the end of this flight is

$$p(t) = \Gamma e^{-\Gamma t} \quad (9)$$

From equation (8)

$$r = \int_0^t \Gamma e^{-\Gamma t'} dt' = 1 - e^{-\Gamma t}, \quad (10)$$

so that the random flight times are given by

$$t = -\frac{1}{\Gamma} \ln(1-r) = -\frac{1}{\Gamma} \ln(r) \quad (11)$$

Note that, since r is uniformly distributed, $\ln(1-r)$ is equivalent to $\ln(r)$.

In effect, what happens in the calculation is that the cumulative probability $P(t)$ is calculated, i.e. the area under the probability curve up to a value t , and its value is then mapped on to a uniform random number distribution from which t is directly selected. This process is illustrated in Figures 3 and 4. Similar manipulations provide values for any other physical parameter

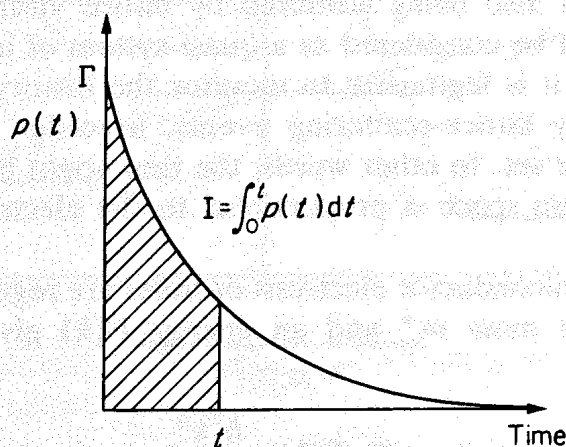


Figure 3. Simple probability density as a function of time

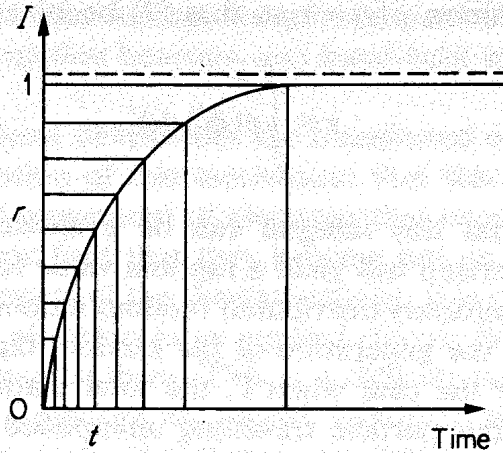


Figure 4. Cumulative probability obtained from Figure 3 mapped on to a uniformly distributed random distribution lying between 0 and 1

whose instantaneous value can be described by a probability density distribution, an example being the angular deviation of a particle in a scattering interaction.

3. ELECTRON MOTION

Before this simulation technique is applied to the problem of charge carrier transport in semiconducting solids, it is helpful to examine, briefly, the manner in which charge carriers move through a semiconductor and determine those features of the motion that are governed by probability distributions of the kind discussed in the previous section.

A conductor contains a large number of charge carriers and it is impossible to directly simulate such a many-body distribution of mutually interacting particles that are also being scattered by lattice vibrations. However, the actual system can be considered as a quasi-system of independent particles. This means that it is legitimate to monitor the history of a single particle, undergoing many lattice-scattering events, in order to generate the behaviour of a large set. In other words, the time spent by an electron in each part of momentum space is proportional to the electron distribution function.

In a simple semiconductor electrons or holes are regarded as free particles with an effective mass m^* and an energy $E(k)$ given by the parabolic dispersion law

$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m^*}, \quad (12)$$

where $\hbar = h/2\pi$, $h = 6.625 \times 10^{-34}$ J s is Planck's constant and \mathbf{k} labels the state of the particle. Thus $\hbar\mathbf{k}$ is interpreted as particle momentum and, in the case of electrons, m^* is usually considerably smaller than the free-electron mass $m_0 = 9.11 \times 10^{-31}$ kg. Many semiconductors are not as simple as this but, if they are not, it is sometimes possible, as in the case of GaAs, to provide a description in terms of two effective masses.

In the semiconductor to be simulated here, individual electrons are pictured as drifting under the action of an applied electric field through a lattice of atoms or ions that act as scattering agents. Under these circumstances an electron moves, under the influence of an external electric field, for a time dependent upon the total probability of scattering due to any of the interaction processes with the surrounding material.

The motion is most usefully described in 'momentum space'; here the particle moves at a constant rate between collisions and changes its momentum state from one value to another instantaneously during a collision, as illustrated in Figure 5.

The momentum space is really the space defined by $\hbar\mathbf{k}$ but, since \hbar is a constant scaling factor, only the motion in \mathbf{k} -space is considered. If the carriers are electrons with a charge $-e$ then a constant, uniform electric field $\mathbf{F} = (0, 0, -F)$ causes them to drift in the positive k_z direction and the equation of motion of the electron has a solution

$$\mathbf{k}_f(t) = \mathbf{k}_i - \frac{e\mathbf{F}}{\hbar} t, \quad (13)$$

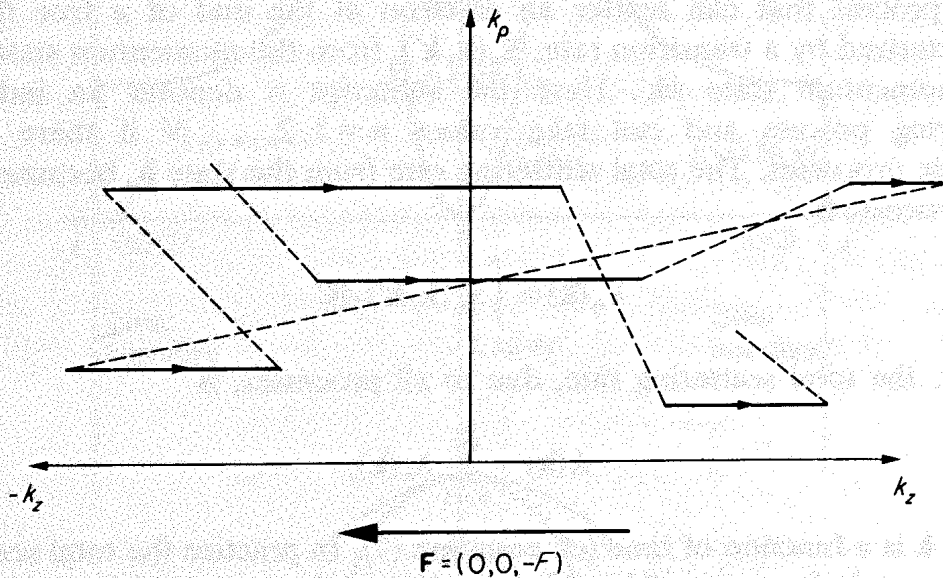


Figure 5. Electron motion in momentum space. The axes are $k_p = (k_x^2 + k_y^2)^{1/2}$, k_z , and the scaling factor \hbar is omitted

where \mathbf{k}_i is the value at the start of the electron flight, $\mathbf{k}_f(t)$ is the value at the end of the flight (drifting time), and t is the flight time.

Since the \mathbf{k} -space of the electrons is symmetric about \mathbf{F} we can use an equivalent two-dimensional (k_ρ, k_z) -space, where $k_\rho = (k_x^2 + k_y^2)^{1/2}$, instead of the three-dimensional (k_x, k_y, k_z) -space. Hence k_ρ remains fixed during an electron flight from an initial position (k_ρ, k_{zi}) to a final position (k_ρ, k_{zf}) and only the z -component of equation (13) needs to be considered, i.e.

$$k_{zf} = k_{zi} + \frac{eF}{\hbar} t. \quad (14)$$

The simulation is started by choosing an arbitrary starting position and is then allowed to proceed until many flight times have occurred between scattering events. If enough flight times are considered, i.e. if the electron path is long enough, then the starting position has no influence on the final results. A flight is terminated by a scattering process that, since there are several competing mechanisms, is selected by another Monte Carlo procedure. The scattering mechanism automatically specifies the electron energy after scattering; however, the determination of the new position of the electron in momentum space requires a knowledge of the scattering angle. Since this angle has a probability distribution that depends on the scattering probability, the scattering angle is also generated by a Monte Carlo method. This is described later.

4. THE ELECTRON-PHONON SCATTERING PROCESSES

Each process that can scatter an electron at the end of a free flight is characterized by a transition rate, $S_n(\mathbf{k}, \mathbf{k}')$, from the momentum state $\hbar\mathbf{k}$ to the momentum state $\hbar\mathbf{k}'$. Here the subscript n denotes an individual scattering process and can take values $n=1, 2, \dots, N$ if there are N possible processes. The total scattering rate from the state \mathbf{k} , because of the n th process, is

$$\lambda_n(\mathbf{k}) = \int S_n(\mathbf{k}, \mathbf{k}') d\mathbf{k}' \quad (15)$$

Hence, the total scattering rate, due to all processes, is

$$\lambda(\mathbf{k}) = \sum_{n=1}^N \lambda_n(\mathbf{k}), \quad (16)$$

where \mathbf{k} is a function of time (cf. equation (7)). In practice the total scattering rates are only functions of $k = |\mathbf{k}|$ so, by virtue of equation (12), $\lambda(\mathbf{k})$ is easily transformed to $\lambda(E)$.

As an illustration of hot electron behaviour in semiconductors we consider

the important material GaAs, whose energy-momentum band structure ($E(k)$ versus $\pm k$) is sketched in Figure 6, in the vicinity of the band extremities, along the $\langle 100 \rangle$ directions. There are energy minima, located at the zone centre, and at the edges, that we will call valleys. There is one central valley, with a small radius of curvature, where electrons have a low effective mass equal to $0.067 m_0$, and there is a shallow satellite valley at the equivalent $\langle 100 \rangle$ Brillouin zone edges. By symmetry, however, two other, identical, satellite valleys are located at the $\langle 010 \rangle$ and $\langle 001 \rangle$ edges as well. Electrons associated with these satellite valleys have an effective mass equal to $0.35 m_0$. Thus the conduction band has valley structure and, at zero applied electric field ($\mathbf{F}=0$) and room temperature (or less), the free electrons are located in the bottom regions of the central valley. The valence band is well separated from the conduction band so the transport of holes need not be considered.

In a non-degenerate sample of GaAs, the electron density is quite small ($\sim 10^{21} \text{ m}^{-3}$) so that the Pauli exclusion principle does not have to be taken into account. This is what we assume here although, within the framework of a Monte Carlo calculation, it is reasonably straightforward to include

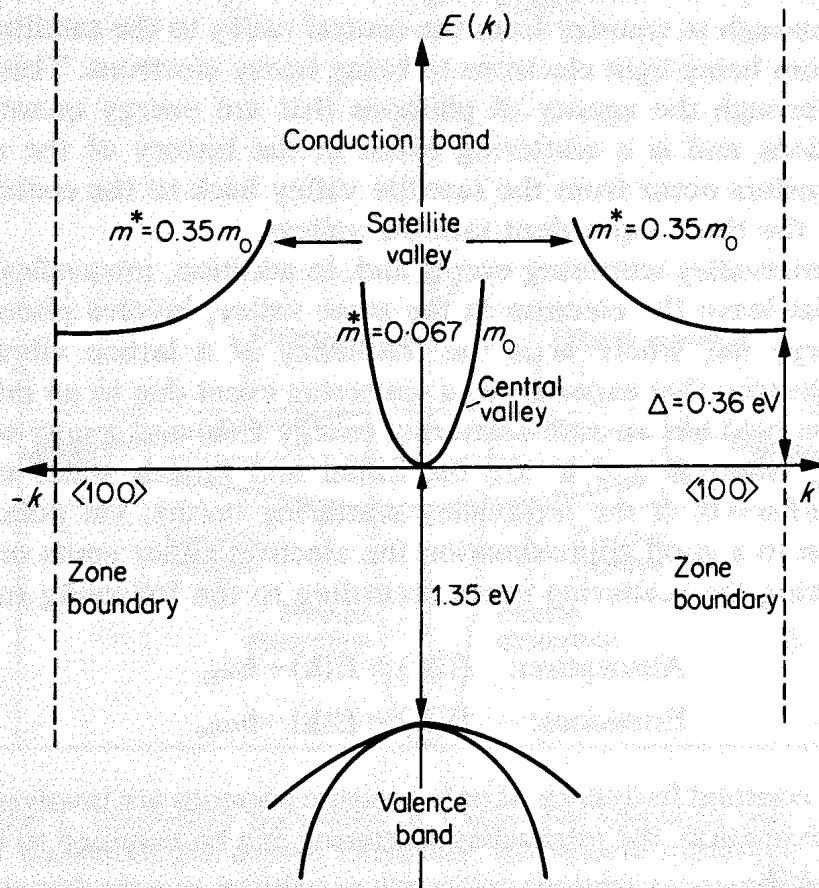


Figure 6. Sketch of the band structure of GaAs

degeneracy. A reasonable approximation, for a student exercise such as this, is to assume that both types of valleys are parabolic, i.e. that the electron energy minima are described by equation (12). Nevertheless the central valley of GaAs is really non-parabolic and, strictly speaking, equation (12) should be modified by the addition of a term of the form αk^4 , where α is a constant.⁶ This non-parabolicity, on its own, turns out to be quite important but it is, in fact, partially offset by a wave-number dependence that should be included in $S_n(\mathbf{k}, \mathbf{k}')$ if Bloch wave functions, as opposed to plane waves, are used. For these reasons it is a consistent, quite good approximation, to use parabolic valleys and a plane wave representation of the free-electron states.

If the applied electric field is zero the electrons are in equilibrium with the vibrating solid atoms which have a mean energy $\sim (k_B T/1.6) \times 10^{19}$ eV, where T is the absolute temperature of the semiconductor and k_B is Boltzmann's constant 1.38×10^{-23} J K⁻¹. For a material at 300 K the mean electron energy is therefore ~ 0.03 eV. The application of an electric field causes the electrons to cease to be in equilibrium with the solid lattice and to increase in energy until they acquire a temperature in excess of that of the solid. The electrons become hot, therefore, and occupy the upper regions of the central valley. At sufficiently high electric fields the electrons may become hot enough to transfer from the central valley to the satellite valleys and switch from being light electrons to being heavy electrons. This transfer is achieved through the agency of phonons that are energy quanta of the lattice vibrations and is a scattering event in the history of the electron. Similarly, transfers occur from the satellite valley back to the central valley and between the three equivalent satellite valleys.

All these intervalley scattering events and, in addition, intravalley scattering events that leave the electron in the same valley, involve phonons that have an energy $\hbar\omega$, where ω is the frequency of a lattice vibration. In general, an electron that experiences a scattering event due to an interaction with a phonon field has an ante-scattering energy $E(\mathbf{k})$ and a post-scattering energy $E(\mathbf{k}')$, where \mathbf{k} and \mathbf{k}' are the initial and final \mathbf{k} states such that $E(\mathbf{k}') - E(\mathbf{k}) \pm \hbar\omega = 0$. If the intravalley scattering occurs, via polar optical phonons, then to a good approximation the electron either emits or absorbs a phonon during the scattering event according to the following rules:

$$\text{Absorption: } E(\mathbf{k}') = E(\mathbf{k}) + \hbar\omega_0 \quad (17a)$$

$$\text{Emissions: } E(\mathbf{k}') = E(\mathbf{k}) - \hbar\omega_0, \quad (17b)$$

where ω_0 is a constant frequency. If only acoustic phonons are involved then, to a good approximation, the intravalley scattering can be assumed to be elastic with $E(\mathbf{k}') = E(\mathbf{k})$.

For GaAs the important intravalley scattering mechanism between states

inside the central valley and between states inside a satellite valley is polar optical phonon scattering. Obviously, acoustic phonon scattering also takes place within the central and satellite valleys but it has a minor influence on the electron distribution.⁶

If scattering between the central and satellite valley occurs then the electrons must acquire at least an energy Δ before the transition becomes

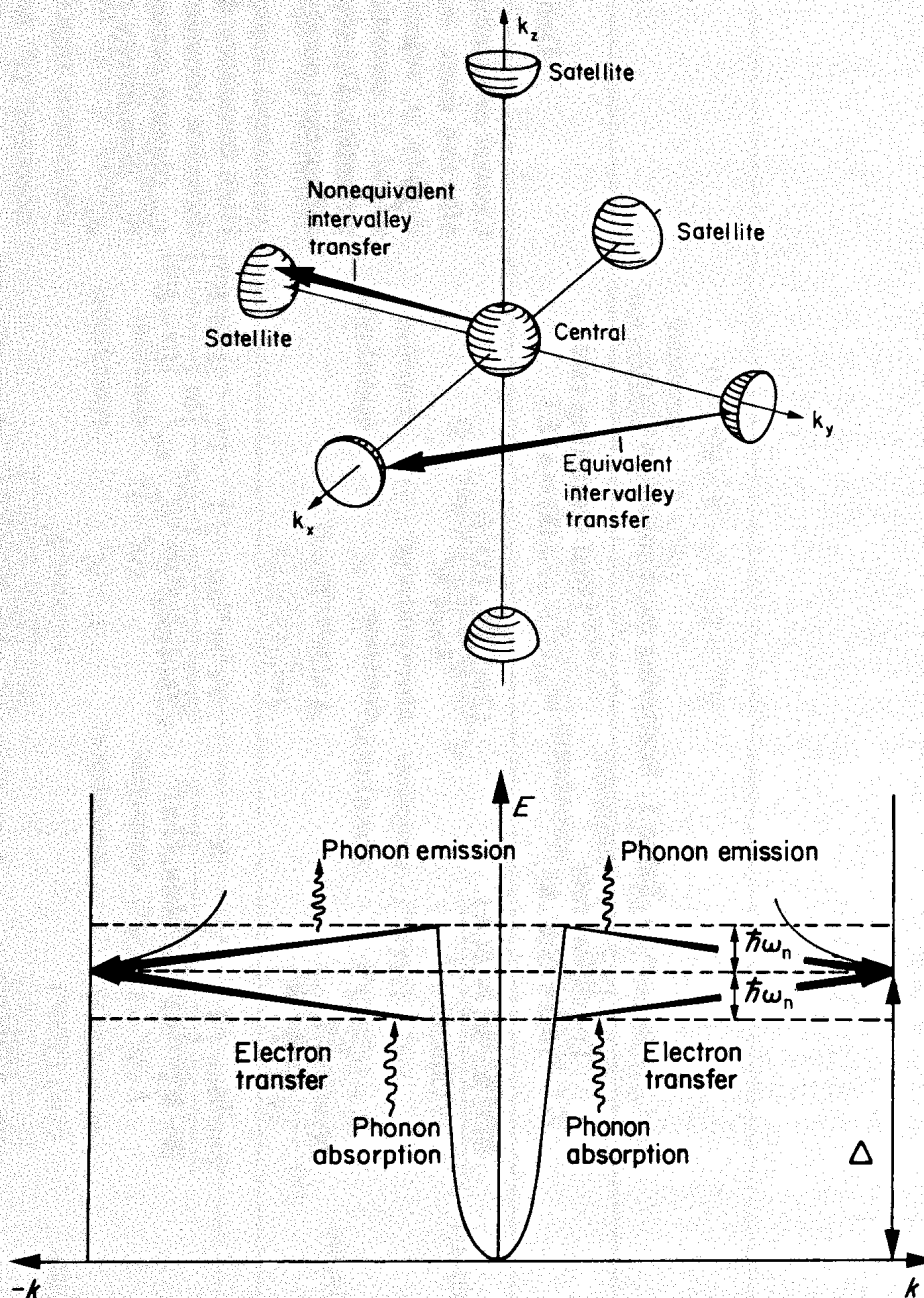


Figure 7. Intervalley transitions on GaAs. For simplicity only one-way transitions are shown. Obviously, the reverse transitions also occur with phonon emission or absorption changing to absorption or emission

Table 1. Scattering mechanisms in GaAs

Scattering mechanism	Transition rate $(\hbar/2\pi)S(\mathbf{k}', \mathbf{k})$	Total scattering rate $\lambda(\mathbf{k}) \equiv \lambda(E)$	Definitions
Acoustic phonon for either absorption or emission (intravalley)	$\frac{\hbar D_a^2 \mathbf{k} - \mathbf{k}' N_a \delta(A)}{(2\rho s)(2\pi)^3}$ $N_a \approx \frac{k_B T}{\hbar s \mathbf{k} - \mathbf{k}' }$	$\frac{(2m_{cs}^*)^3 k_B T D_a^2 E^{\frac{1}{2}}}{4\pi \rho s^2 \hbar^4}$ absorption or emission $A = E' - E = 0$	Central or satellite valley effective mass, m_{cs}^* ; density, ρ ; velocity of sound, s ; acoustic deformation potential, D_a ; phonon occupation number, N_a .
Polar optical phonon (intravalley)	$\frac{2\pi e^2 \hbar \omega_0}{ \mathbf{k} - \mathbf{k}' ^2} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) \frac{X}{4\pi \kappa_0 (2\pi)^3}$	$\frac{Y e^2 m^* \omega_0}{\sqrt{2\hbar(4\pi \kappa_0)^2 E^{\frac{1}{2}}}} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) \ln \frac{ E^{\frac{1}{2}} + E^{\frac{1}{2}} }{ E^{\frac{1}{2}} - E^{\frac{1}{2}} }$	High frequency and static dielectric constants, ϵ_∞ , ϵ_0 ; phonon occupation number, N_o ; permittivity of free space, κ_o .

$$X = N_o \delta(A_a) \quad \text{absorption}$$

$$(N_o + 1) \delta(A_e) \quad \text{emission}$$

$$N_o = [\exp(\hbar \omega_o / k_B T) - 1]^{-1}$$

$$Y = N_o \quad \text{absorption}$$

$$(N_o + 1) \quad \text{emission}$$

$$A_{a,e} = E' - E \mp \hbar \omega_o = 0$$

Equivalent intervalley (satellite \rightleftharpoons satellite)	$\frac{(Z-1)\hbar D_e^2 X}{(2\pi)^3(2\rho\omega_e)^3}$ $X = N_e \delta(A_e)$ $N_e = [\exp(\hbar\omega_e/k_B T) - 1]^{-1}$	$\frac{(Z-1)m_e^{*3} D_e^2 E^{1/2} Y}{\sqrt{2\pi\rho\omega_e}\hbar^3}$ $Y = N_e$ $A_{a,e} = E' - E \mp \hbar\omega_e$	absorption emission	Intervalley deformation potential, D_e ; number of equivalent valleys, Z (for GaAs, $Z=3$); phonon occupation number, N_e .
Non-equivalent intervalley				Intervalley deformation potential D_n ; phonon occupation number, N_n .
(a) central \rightarrow satellite	$(a) \quad \frac{3\hbar D_n^2 X}{2\rho\omega_n(2\pi)^3}$ $X = N_n \delta(A_n)$ $(N_n + 1)\delta(A_n)$ $\frac{\hbar D_n^2 X}{2\rho\omega_n(2\pi)^3}$	$\frac{3m_n^{*3} D_n^2 E^{1/2} Y}{\sqrt{2\pi\rho\omega_n}\hbar^3}$ $Y = N_n$ $(N_n + 1)$ $A_{a,e} = E' - E + \Delta \mp \hbar\omega_n = 0$	absorption emission absorption emission	
(b) satellite \rightarrow central	$(b) \quad \frac{\hbar D_n^2 X}{2\rho\omega_n(2\pi)^3}$ $X = N_n \delta(A_n)$ $(N_n + 1)\delta(A_n)$ $N_n = [\exp(\hbar\omega_n/k_B T) - 1]^{-1}$	$\frac{m_n^{*3} D_n^2 E^{1/2} Y}{\sqrt{2\pi\rho\omega_n}\hbar^3}$ $Y = N_n$ $(N_n + 1)$ $A_{a,e} = E' - E - \Delta \mp \hbar\omega_n = 0$	absorption emission absorption emission	

possible. However, in the satellite valley the electron energy is measured from its minimum so it is necessary to add Δ to the electron energy if scattering from the satellite to the central valley occurs. Such non-equivalent intervalley transitions are shown in Figure 7 and are summarized as:

Central \rightarrow Satellite:

Absorption: $E_s(\mathbf{k}') = E_c(\mathbf{k}) - \Delta + \hbar\omega_n;$ (18a)

Emission: $E_s(\mathbf{k}') = E_c(\mathbf{k}) - \Delta - \hbar\omega_n.$ (18b)

Satellite \rightarrow Central:

Absorption: $E_c(\mathbf{k}') = E_s(\mathbf{k}) + \Delta + \hbar\omega_n;$ (19a)

Emission: $E_c(\mathbf{k}') = E_s(\mathbf{k}) + \Delta - \hbar\omega_n$ (19b)

where ω_n is a constant frequency. The other transitions that must be considered take place between the satellite valleys and involve the emission or absorption of a phonon of energy $\hbar\omega_e$ where ω_e is also a constant frequency. The energy relationship for satellite \rightleftharpoons satellite transitions has the same form as equations (17a) and (17b).

The complete list⁶ of electron-phonon scattering processes for plane wave states in parabolic valleys is given in Table 1. It should be noted that if V is the volume of the crystal then a factor $V/8\pi^3$ should appear in front of the integral of equation (15). This factor has been absorbed into the definition of $S_n(\mathbf{k}, \mathbf{k}')$. The formulae are presented without proof, but the references at the end of this chapter and a good textbook on solid-state physics for

Table 2. Data for GaAs⁶

Parameter	Value
Density	5.37 g/cm ³
Velocity of sound, s	5.22×10^5 cm/s
High frequency dielectric constant, ϵ_∞	10.82
Static dielectric constant ϵ_0	12.53
Polar optical phonon frequency, ω_0	5.37×10^{13} rad.S ⁻¹
Equivalent intervalley phonon frequency, ω_e	4.54×10^{13} rad.S ⁻¹
Non-equivalent intervalley phonon frequency, ω_n	4.54×10^{13} rad.S ⁻¹
Acoustic deformation potential in central and satellite valleys	7 eV
Equivalent intervalley deformation potential, D_e	10^9 eV/cm
Non-equivalent intervalley deformation potential, D_n	10^9 eV/cm
Central valley effective mass, m_c^*	$0.067 m_0$
Satellite valley effective mass, m_s^*	$0.35 m_0$
Valley separation	0.36 eV

Note. If SI units are used to calculate $\lambda_n(E)$ then care must be exercised with quantities measured in eV/cm.

advanced students, will enable the reader to check them without too much difficulty. Each process is governed by an energy-conserving delta-function condition $\delta(A)$ in which we write $E' \equiv E(\mathbf{k}')$ and $E \equiv E(\mathbf{k})$. Data for GaAs that are required to evaluate these formula are given in Table 2. The computer program given at the end of this chapter, however, can be run with any set of data required, even if it does not correspond to a real substance.

5. COMPUTATION OF ELECTRON FLIGHT TIMES AND SCATTERING CHANNEL SELECTION

If $p(t)$ is the probability per unit time that an electron has a flight, of duration time t , terminated by some scattering process (i.e. has a drift time t in momentum space and is then scattered) then the solution of equation (8) in the form

$$r = \int_0^t p(t') dt'$$

will enable a random distribution of such flight times to be generated.

Now suppose that the electron drifts for a time t before being scattered and that this time consists of n tiny increments $\delta t_1, \delta t_2, \dots, \delta t_n$. The probability of the electron being scattered, within the time interval δt_i , is $\lambda(\mathbf{k})\delta t_i$, where $\lambda(\mathbf{k})$ is the total scattering rate defined by equation (16). The probability that there will not be any scattering during δt_i is thus $(1 - \lambda(\mathbf{k})\delta t_i)$. Therefore, the probability of an electron drifting in momentum space, for a time t , is

$$S(t) = \prod_{i=1}^n (1 - \lambda(\mathbf{k})\delta t_i) \quad (20)$$

so that

$$\log\{S(t)\} = \sum_{i=1}^n \log(1 - \lambda(\mathbf{k})\delta t_i). \quad (21)$$

However, since $\lambda(\mathbf{k})\delta t_i \ll 1$ equation (21) reduces to

$$\log\{S(t)\} = - \sum_{i=1}^n \delta t_i \lambda(\mathbf{k}) \quad (22)$$

which gives, immediately,

$$S(t) = \exp\left\{- \int_0^t \lambda(\mathbf{k}) dt'\right\} \quad (23)$$

where $\lambda(\mathbf{k})$ is a function of time through equation (13). The probability density $p(t)$ is therefore

$$p(t) = \lambda(\mathbf{k}) \exp \left\{ - \int_0^t \lambda(\mathbf{k}) dt' \right\} \quad (24)$$

Using equation (24) and a uniformly distributed random number distribution gives

$$r = 1 - \exp \left\{ - \int_0^t \lambda(\mathbf{k}) dt' \right\}. \quad (25)$$

Equation (25) is very complicated and cannot, for the scattering mechanisms discussed in section 3, be solved analytically for t . There is no conceptual difficulty here, however, because, if necessary, the integrations could be performed by numerical quadrature to produce r and t in tubular form for each value of electron energy. Such a process involves several sub-routines and, spread over thousands of scattering events, involves a significant amount of computer time and store. It is also rather inconvenient to program.

A new technique for circumventing this difficulty has been found^{5,6} and involves supplementing the real scattering processes of section 3 by the addition of a virtual scattering process that does not affect the state of the electron. Suppose a virtual scattering transition probability $S_v(\mathbf{k}', \mathbf{k})$ is defined as

$$S_v(\mathbf{k}', \mathbf{k}) = \lambda_v(\mathbf{k}) \delta(\mathbf{k} - \mathbf{k}'), \quad (26)$$

where, since the electron state is unaltered, the electron distribution remains unaffected so that $\lambda_v(\mathbf{k})$ is quite arbitrary. We are then at liberty to choose

$$\lambda_v(\mathbf{k}) = \Gamma - \lambda - \lambda(\mathbf{k}), \quad (27)$$

where $\lambda(\mathbf{k})$ is the total real scattering rate and Γ is some constant sufficiently large to avoid negative probabilities. Thus $\lambda_v(\mathbf{k}) > 0$ for all values of \mathbf{k} that could be involved in the situation and the new total scattering rate for the electron that now includes the virtual process is simply

$$\lambda_T(\mathbf{k}) = \lambda(\mathbf{k}) + \lambda_v(\mathbf{k}) = \Gamma. \quad (28)$$

Equation (25) now reduces to the elementary form

$$r = 1 - e^{-\Gamma t}, \quad (29)$$

giving the amazing result that

$$t = -\frac{1}{\Gamma} \ln(1-r) = -\frac{1}{\Gamma} \ln(r). \quad (30)$$

The time given by equation (30) is not usually the flight time between real scattering processes but is more likely to be the time between one virtual scattering process and another. During the simulation a flight time t_1 , say, is generated by a certain random number in accordance with equation (30). A further random number is then used to determine which scattering process (i.e. scattering channel) is to be selected for possible termination of the flight. This selection normally uses random numbers lying between 0 and 1 so that all the scattering rates are usually normalized with Γ . Hence, if the electron, at the moment of scattering, has an energy E , $\lambda_n(E)/\Gamma$ are calculated and a uniformly distributed random number is used, in the manner of Figure 8, to select the appropriate scattering channel.

If a virtual process is encountered the flight is not terminated and the flight time t_1 is stored. A new flight time t_2 is then selected, in the same way

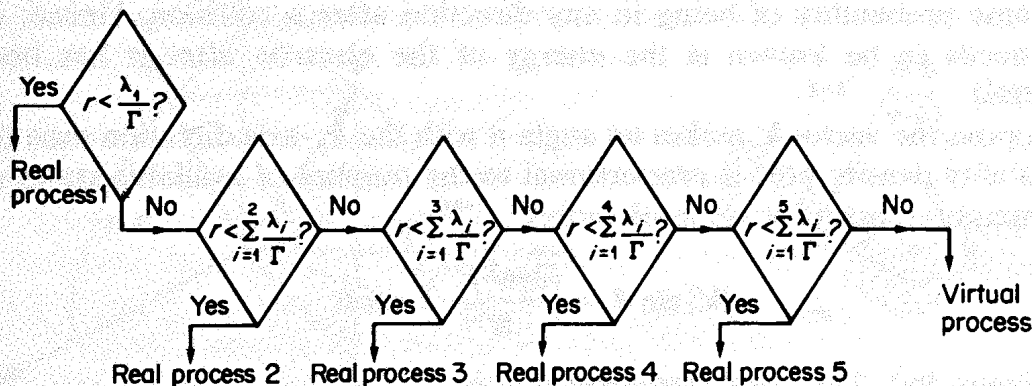
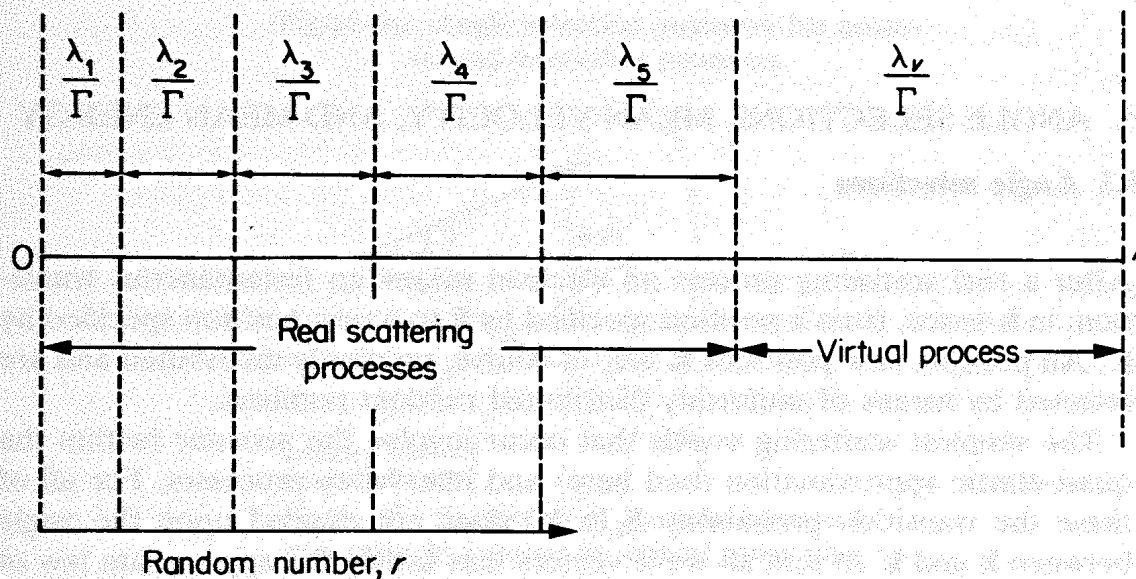


Figure 8. Scattering channel selection assuming that $N = 5$

as t_1 , and another scattering channel is selected. If a virtual process is encountered, once again, then t_2 is added to t_1 and a further flight time t_3 is calculated. This process goes on until the flight is finally terminated by the selection of a real scattering mechanism. It is clearly advisable to have as few virtual processes as possible, but the penalty that has to be paid here is that many virtual processes occur. This means that we have to accumulate, say, M subflights t_i until the real flight time $t = \sum_{i=1}^M t_i$ is obtained. This penalty, in computing terms, is relatively minor compared to using equation (25) together with only real scattering mechanisms. Nevertheless, the number of virtual processes can be minimized by making Γ as small as possible, without making $\lambda_v < 0$. In the program given here we set $\Gamma = \{\sum_{n=1}^N \lambda_n(E)\}_{\max}$ that, for two-valley GaAs processes, happens to be $\sum_{n=1}^N \lambda_n(E_{\max})$, where $E_{\max} \sim 1$ eV is the maximum energy allowed during the simulation.

5. ANGLE SELECTIONS, MEAN VELOCITY, AND MEAN ENERGY

5.1 Angle selections

After a real scattering process an electron makes an instantaneous transition, in \mathbf{k} -space, from a position specified by \mathbf{k} to a new position specified by \mathbf{k}' . All possible new positions \mathbf{k}' are, of course, randomly distributed and are selected by means of uniformly distributed random numbers.

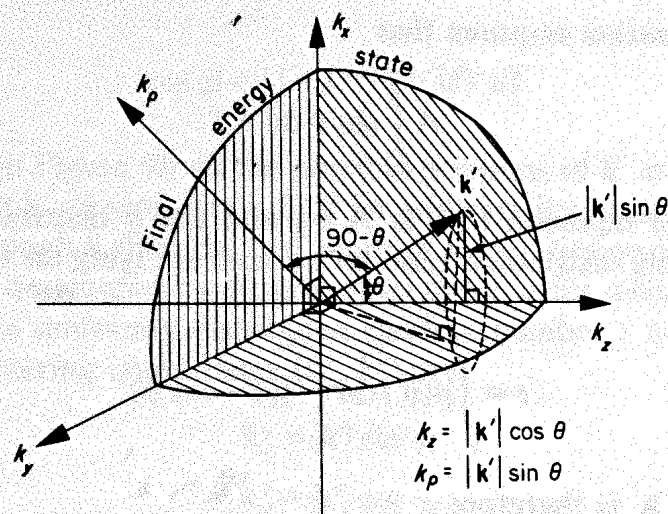
The simplest scattering events that occur involve the acoustic (within the quasi-elastic approximation used here) and intervalley processes. For all of these the transition probability $S_n(\mathbf{k}, \mathbf{k}')$ does not depend upon the angle between \mathbf{k} and \mathbf{k}' so that all wave vectors that satisfy the appropriate law of conservation of energy are equally probable. Such scattering processes are called randomizing, or isotropic, which means that the scattered electron has the same probability of being in any direction after a collision. Hence, all that needs to be known is the energy of the electron after it has been scattered.

Suppose the vector \mathbf{k}' makes an angle θ with the k_z -axis direction then the probability density $p(\theta)$ is proportional to the number of available states on the circumference of a circle of radius

$$|\mathbf{k}'| \sin \theta = \left(\frac{2m^*E'}{\hbar^2} \right)^{\frac{1}{2}} \sin \theta$$

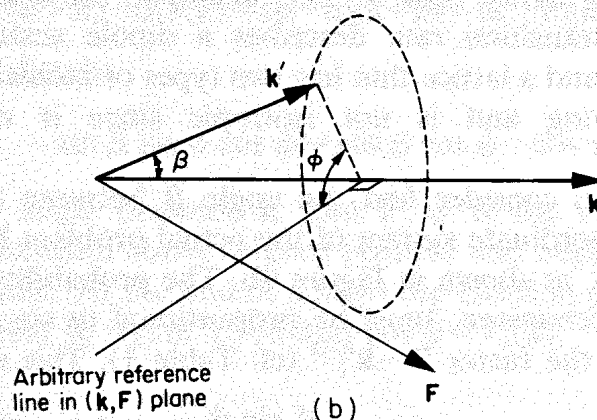
(cf. Figure 9a). The basic statement is that

$$p(\theta) = A \sin \theta, \quad (31)$$



(a)

Figure 9a. Angle selection geometry for acoustic and intervalley processes



(b)

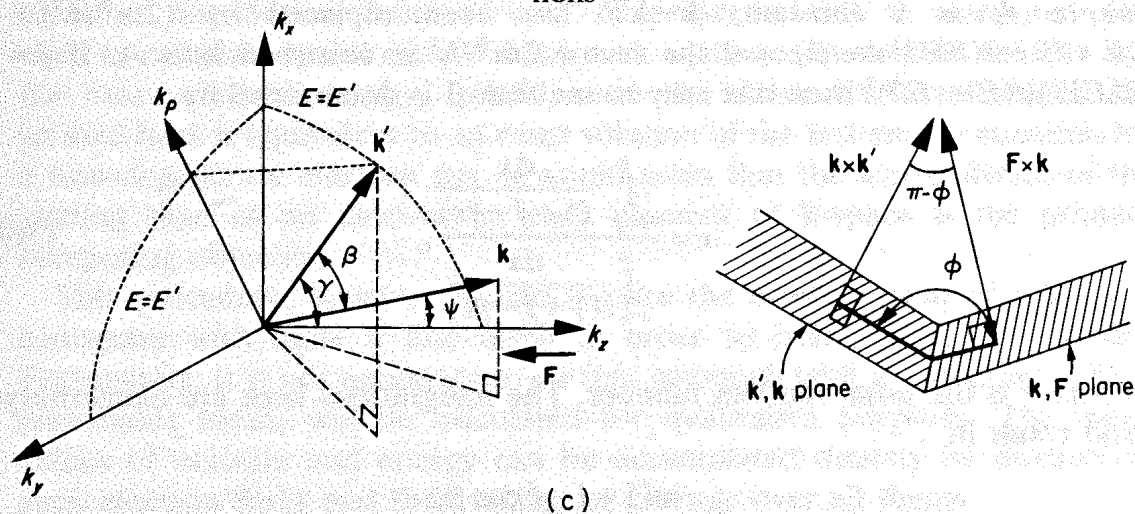
Figure 9b. Scattering of electron in state \mathbf{k} to a state \mathbf{k}' induced by optical polar phonons

Figure 9c. Full geometry of electron scattering by optical polar phonons

where normalization requires that

$$A \int_0^\pi \sin \theta \, d\theta = 1. \quad (32)$$

The solution of equation (32) is $A = \frac{1}{2}$ and the θ distribution is obtained from a uniformly distributed random number set lying on the interval (0, 1) by inverting

$$r = \int_0^\theta p(\theta') \, d\theta' = \frac{1}{2}(1 - \cos \theta). \quad (33)$$

The new state \mathbf{k}' is therefore

$$\mathbf{k}' = (|\mathbf{k}'| \sin \theta, |\mathbf{k}'| \cos \theta) \quad (34)$$

The situation for polar optical phonon scattering is much more difficult because, as Table 1 shows, $S_n(\mathbf{k}, \mathbf{k}')$ depends upon the angle between \mathbf{k} and \mathbf{k}' . Actually this transition rate describes a dipole scattering interaction between electrons and a lattice that has two types of atoms. This is a form of Coulombic scattering and is not isotropic since it emphasizes small angle deviations.

It is necessary to consider first the angle β between \mathbf{k} and \mathbf{k}' without reference to the coordinate system of the actual problem but using \mathbf{k} as the reference direction, as shown in Figure 9b. The probability density $p(\beta)$, as in the previous mechanisms, must be proportional to $\sin \beta$, but it must be weighted, also, by the factor $|\mathbf{k} - \mathbf{k}'|^{-2}$ (cf. Table 1). This means that

$$p(\beta) = \frac{A \sin \beta}{E + E' - 2(EE')^{\frac{1}{2}} \cos \beta}, \quad (35)$$

where A is a constant, $|\mathbf{k} - \mathbf{k}'|^2$ has been replaced by $(2m^*/\hbar^2) \times (E + E' - 2(EE')^{\frac{1}{2}} \cos \beta)$ and the factor $2m^*/\hbar^2$ is absorbed into A . If $f = 2(EE')^{\frac{1}{2}}/(E^{\frac{1}{2}} - E'^{\frac{1}{2}})^2$ then it is easy to see that β is determined by

$$r = \frac{\int_{\cos \beta}^1 \frac{dx}{(1+f-fx)}}{\int_{-1}^1 \frac{dx}{(1+f-fx)}}, \quad (36)$$

where r is the usual random number. The integrations here are elementary and result in

$$r = \frac{\ln(1+f-f \cos \beta)}{\ln(1+2f)}, \quad (37)$$