CHAPTER II

'ELECTRONIC TRANSPORT PROPERTIES'
2.1 Kinetic Method

In this section, we will present the transport theory of charge carriers, (unless otherwise mentioned we shall mean electrons) in semiconductors. The purpose of any transport theory is to build a link between the measured transport coefficients and internal microscopic scattering mechanisms envisaged in the foregoing chapter. For this purpose we invoke the kinetic method. The basic idea is the following: When electrons are subjected to an external electric field, they gain energy and momentum from the applied field; further the charge carriers exchange energy and momentum, through collisions, with heat bath with which they are in intimate contact. Consequently, the electron distribution function deviates from the equilibrium value. Then in steady state, the rate of change of the distribution of electrons due to applied field must balance the rate of change due to collisions, and is given by the well known Boltzmann transport equation, /1/

\[
\frac{\delta f_k}{\delta t} = \left( \frac{\delta f_k}{\delta t} \right)_F + \left( \frac{\delta f_k}{\delta t} \right)_C = 0 .
\]  

(2.1.1)

The first and second term on r.h.s of (2.1.1) are due to field and collisions, respectively. The collision term arises due to the various scattering mechanisms viz.
impurities (I), lattice (L) and interelectronic collisions (e-e). This is given by

\[
\frac{\delta f_k}{\delta t} = \left( \frac{\delta f_k}{\delta t} \right)_I + \left( \frac{\delta f_k}{\delta t} \right)_L + \left( \frac{\delta f_k}{\delta t} \right)_{e-e}.
\]

Further, we have assumed that the phonons are in thermal equilibrium at lattice temperature and the phonon distribution (1.2.7) is unaffected by the applied field.

The quantitative aspects of the transport properties can be obtained by solving the Boltzmann equation. An analytical solution of (2,1,1) is exceedingly complicated and one needs to introduce model distribution functions and simplifying assumptions /17,44,45/. A numerical solution of (2,1,1) has been obtained using Monte Carlo technique /46,47/. But in such calculations it has been generally felt that it would be difficult to ascertain a priori the effects which individual processes will produce on the distribution function. In view of this, we shall work with a model distribution function. Frohlich and Paranjape (here onwards called as F-P) /48/ assumed a Maxwellian distribution function, displaced in momentum space i.e.,

\[
f_k = \Lambda \exp \left[ -\hbar^2 \left( \frac{|k-k_0|}{2mk_BT_e} \right)^2 / 2m_kT_e \right].
\]
as a solution of the Boltzmann equation. In (2.1.3) \( h_k^0 \) is the displacement of electron momentum due to applied field \( P \), and \( T_e \) is the 'electron temperature'. This distribution function can be expanded in Legendre polynomials, and truncating it to the first order, for \( \hbar^2 k^2 / 2mk_B T_e \ll 1 \), we write

\[
f_k = f_0 + f_1 \quad (2.1.4)
\]

where

\[
f_1 = (h_k k^0 / m k_B T_e) f_0 \quad (2.1.4a)
\]

and \( f_0 \) is the spherical part of the distribution function, which is Maxwellian at electron temperature \( T_e \). Usually (2.1.4) is a reasonable approximation for most of the situations which we will consider.

Now, we shall give F-P approach to the transport problem. In interelectronic collisions the momentum and energy are conserved i.e.

\[
\sum_k \hbar k \left( \frac{\partial f_k}{\partial t} \right)_{e-e} = 0 \quad (2.1.5)
\]

and

\[
\sum_k \hbar k \left( \frac{\partial f_k}{\partial t} \right)_{e-e} = 0 \quad (2.1.6)
\]

Making use of (2.1.1), (2.1.2), (2.1.5) and (2.1.6) we
Equations (2.1.7) and (2.1.8) are, respectively, called as the momentum and energy balance equations. Converting the summations to the integral, and using the distribution function (2.1.4), the field terms in (2.1.7) and (2.1.8) yield, respectively, $e_{\text{Fn}}$ and $e_{\text{Vd}}$. $\text{En}$ /48/, where $\text{Vd}$ is given by $(\hbar k_0/m)$. Now (2.1.7) and (2.1.8) can be written as:

$$- \int h_k \left[ \left( \frac{\partial h_k}{\partial t} \right)_L + \left( \frac{\partial h_k}{\partial t} \right)_I \right] \, d^3k = e_{\text{Fn}} \quad (2.1.9)$$

and

$$- \int E_k \left[ - \frac{\partial f_k}{\partial t} \right] \, d^3k = e_{\text{Vd}} \cdot \text{En} \quad (2.1.10)$$

These two equations facilitate the calculation of electrical transport properties. In F-P method one needs to invoke distribution function in the beginning only to calculate $\left( \frac{\partial f_k}{\partial t} \right)_L, I$. There exists another method /17,49/,

* In view of the elastic nature of the impurity scattering energy loss rate due to impurity does not arise.
which is exactly equivalent to F-P approach, wherein the rate of loss of momentum and energy of an electron to the lattice and impurity* are averaged over the electron distribution function. Then (2.1.9) and (2.1.10) lead to

$$\left( \frac{d\mathbf{n}_k}{dt} \right) = - \frac{\int \left\{ (\frac{d\mathbf{k}}{dt})_L + (\frac{d\mathbf{h}_k}{dt})_I \right\} f_k d^3k}{\int f_k d^3k} = e\mathbf{F} \quad (2.1.11)$$

and

$$\left( \frac{d\mathbf{p}_k}{dt} \right) = - \frac{\int (\frac{d\mathbf{p}_k}{dt})_L f_k d^3k}{\int f_k d^3k} = e\mathbf{V}_d \cdot \mathbf{F} \quad . \quad (2.1.12)$$

This method is convenient than the F-P approach because the distribution function need not be invoked until the last averaging process over $f_k$.

In pausing, it is expedient to know more about the displaced Maxwellian distribution function (2.1.3). This form of distribution requires electron density so high that the rate of energy exchange between electrons through the mutual collisions, is large compared with the rate of energy exchange between electrons and lattice. Then electrons will be in thermal equilibrium at a temperature $T_e$ which may be

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* The foot note in the preceding page.
higher than lattice temperature $T$. Then electrons are said to be hot. The situation in which $T_e$ goes below $T$, has been demonstrated by Paranjape and co-workers /50,51/ and this is called as electron cooling. This requires the inclusion of higher order terms in the distribution function.
PART I
2.2 Parabolic Band with Spherical Energy Surface

In this section we shall calculate expressions (2.1.11) and (2.1.12) for a simple parabolic band model with spherical energy surface having conduction band minimum at k = 0. Further, we shall restrict ourselves to the scattering of electrons within the central valley.

2.2a Ionized Impurity Scattering

It is well known that the ionized impurity scattering is elastic in view of the greater mass of the ionized impurity atom than that of an electron. Electron loses only momentum in the scattering process. Using the matrix element given by (1.3.2) the rate of loss of momentum of electron is /52/

\[
\langle \frac{dhk}{dt} \rangle = \frac{-\hbar^2 N N \epsilon^4}{2^{1/2} \epsilon_o^2 m^{1/2} \epsilon_b^{3/2}} \left[ \ln(1+z) - z/(1+z) \right].
\]

Averaging this over the steady state distribution (2.1.4) the momentum loss rate is

\[
\langle \frac{dhk}{dt} \rangle = \frac{2^{3/2} N N \epsilon^4 m^{1/2} \epsilon_d}{3 \pi^{1/2} \epsilon_o^2 (k_B \epsilon) B^{3/2}} \frac{6 \hbar^2 \epsilon_B^2 \epsilon_o}{e^2 n^2} \left( \ln \frac{6 \hbar^2 \epsilon_B^2 \epsilon_o}{e^2 n^2} - 1 \right),
\]

... (2.2.2)
where $N_i$ stands for the number of impurities. It was assumed that $z = \frac{4k^2}{R^2} \gg 1$.

2.2b Lattice Scattering

Now, we shall calculate the average momentum and energy loss rate due to lattice scattering. We have already mentioned in first chapter that lattice scattering occurs both by one-phonon (1p) and two-phonon (2p) processes. Then, we can write

$$
\left( \frac{d\mathbf{k}}{dt} \right)_L = \left( \frac{d\mathbf{k}}{dt} \right)_{1p} + \left( \frac{d\mathbf{k}}{dt} \right)_{2p}
$$

(2.2.3)

and

$$
\left( \frac{dE}{dt} \right)_L = \left( \frac{dE}{dt} \right)_{1p} + \left( \frac{dE}{dt} \right)_{2p}.
$$

(2.2.4)

Therefore in (2.1.11) and (2.1.12), on r.h.s., we have to calculate average momentum and energy loss rates due to one-phonon and two-phonon processes. We briefly outline the calculations due to the former process, since there exists sufficient calculation in the literature /17/. We will deal in detail with the two-phonon processes, in particular, scattering by two-short wavelength phonons for the reasons mentioned in the last three sections of the chapter.
A. One-Phonon Processes

We shall now consider momentum and energy loss rates due to one-phonon processes described by the interaction (1.3.6). These loss rates are well known and are given by

\[ \left( \frac{d\mathbf{k}}{dt} \right)_{\text{lp}} = \frac{\hbar}{q} \mathbf{g}_k \left[ P_a(k \rightarrow k + q) - P_e(k \rightarrow k - q) \right] \]

... (2.2.5)

and

\[ \left( \frac{dE}{dt} \right)_{\text{lp}} = \frac{\hbar}{q} \mathbf{g}_k \left[ P_a(k \rightarrow k + q) - P_e(k \rightarrow k - q) \right], \]

... (2.2.6)

where \( \mathbf{g}_k = (q, \mathbf{k}) \mathbf{k}; \mathbf{k} \) being the unit vector associated with \( k \). The probabilities of absorption, \( P_a \), and emission, \( P_e \), of one-phonon process are well known and are given by

\[ P_a = \frac{2\pi}{\hbar} \left| \langle k + q, N_q - 1 \mid H_{\text{int}}(i) \mid k, N_q \rangle \right|^2 \times \delta(E_{k+q} - E_k - \hbar\mathbf{g}_q) \]

... 2.2.7

and

\[ P_e = \frac{2\pi}{\hbar} \left| \langle k - q, N_q + 1 \mid H_{\text{int}}(i) \mid k, N_q \rangle \right|^2 \times \delta(E_{k-q} - E_k + \hbar\mathbf{g}_q) \]

... 2.2.8
We now insert (2.2.7) and (2.2.8) in (2.2.5) and (2.2.6) and change the summation over \( g \) into an integration by well-known transformation

\[
\mathcal{M} \rightarrow (1/8\pi^3) \int \int q^2 \sin \theta \, d\theta \, d\phi , \quad (2.2.9)
\]

where \((q, \theta, \phi)\) is the polar co-ordinate representation of \( q \) w.r.t. \( k \). Then the absolute square of the matrix elements contained in (2.2.7) and (2.2.8) are substituted depending on the types of one-phonon processes envisaged in section (1.3). Next, we perform the angular integration, making use of the momentum and energy conservation conditions given by (1.3.8) and (1.3.10), respectively. In doing so it becomes essential to use one of the properties of Dirac-delta function \( /16/ \), namely, \( \int_{-\infty}^{\infty} \delta(x) \delta(x - a) = \delta(a) \). Further, the conditions (1.3.8) and (1.3.10) put upper and lower limits on phonon wave vectors involved in the scattering as described in section (1.3). Between these limits, integration over \( q \) is performed. The momentum and energy loss rates so obtained are averaged making use of the distribution function (2.1.4) by considering the field direction as the polar axis. This procedure leads to the following expressions for the various one-phonon processes described in (1.3).

(i) **Acoustic Phonon Deformation Potential Scattering**

Making use of (1.3.14), the average momentum and
energy loss rates, due to acoustic deformation potential type of scattering, are respectively /52, 17/

\[
\left\langle \frac{\text{d}k}{\text{d}t} \right\rangle_{\text{ac-def}} = - \frac{2^{7/2} \varepsilon_1^2 m^{5/2} k_B \beta_1^2 v_d T_e T_{e}^{1/2}}{3 \pi^{3/2} \rho s_1^2 \hbar^4}
\]

and

\[
\left\langle \frac{\text{d}E_k}{\text{d}t} \right\rangle_{\text{ac-def}} = - \frac{2^{7/2} \varepsilon_1^2 m^{5/2} k_B \beta_1^2 \varepsilon_1 v_d (k_B T_e)^{1/2}}{3 \pi^{3/2} \rho \hbar^4}
\]

where \( \rho = M N \).

(ii) **Acoustic Phonon Piezoelectric Scattering**

Making use of (1.3.21) for the interaction matrix element we get /53, 54/

\[
\left\langle \frac{\text{d}h}{\text{d}t} \right\rangle_{\text{ac-piezo}} = \frac{16 \pi m^{3/2} e^2 \beta_1^2 a_1 v_d (k_B T_e)^{1/2}}{3 (2)^{1/2} \hbar^2 \rho \varepsilon_0^2}
\]

and

\[
\left\langle \frac{\text{d}E_k}{\text{d}t} \right\rangle_{\text{ac-piezo}} = - \frac{32 (2 \pi k_B)^{1/2} \rho^2 e^2 m^{3/2} a_1 (k_B T_e)^{1/2}}{\varepsilon_0^2 \hbar^2 \rho}
\]

In the above two cases we have made use of
equipartition of energy for the lattice oscillators i.e.,
\[ N_q = \frac{k_B T}{N_q} \] and also the fact that \[ \overline{W_q} = S_1 q. \]

(iii) Polar Optical Mode Scattering

Similarly, making use of (1.3.20) one gets the average momentum and energy loss rates due to polar optical modes /55/, and they are given by

\[
\left\langle \frac{\text{d} p}{\text{d} t} \right\rangle_{\text{po}} = - \frac{(2k_B e)^{1/2} e^2 m^{3/2} (\varepsilon_{\infty}^{-1} - \varepsilon_{\infty}^{-1}) N V \int M_1(x_e/2)}{3 \hbar^2 \pi^{1/2}}
\]

and

\[
\left\langle \frac{\text{d} E}{\text{d} t} \right\rangle_{\text{po}} = - \frac{2^{1/2} e m^{1/2} (k_B e)^{3/2} (\varepsilon_{\infty}^{-1} - \varepsilon_{\infty}^{-1}) N M_2(x_e/2)}{\pi^{1/2} \hbar^2}
\]

where

\[
M_1(x_e/2) = x_e^{3/2} e^{x_e/2} \left\{ (e^{x_e} - 1) K_1(x_e/2) \right\}
\]

and

\[
M_2(x_e/2) = (e^{x_e} - 1) x_e^{1/2} e^{x_e/2} K_0(x_e/2)
\]
and \( e \) is the optical phonon equivalent temperature defined by \( \hbar W = k_B e \), \( x = e/T \), \( x_e = e/T_e \) and \( N \) is the polar optical phonon equilibrium distribution function; \( K_0 \) and \( K_1 \) are modified Bessel functions /56/. Further it is assumed that \( W_q \) is independent of the wave vector (i.e., \( W_q = W \)).

(iv) Non-Polar Optical Mode Scattering

Electron scattering by non-polar optical modes in polar semiconductors was first treated by Stratton /57/. Assuming \( W_q \) to be independent of \( q \) and using (1.3.19) one gets /51/

\[
\left\langle \frac{\text{d}n_k}{\text{d}t} \right\rangle_{\text{npo}} = - \frac{2(DK)^2 m^{5/2} v_d N G_1(x_e/2)}{3 \pi^{3/2} \hbar^2 \rho (k_B e)^{1/2}}
\]  \hspace{1cm} (2.2.16)

and

\[
\left\langle \frac{\text{d}E_k}{\text{d}t} \right\rangle_{\text{npo}} = - \frac{(DK)^2 (k_B e)^{1/2} m^{3/2} N G_2(x_e/2)}{\pi^{3/2} \hbar^2 \rho},
\]  \hspace{1cm} (2.2.17)

where

\[
G_1(x_e/2) = e^{x_e/2} (x_e/2)^{3/2} \left[ (e^{x_e} - 1) K_1(x_e/2) + (e^{x_e} + 1) \left\{ (4/x_e) K_1(x_e/2) + K_0(x_e/2) \right\} \right].
\]  \hspace{1cm} (2.2.16a)
Here $e$, $x$ and $x_e$ have the same meaning as in polar optical mode scattering case.

B. Two-phonon Scattering /58,59/

Let us consider a semiconductor with the simple band model described in the beginning of section (2.2). The transition probability for an electron going from an initial state $k$ to a final state $k'$, with the assistance of two phonons, may be written as

$$P_{aa} = \frac{2\pi}{\hbar} \left| \langle k+q+q', N_q, N_{q'} \mid H_{int}(ii) \mid k, (N_q+1), (N_{q'}+1) \rangle \right|^2$$

$$\times \delta(E_{k+q+q'} - E_k - \hbar (N_q + N_{q'})) \quad (2.2.18)$$

$$P_{ee} = \frac{2\pi}{\hbar} \left| \langle k-q-q', (N_q+1), (N_{q'}+1) \mid H_{int}(ii) \mid k, N_q, N_{q'} \rangle \right|^2$$

$$\times \delta(E_{k-q-q'} - E_k + \hbar (N_q + N_{q'})) \quad (2.2.19)$$

$$P_{ae} = \frac{2\pi}{\hbar} \left| \langle k+q-q', N_q, (N_{q'}+1) \mid H_{int}(ii) \mid k, (N_q+1), N_{q'} \rangle \right|^2$$

$$\times \delta(E_{k+q-q'} - E_k - \hbar (N_q + N_{q'})) \quad (2.2.20)$$
and

\[ P_{ea} = \frac{2\pi}{\hbar} \left| \langle k, q+q', (N+1), N_g', \int \right| \int | k, N_g, (N_g+1) \rangle \right|^2 \]

\[ \times \delta (E_k - q+q', - E_{k+q} - (N - N_g')) \]

(2.2.21)

where the subscripts aa, ee, ae and ea refer to absorption of two phonons, emission of two phonons, one phonon absorption—another phonon emission and one phonon emission—another phonon absorption, respectively. The rate of loss of momentum and energy to the lattice due to the two-phonon process described by equations (2.2.18) to (2.2.21) may be written, respectively, as

\[
(\frac{d(\hbar k)}{dt})_{2p} = \sum_{q, q'} \left\{ \hbar (q+q') \left[ P_{aa}(k \rightarrow k+q+q') - P_{ee}(k \rightarrow k-q-q') \right] + \hbar (q-q') \left[ P_{ae}(k \rightarrow k+q-q') - P_{ea}(k \rightarrow k-q+q') \right] \right\}
\]

... (2.2.22)

and

\[
(\frac{dE_k}{dt})_{2p} = \sum_{q, q'} \left\{ \hbar (q+q') \left[ P_{aa}(k \rightarrow k+q+q') - P_{ee}(k \rightarrow k-q-q') \right] + \hbar (q-q') \left[ P_{ae}(k \rightarrow k+q-q') - P_{ea}(k \rightarrow k-q+q') \right] \right\}
\]

... (2.2.23)
where \((g + g')_k = [(g + g') \cdot \hat{k}] \hat{k} = \hat{k} (g + g') \cos \theta\) is the angle between \(k\) and \(g + g'\) and \(\hat{k}\) is a unit vector along \(k\). To proceed with the further calculation, we shall assume that \(g + g' = \Omega\) or \(g - g' = \Omega\) corresponding to the two types of situations described in (2.2.22) and (2.2.23). Now we substitute (1.3.23), (2.2.18) to (2.2.21) in (2.2.22) and (2.2.23) and replace the summation over \(g\) and \(Q\) by integration (i.e. \(N \rightarrow \int_{Q} \frac{1}{8\pi^{3}} \int d^{3}q\) and \(\frac{1}{8\pi^{3}} \int d^{3}Q\)).

Thus we get

\[
\left( -\frac{d\mathbf{k}}{dt} \right)_{2p} = \left( \frac{1}{8\pi^{3}} \int d^{3}Q \int d^{3}q \right) \left| V_{2}(g, Q-g) \right|^{2} \hbar Q_{k} \{ N \frac{N}{N} d-g \} \delta(E_{k} - E_{k} - \hbar (W + W_{Q-g}))

- \frac{(N+1)(N Q - g + 1)}{(N Q + g + 1)} \delta(E_{k} - E_{k} + \hbar (W + W_{Q+g}))

+ \left( \frac{1}{8\pi^{3}} \int d^{3}Q \int d^{3}q \right) \left| V_{2}(g, Q+g) \right|^{2} \hbar Q_{k} \{ N \frac{N}{N} d+g \} \delta(E_{k} - E_{k} - \hbar (W - W_{Q+g}))

- \frac{(N+1)(N Q + g)}{(N Q - g + 1)} \delta(E_{k} - E_{k} + \hbar (W - W_{Q+g})) \}

(2.2.24)

and

\[
\left( -\frac{d\mathbf{E}_{k}}{dt} \right)_{2p} = \left( \frac{1}{8\pi^{3}} \int d^{3}Q \int d^{3}q \right) \left| V_{2}(g, Q-g) \right|^{2} \hbar (W + W_{Q-g})

\{ N \frac{N}{N} d-g \} \delta(E_{k} - E_{k} - \hbar (W + W_{Q-g}))

- \frac{(N+1)(N Q - g + 1)}{(N Q + g + 1)} \delta(E_{k} - E_{k} + \hbar (W + W_{Q-g+g}))

- \frac{(N+1)(N Q + g + 1)}{(N Q - g + 1)} \delta(E_{k} - E_{k} + \hbar (W + W_{Q+g})) \} \}

(2.2.24)
Since we are interested in phonons of short wavelength region, belonging to the same branch, it is reasonable to assume that $W_q$ and $W_{q+Q}$ are independent of the phonon wave vectors in as much as some of the phonon branches are relatively flat in the short wavelength region in certain semiconductors. Thus, we may write $W_q = W_{k'} = W_s/2$. $W_s$ is the two-phonon frequency in the short wavelength region.

Further $|V_2(q, q+q)|^2$ is independent of $q$ and $Q$ and it may be taken out of the integrals in (2.2.24) and (2.2.25).

The phonon distribution functions are also independent of $q$ and as the phonons are in thermal equilibrium we may write

$$N_q = N_q, N_{q+Q} = N_q and N_{q+1} = N_q \exp \left( \frac{-\hbar \omega}{k_B T} \right).$$

Then in (2.2.24) and (2.2.25) the $q$ integration is straightforward and we get

$$\int_{q=0}^{q_z} d^3q = \left( \frac{4\pi}{3} \right) (q_z^3 - q_0^3) = \left( \frac{4\pi}{3} \right) q_z^3.$$

$q_0$ denotes the value of $q$ at which the phonon branch starts.
flattening and \( q_z \) is the value at zone edge. In order to integrate over \( \Omega \), we express \( d^3 \Omega \) in terms of polar coordinates \((Q, \theta, \phi)\) w.r.t. \( k \) as the polar axis. Then, we may write (2.2.24) and (2.2.25)

\[
\left( \frac{d^2 \mathbf{k}}{dt} \right)_{2p} = \frac{(hD_s)^2 q_z^3 N N^i \xi}{3 \left( 2 \pi a^2 \right)^2 \pi^3} \left\{ \left( M_{1+} - e^{-i \frac{hW_s}{k_B T}} M_{1-} \right) * \left( M_{2+} - e^{-i \frac{hW_s}{k_B T}} M_{2-} \right) \right\} \exp \left( i \frac{hW_s}{k_B T} \right)
\]

and

\[
\left( \frac{d^2 \mathbf{A}}{dt} \right)_{2p} = \frac{(hD_s)^2 q_z^3 W_s N N^i}{3 \left( 2 \pi a^2 \right)^2 \pi^3} \left( I_{1+} - e^{-i \frac{hW_s}{k_B T}} I_{1-} \right).
\]

where

\[
M_{1+} = \int Q^3 dQ \int \cos \theta \delta(E_{k+Q} - E_k + \frac{hW_s}{k_B T}) \sin \theta d\theta,
\]

\[
M_{2+} = \int Q^3 dQ \int \cos \theta \delta(E_{k+Q} - E_k) \sin \theta d\theta \quad (2.2.30)
\]

and

\[
I_{1+} = \int Q^2 dQ \int \sin \theta \delta(E_{k+Q} - E_k + \frac{hW_s}{k_B T}) d\theta. \quad (2.2.31)
\]

Now we express the Dirac delta function contained in (2.2.30) and (2.2.31) respectively, as

\[
\delta(E_{k+Q} - E_k + \frac{hW_s}{k_B T}) = \frac{m}{\hbar^2 k Q} \delta(\cos \phi \pm \frac{Q}{2k} \mp \frac{mW_s}{\hbar k Q})
\]

\[
\ldots \quad (2.2.32)
\]
and
\[
\delta\left(E_{k+Q} - E_k\right) = \frac{m}{\hbar^2 k_Q} \delta(\cos \theta \pm \frac{Q}{2k}) \ , \quad (2.2.33)
\]

As mentioned in the earlier section we make use of the delta function and integrate over \( \theta \) in (2.2.30) and (2.2.31). In order to perform \( Q \) integration in these expressions we obtain the limits of integration from the arguments of delta functions which ensure the energy conservation. The limits of integration are the following:

\[
M_{1+}, I_+ \implies Q_l = -k + (k^2 + \frac{2mW}{\hbar})^{1/2},
\]
\[
Q_u = k + (k^2 + \frac{2mW}{\hbar})^{1/2} \quad (2.2.34)
\]
\[
M_{1-}, I_- \implies Q_l = k - (k^2 - \frac{2mW}{\hbar})^{1/2},
\]
\[
Q_u = k + (k^2 - \frac{2mW}{\hbar})^{1/2} \quad (2.2.35)
\]
\[
M_{2+}, M_{2-} \implies Q_l = 0,
\]
\[
Q_u = 2k \quad , \quad (2.2.36)
\]

where subscripts \( l \) and \( u \) denote the lower and upper limits, respectively. Now we simplify \( M_{1+}, M_{1-}, M_{2+}, M_{2-}, I_{1+} \) and \( I_{1-} \) by integrating over \( Q \) and substituting in (2.2.28) and (2.2.29), we get
Proceeding further, we shall now calculate the average rate of loss of momentum and energy. The average loss rates can be written as

$$\left\langle \frac{\partial \mathbf{H}_k}{\partial t} \right\rangle_{2p} = \frac{(D_{sm})^2 q_{2z}^3 \hat{k} N N'}{3 \left( \hbar \rho a^2 W_s \right)^2 \pi}$$

and

$$\left\langle \frac{\partial E_k}{\partial t} \right\rangle_{2p} = -\frac{D_{sm}^2 q_{2z}^3 m_{3/2} \beta N N'}{3 \left( 2 \right)^{1/2} \pi \rho a^4 \hbar W_s}$$

Proceeding further, we shall now calculate the average rate of loss of momentum and energy. The average loss rates can be written as

$$\left\langle \frac{\partial \mathbf{H}_k}{\partial t} \right\rangle_{2p} = \hat{k}_0 \int \frac{\partial \mathbf{H}_k}{\partial t} \cdot \hat{k}_0 f_k d^3k / \int f_k d^3k$$

and

$$\left\langle \frac{\partial E_k}{\partial t} \right\rangle_{2p} = \int (\frac{\partial E_k}{\partial t}) f_k d^3k / \int f_k d^3k. \quad (2.2.39)$$

Now, we substitute (2.1.4) for $f_k$ and express $d^3k$ in terms of polar co-ordinates $(k, \gamma, \psi)$ w.r.t. $\hat{k}_0$ as the polar axis; then we express $k$ in terms of $E$ making use of the parabolic
relation (1.1,8) and substitute (2.2.37) and (2.2.38) in (2.2.39) and (2.2.40), respectively, and integrate over the angular variable \( \gamma \) and \( \psi \). Then we get

\[
\left\langle \frac{dk}{dt} \right\rangle = - \frac{2^{3/2} D_s^2 \frac{m^{3/2}}{h^2} \frac{a^3}{p^2} \frac{k_o}{N^2} N^1}{9 \pi^{7/2} \hbar^2 \frac{2^2}{a^2} \frac{4}{(k_B T_e)^{5/2}}}
\]

\[
x \left\{ \int_0^\infty E^{3/2} (E+\hbar W_s)^{1/2} e^{-E/k_B T_e} dE 
+ \frac{\hbar W_s}{k_B T} \int_0^\infty E^{3/2} (E-\hbar W_s)^{1/2} e^{-E/k_B T_e} dE 
+ 2 e^{\frac{\hbar W_s}{2k_B T}} \left[ \int_0^\infty E^2 e^{-E/k_B T_e} dE \right] \right\}
\frac{\hbar W_s}{2}

\]

\[ \ldots \quad (2.2.41) \]

and

\[
\left\langle \frac{dE_k}{dt} \right\rangle = - \frac{2^{1/2} D_s^2 \frac{m^{3/2}}{h^2} \frac{a^3}{p^2} \frac{k_o}{N^2} N^1}{3 \pi^{7/2} \frac{2^2}{a^2} \frac{4}{(k_B T_e)^{3/2}}}
\]

\[
x \left\{ \int_0^\infty E^{1/2} (E+\hbar W_s)^{1/2} e^{-E/k_B T_e} dE 
- \frac{\hbar W_s}{k_B T} \left[ \int_0^\infty \frac{dE}{\hbar W_s} E^{1/2} (E-\hbar W_s)^{1/2} e^{-E/k_B T_e} \right]\right\}
\ldots \quad (2.2.42)
\]

Let us now write \( y' = E/k_B T_e \) in (2.2.41) and (2.2.42). Then
we shall make change of variable from \( y' \rightarrow y' + \frac{2nW}{k_BT_e} \) in the second integral of both (2.2.41) and (2.2.42) and \( y' \rightarrow y' + (N_{W_s}/2k_BT_e) \) in the third integral of (2.2.41).

We shall now define \( \Theta_s = \frac{N_{W_s}}{k_B}, \frac{\Theta_s}{T_e} \text{ and } r = \frac{\Theta_s}{T}; \) then rewrite (2.2.41) and (2.2.42) as

\[
\langle \frac{dk}{dt} \rangle_{2p} = - \frac{2 \pi k_0^2 q_s^3 m^{3/2} N N'}{g} \frac{N}{r/2} \left( \frac{\pi}{2} \right)^2 a^4 \left( k_B \Theta_s \right)^{3/2} \left\{ G_1\left( \frac{r}{2} \right) + G_2\left( \frac{r}{2} \right) \right\}
\]

\[
\text{(2.2.43)}
\]

and

\[
\langle \frac{dE_k}{dt} \rangle_{2p} = - \frac{p_s^2 q_s^3 m^{3/2} N N'}{3 \left( k_B \Theta_s \right)^{1/2}} \frac{N}{r/2} \left( \frac{\pi}{2} \right)^2 a^4 G_2\left( \frac{r}{2} \right),
\]

\[
\text{(2.2.44)}
\]

where \( G_1(r/2) \) and \( G_2(r/2) \) are of the same form as defined in (2.2.16a) and (2.2.17a), respectively, and

\[
G_3(r/2) = 2(r/2)^{3/2} e^{-2(r-r_e)^2} \left( 1 + 4r_e^{-1} + 8r_e^{-2} \right).
\]

\[
\text{(2.2.43a)}
\]

The two expressions (2.2.43) and (2.2.44) are the basic results of the present work. These two expressions together with the similar loss rates due to one-phonon
processes and impurity will facilitate calculations of various transport properties. In the next section we will consider the method of obtaining zero field mobility ($\mu_0$), warm electron coefficient ($\beta$), energy relaxation time ($\tau_e$), electron drift velocity ($V_d$), and electron temperature ($T_e$) from the momentum and energy balance equations.
2.3 Method of Obtaining $\nu_0, \tau_e, \beta, V_d$ and $T_e$ /17/

Let us first consider zero field mobility. The drift mobility of an electron is defined as the drift velocity per unit electric field. The total average momentum loss rate is obtained by addition of average momentum loss rates due to all individual scattering mechanisms and this is equated to $eF$ as in (2.1.11). This expression relates $V_d$, $F$ and $T_e$. It is then possible to calculate $V_d/F$ in the limit as $F \to 0$. This is the well known zero field mobility.

Next, we shall consider energy relaxation time $\tau_e$ and warm electron coefficient $\beta$. It is convenient to describe the energy loss process of electrons by invoking the energy relaxation time. This concept may be introduced by writing the average rate of change of energy of electron as

$$\left\langle \frac{dE}{dt} \right\rangle = \left\langle \frac{dE}{dt} \right\rangle_F + \left\langle \frac{dE}{dt} \right\rangle_L$$

$$= eV_d \cdot F - \frac{3 k_B}{2} \left( \frac{T_e - T}{T_e} \right), \quad (2.3.1)$$

where $3k_B (T_e - T)/2$ is the average excess energy of electrons over the thermal equilibrium value and $\tau_e$ is introduced as decay time of heated spherical part, $f_0$, of the
distribution function (2.1.4). In the steady state, it is well known that the power loss

\[ P = \left\langle \frac{\partial E}{\partial t} \right\rangle_L = \sigma^* (T_e) F^2, \] (2.3.2)

where \( \sigma^* (T_e) \) is the conductivity at electron temperature \( T_e \). Now for small electric field, we may expand \( \sigma^* (T_e) \) in Taylor series around \( (T_e - T) \) as

\[ \sigma^* (T_e) = \sigma(T) \left\{ 1 + \frac{T_e - T}{\sigma(T)} \left[ \frac{d \sigma(T_e)}{dT_e} \right]_{T_e = T} \right\} . \] (2.3.3)

Taking the product of the total average momentum and energy loss rate equations envisaged in section (2.2) it is straightforward but lengthy procedure to show that for small electric field (i.e. in the warm electron range) \( T_e - T \propto F^2 \). Making use of this argument, we may rewrite (2.3.3) as

\[ \sigma^* (T_e) = \sigma(T) (1 + \beta F^2), \] (2.3.4)

where

\[ \beta(T) = \frac{T_e - T}{\sigma(T) F^2} \left[ \frac{d \sigma(T_e)}{dT_e} \right]_{T_e = T} . \] (2.3.5)

In (2.3.5) \( \beta \) is independent of \( F \). The equation (2.3.4)
may be expressed in terms of mobility as

\[ \mu (F) = \mu_0 (1 + \beta F^2) \]  \hspace{1cm} (2.3.6)

and in this sense \( \beta \) is a measure of departure of field dependent mobility from its Ohmic value. In the warm electron region, it is evident from (2.3.1) to (2.3.6) that

\[ \frac{1}{\tau_e} = \frac{2}{3k_B} \left( \frac{3}{dT_e} \left\langle \frac{dE}{dt} \right\rangle_L \right) T_e = T \]

\[ = \frac{2}{3k_B} \left( \frac{dP}{dT_e} \right) T_e = T \]  \hspace{1cm} (2.3.7)

Now combining (2.3.5) and (2.3.7) we get

\[ \beta = \frac{2 e \mu_0 \tau_e}{3 k_B T} \]  \hspace{1cm} (2.3.8)

Thus, one can use (2.3.7) to calculate energy relaxation time \( \tau_e \), which in turn can be used along with \( \mu_0 \) to calculate warm electron coefficient \( \beta \).

Now we will consider the calculation of \( V_d \) and \( T_e \) as a function of electric field \( F \). In order to achieve this we make use of the two simultaneous equations (2.1.11) and (2.1.12). These two equations may be formally written respectively, as
\[
\frac{\mathrm{eF/V}_d}{a} = Z_1 (T_e, T) \quad (2.3.9)
\]

and
\[
\mathrm{eFV}_d = Z_2 (T_e, T), \quad (2.3.10)
\]

where \(Z_1 (T_e, T)\) and \(Z_2 (T_e, T)\) are known functions. From these two equations, we get
\[
V_d^2 = \frac{Z_2 (T_e, T)}{Z_1 (T_e, T)} \quad (2.3.11)
\]

and
\[
(eF)^2 = Z_2 (T_e, T) \cdot Z_1 (T_e, T). \quad (2.3.12)
\]

Now for various values of \(T_e\) and a fixed value of \(T\) both \(Z_1 (T_e, T)\) and \(Z_2 (T_e, T)\) are calculated. Making use of these calculated values in (2.3.11) and (2.3.12) it is possible to obtain \(V_d\) and \(T_e\) as a function of \(F\).
2.4 Application to n-InSb

In previous sections we have given the transport theory for semiconductor with a simple band structure incorporating both one-phonon and two-phonon processes. We will apply the theory in the present section.

InSb is a polar semiconductor with conduction band minimum located at the center of Brillouin zone and the constant energy surfaces are approximately spherical. The conduction band is parabolic for electron energies less than 0.023 eV /60/. In view of these features we shall apply the theory to n-InSb, particularly below 30K for the reasons given in section (1.4).

The scattering mechanisms in InSb at low temperatures are of considerable importance in view of its application as a detector of millimeter and sub millimeter wave radiation /61/. One way of obtaining information about the possible scattering mechanisms is to compare semiconductor transport experiments with the theoretical calculations incorporating the lattice and impurity scattering mechanisms. From the existing investigations (see for details /62-64/) the following scattering mechanisms are known to be important: They are (i) acoustic-mode deformation potential type, piezoelectric type, (ii) polar optical phonon scattering, and (iii) ionized impurity scattering. As mentioned in
chapter I, these mechanisms are inadequate in describing
the energy loss process particularly below 20K. So we
incorporate the scattering due to two-short wavelength
transverse acoustic phonons (hence forth denoted by 2CA) in
view of the recent magneto-phonon experimental observations
/37/.

Assuming these scattering mechanisms and utilizing
the expressions (2.2.2), (2.2.10), (2.2.12), (2.2.14) and
(2.2.43) for momentum loss and (2.2.11), (2.2.13), (2.2.15)
and (2.2.44) for energy loss, we now write the momentum and
energy balance equations, (2.1.11) and (2.1.12), respectively,
as

\[ \frac{eF}{V_d} = \frac{2^{3/2} N I e^4 m^{1/2}}{3 \pi^{1/2} \varepsilon_o^2 (\gamma_B T_e)^{3/2}} \left( \ln \frac{6 m k_B^2 T_e^2 \varepsilon_o}{\pi e^2 h^2 n} + \frac{2^{7/2} e^2 m^{5/2} k_B^3 T_e^{1/2}}{3 \pi^{3/2} p s_l h^4} \right) \]

\[ + \frac{16 \pi m^{3/2} e^2 a_1 (k_B T_e)^{1/2}}{3 (2)^{1/2} h^2 \varepsilon_o^2 \phi} \]  

\[ + \frac{(2 k_B \varepsilon_1)^{1/2} e^2 m^{3/2} (\varepsilon_1^{1/2} - \varepsilon_o^{1/2}) N}{3 h^2 \pi^{1/2}} M_1(x_e/2) \]

\[ + \frac{2D_s^2 m^{5/2} q_z N N'}{9 \pi^{7/2} \rho^2 a_4 (k_B \varepsilon_s)^{3/2}} \left\{ G_1(x_e/2) + G_3(x_e/2) \right\} \]

..... (2.4.)
TABLE 1
Scattering mechanisms and physical parameters used in the present work in n-InSb.

<table>
<thead>
<tr>
<th>Scattering mechanism</th>
<th>Phonon equivalent temperature in K</th>
<th>Coupling constant*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Ionized impurity scattering</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2. Lattice scattering</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. One-phonon processes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Acoustic phonon</td>
<td>-</td>
<td>$E_1 = 7.2$ eV</td>
</tr>
<tr>
<td>Polar optical phonon</td>
<td>$278^\text{/63/}$</td>
<td>-</td>
</tr>
<tr>
<td>B. Two-phonon process</td>
<td>$124^\text{/65/}$</td>
<td>$D_M = 1240$ eV**</td>
</tr>
<tr>
<td>(2TA at $\omega = \infty$)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$a = 6.4789$ Å, $m = 0.0139 m_o$, $\rho = 5.82$ gm cm$^{-3}$, $\varepsilon_o = 17.5$ 
$\varepsilon_\infty = 15.88$, $S_1 = 2.3 \times 10^5$ cm s$^{-1}$, $n = 5.4 \times 10^{13}$ cm$^{-3}$, and $N_I = 6.7 \times 10^{14}$ cm$^{-3}$ /64/.

* Parameters selected in the present work.

** Note that in our published work /58,59/, we have taken $(D_M / 2) = 620$ eV in as much as a factor 2 was left over in denominator in the definition of $D_M$. 
and

\[ e_{PV_d} = \frac{2^{7/2} \varepsilon_1^{5/2} \kappa_B^{3/2} \tau^{1/2}}{\pi^{3/2} \rho \hbar^4} \left[ \frac{T_e - T}{T_e^{1/2}} \right] \]

\[ + \frac{32 (2\pi \kappa_B)^{1/2} \varepsilon_1^{2} \varepsilon_m^{3/2} a_1}{\varepsilon_0^2 \hbar^2 \rho} \left[ \frac{T_e - T}{T_e^{1/2}} \right] \]

\[ + \frac{2^{1/2} \varepsilon_2^{1/2} (\kappa_B \varepsilon_1)^{3/2}}{\pi^{1/2} \hbar^2} \left[ \varepsilon_0^{-1} - \varepsilon_1^{-1} \right] N M_2(x_e/2) \]

\[ + \frac{D_s^2 \varepsilon_2^{3/2} \varepsilon_m^{3/2}}{3 (k_B \varepsilon_1)^{1/2} \pi^{1/2} \rho^2 a^4} \quad (2.4.2) \]

Now we shall calculate numerically \( \mu_0, T_e, \beta, V_d \) and \( T_e \) following the method described in section (2.3) in the temperature range 4.2 to 30 K, using the physical parameters given in Table 1. For the purpose of calculation, we have taken the two-phonon frequency \( \omega_0 \) at the two phonon critical point \( \pi = XX \) and the corresponding wave vectors have been used in view of the relatively flat TA branch \( /67/ \). We denote simply \( D_s \) by \( D_2 \) even though \( D_s \) selected here is for the entire short wavelength region.

(i) Zero Field Mobility

The variation of \( \mu_0 \) with \( T \) is shown in figure 1 along with the experimental data \( /64/ \). Our calculations indicate that in the temperature range considered i.e. 4.2
Zero field mobility vs lattice temperature in InSb. Theoretical: solid line. Experimental data: 0 ($n = 5.4 \times 10^{13} \text{ cm}^{-1}$) /64/.
to 30K only ionized impurity scattering is the dominant momentum loss process in conformity with the existing analysis /64,68/. Further, it is evident from our calculations that both one-phonon and two-phonon processes make insignificant contributions to $\mu_0$. For eg. $\mu_0$ (due to ZTA) at 25K is $6.6 \times 10^3 \text{ cm}^2 \text{ v}^{-1} \text{ s}^{-1}$ whereas the observed $\mu_0 = 3.2 \times 10^5 \text{ cm}^2 \text{ v}^{-1} \text{ s}^{-1}$, and that due to one-phonon mechanisms are two or three order of magnitude higher than the observed one /69/. Moreover for lattice scattering mechanisms $\mu_0$ decreases with increase of temperature whereas for ionized impurity scattering it is an increasing function of temperature. In the temperature range 20-30K, the agreement between theory and experiment is reasonable and for temperatures below 15K there is departure and the exact mechanism for mobility is not known. The suggestion of Kinch /64/, that electron-electron interaction plays an important role in this range, is yet to be tested. However, we wish to point out that the two-phonon mechanism in question does not play a significant role in the momentum loss in the temperature range 4.2 to 30K.

(ii) **Energy Relaxation Time ($\tau_e$) /58/**

We have seen that $\tau_e$ is proportional to the temperature derivative of power loss (P) through the expression (2.3.7) in the warm electron range. We have calculated
FIGURE 2

\( \frac{dP}{d\tau_e} \) (W K\(^{-1}\))

\( \tau_e \) (K)

FIGURE 2
(dP/dT)T=T vs (100/T_e) in n-InSb. Solid lines represent theoretical calculations due to: (1) acoustic + polar optical +ZA, (2) ZTA and (3) polar optical. Experimental data: O (n=5.4x10^{13} \text{cm}^{-3}) , X (n=2.2x10^{14} \text{cm}^{-3}) , □ (n=1.1x10^{15} \text{cm}^{-3}) , ▽ (n=6.8x10^{13} \text{cm}^{-3}) /35/ and △ (n=5.4x10^{13} \text{cm}^{-3}) /64/
and plotted against $T_e$ (See Fig. 2) for various independent processes (curve f: acoustic deformation + piezoelectric type, curve e: polar optical, curve c: ZTA) as well as their combinations (curve d: acoustic + polar optical, curve b: acoustic + ZTA and curve a: acoustic + polar optical + ZTA). The experimental results in the range of 1.5 to 30K, of the $(dP/dT_e)_{T_e=T}$ as a function of $T_e$ have been published by many authors /35,62-64,70/. For the purpose of comparison we have shown the experimental data of Sandercock /35/, (for carrier concentrations, viz, $n = 5.4 \times 10^{13}$, $2.2 \times 10^{14}$, $1.1 \times 10^{15}$ and $6.8 \times 10^{13}$ cm$^{-3}$) and Kinch /64/. It is interesting to note that in the temperature range 10 to 20K there is good agreement between curve (a) and the experimental data. The curve (c) indicates that in the temperature range of 12 to 18K the powerloss due to ZTA phonon scattering is dominant over the one-phonon scattering mechanisms and the sudden increase in the observed powerloss is accounted for, in this temperature range by scattering due to ZTA. Curve (d) clearly shows that the one-phonon processes (acoustic and polar optical) alone cannot account for the observed energy loss rate in the temperature range 10 to 20K.

In figure 3 is shown the relation between $(dP/dT_e)_{T_e=T}$ vs $(100/T_e)$ for ZTA, polar optical phonon as well as total powerloss due to all processes. This type
FIGURE 4

Warm electron coefficient vs lattice temperature in n-InSb. Curve (a) $\beta$ is due to calculations using calculated $\mu_0$ and $\tau_\xi$. Curve (b) $\beta'$ is due to calculations using the calculated $\tau_\xi$ and observed $\mu_0$ /64/. Experimental points: o /64/. 

$\beta$ (cm$^2$/V$^2$) vs $T_e$ (K)
of plot clearly exhibits the temperature dependence of \( \frac{1}{\tau_{c}} \). The curve due to ZTA (see curve 2) process is almost parallel to experimental data in the range 12 to 18K giving the temperature dependence \( \frac{1}{\tau^{2}} \exp \left(-\frac{124}{T}\right) \) and this constitutes the best evidence for the scattering by two-zone edge transverse acoustic phonons.

(iii) **Warm Electron Coefficient**

The warm electron coefficient can be calculated making use of the computed values of \( \tau_{c} \) and \( \mu_{0} \), at various temperatures, in the expression (2.3.8). In figure 4 we have shown the plot of \( \beta \) vs T (curve a) along with the available experimental data /64/. In the temperature range 12 to 20K there is a slight departure of the calculated curve (a) from the experimental data as far as magnitude of \( \beta \) is concerned; however, the temperature variation of \( \beta \) for the calculated curve is faster than the experimental behaviour. This is understandable: We know that \( \mu_{0} \) and \( \tau_{c} \) constitute \( \beta \). From figure 2 we see that \( \tau_{c} \) agrees very well with experimental data as far as variation with temperature is concerned. However it is to be noted that there is considerable spread in the magnitude of the available experimental data /35, 62, 64/ itself. For example, the data of Sandercock /35/ and Kinch /64/, for samples with the same carrier concentration \( n = 5.4 \times 10^{13} \text{cm}^{-3} \), have noticeable spread. Consequently,
the use of calculated $\tau_e$ in the calculation of $\beta$ may lead to some departure in magnitude when compared with measured $\beta$. Secondly, the estimation of $\beta$ depends on the behaviour of $\mu_o$ with $T$. From figure 1 we notice that calculated $\mu_o$ is somewhat more than observed value for $T < 15K$. Moreover, the experimental $\mu_o$ increases faster than the calculated one. Thus, even though the right temperature dependence of $\tau_e$ has been used in the calculation of $\beta$, in view of the discrepancy in $\mu_o$ vs $T$ behaviour, one would expect departures in behaviour of $\beta$ vs $T$. Furthermore, the magnitude of $\mu_o$ above $15K$ is in reasonable agreement. Thus, if one calculates $\beta$ using experimental $\mu_o$ very little change (curve b) occurs above $13K$ where as $\beta$ at $10.5K$ reduces from 26.4 to $20 \, \text{cm}^2 \, \text{V}^{-2}$ which is nearer to the experimental value of $19 \, \text{cm}^2 \, \text{V}^{-2}$. From this it is evident that an explanation of $\beta$ vs $T$ requires further study of mobility mechanism below $15K$.

(iv) Drift Velocity and Electron Temperature /59/

Assuming the momentum loss of electron to be entirely due to ionized impurity scattering, we have obtained, numerically, the electron drift velocity and electron temperature $T_e$ as a function of applied field $F$, from equations (2.3.11) and (2.3.12), at lattice temperature $4.2K$. For the purpose of comparison we have used the experimental
Electron drift velocity ($V_d$) and electron temperature ($T_e$) vs electric field at lattice temperature 4.2 K in n-InSb. Theoretical: solid line with 2TA, broken line without 2TA. Experimental data: $\bigcirc$ (n=1.19x10$^{14}$ cm$^{-3}$) /70/, $\square$, 0, (n=3x10$^{14}$ cm$^{-3}$) /71/, X (n=1.12x10$^{14}$ cm$^{-3}$) /72/. 

FIGURE 5
data from /71/ for $V_d$ vs $F$ and from /70-72/ for $T_e$ vs $F$. 
All these calculated and experimental points are shown in 
Figure 5.*

Let us consider the behaviour of $V_d$ vs $F$ first. The 
curve (a*) has the right field variation than curve (b*), 
which excludes the scattering by ZTA, particularly in the 
field range 0.1 to 0.3 V cm$^{-1}$ (electron temperature range 
10-20K). Even though, the magnitude of $V_d$ is in reasonable 
agreement with the experimental data shown therein, the 
comparison is not justified in view of the fact that in the 
calculation we have taken $n = 5.4 \times 10^{13}$ cm$^{-3}$ where as 
the experimental data is for the sample with $n = 3 \times 10^{14}$ cm$^{-3}$. 
We could not calculate $V_d$ vs $F$ for this sample as the value 
of $N_I$ is not available. Hence the experimental data shown 
there-in helps us to compare only the $V_d$ vs $F$ variation which 
we believe to be same for both samples.

In the $T_e$ vs $F$ relation the curve (a) exhibits the 
right field variation than curve (b), which excludes ZTA 
process, in the temperature region 10 to 20K; here again the 
calculation is for the sample with $n = 5.4 \times 10^{13}$ cm$^{-3}$ and 
the experimental data are for samples with carrier concentra-
tions other than the one used for calculation.

Thus, on comparing curves (a') and (a) with (b') 
and (b) respectively, in figure 5, it may be emphasized that
the inclusion of ZTA phonon scattering has lead to the right
dependance of $V_d$ and $T_e$ on $F$. 
2.5 Discussion and Conclusions

In the foregoing sections, we have developed a transport theory for a semiconductor with the standard band model incorporating two-phonon process besides one-phonon and ionized impurity scattering mechanisms. We have compared our results with the experimental data of n-InSb.

As noted earlier in section (1.3) the method assumes the validity of adiabatic principle, Boltzmann transport equation and perturbation theory. The method requires that \((\hbar/k_B T) < T/\tau\), where \(\tau\) is the successive collision time for electrons. Directly related with this condition is \(k_{\text{B}} \ell > 1\). Now let us examine to what extent our method is justified in comparing with the data of particular sample of n-InSb chosen here \((n = 5.4 \times 10^{13} \text{cm}^{-3})\). The values of \(\hbar/k_B T\) at 4.2K and 25K are, respectively, \(1.8 \times 10^{-12}\) and \(3.054 \times 10^{-13}\). The corresponding experimental values of \(\mu_0\), from figure 1, lead to values of \(\tau\) (4.2K) = \(3 \times 10^{-12}\) \(\text{s}^{-1}\) and \(\tau\) (25K) = \(2.78 \times 10^{-12}\) \(\text{s}^{-1}\) for \(n = 5.4 \times 10^{13} \text{cm}^{-3}\). From these estimates it is clear that \(\hbar/k_B T < \tau\) is violated at 4.2K where as at 25K it is satisfied. So for the temperatures below 25K but not too low as 4.2K one is in the cross over region and applicability of the method is weakly violated in the samples we have considered.
Several attempts have been made to overcome this theoretical difficulty (see for eg. /63,70/), and an exact treatment of this case does not exist. Since the criterion for the validity of the method is weakly violated in as much as we are in the crossover region the applicability of the method is assumed in the present work. The above said difficulty can be avoided if one selects a sample which is sufficiently degenerate in which case \( \frac{h}{k_B T} \) may be replaced by \( \frac{h}{E_F} \), where \( E_F \) is fermi energy, and it has been shown that \( \frac{h}{E_F} < T \) for the temperature range of our interest /63/.

In our calculations we have used non-degenerate distribution function. We are justified in using these calculations, in comparing with experimental observations, for the following reason. In the temperature range of our interest (4.2 to 30K) the electrons in most of the n-InSb samples, whose data we have used for the comparison, obey the non-degenerate distribution function (for e.g. for samples of \( n = 5.4 \times 10^{13} \) and \( 2.2 \times 10^{14} \) cm\(^{-3}\) the degeneracy temperatures are, respectively, 4.5 K and 11.4 K). Further, for the above samples the screening of the coupling potentials by the conduction electrons may be neglected in as much as the relevant screening parameter is much less than the phonon wave vector in the temperature range of interest except at very low temperatures. Directly connected with
this condition is $2m e^2/m \xi_0 (k_B T)^2 < 1$ /74/; for e.g. at $T = 10^4K$, for sample with $n = 5.4 \times 10^{13} cm^{-3}$, the value for the same is 0.2.

Now we shall discuss about the coupling constants. In the literature the value for the acoustic deformation potential constant $E_1$ ranges from 3 to 30 eV /17/. The value $E_1 = 30$ eV was determined by fitting the free carrier absorption coefficient /73/ and the same was used by Kinch /64,74/. $E_1 = 15$ eV was also used to calculate electron energy loss /75/. We have used $E_1 = 7.2$ eV in our calculation. This is the value more often used in the literature in transport calculations /62,63,66,76/. The values for the rest of the parameters used by us are well known in the literature (see for e.g. /63,64/).

The two-phonon deformation potential constant selected by us ($D_2 = 1240$ eV) is at variance with those deduced by Ngai ($D_2 = 622$ eV for $E_0$ gap) /34/, from the magneto-phonon experiments /37/, and Cardona and co-workers /77/ ($D_2 = 230$ eV for $E_1$ gap), from the second order resonant Raman scattering experiment. The difference in the value of $D_2$ may be attributed to the following. The $D_2$ values deduced from these resonant experiments make use of the one-phonon coupling constant as standard whereas our $D_2$ value has been obtained by fixing the total energy relaxation time which
includes all possible scattering mechanisms in the temperature range of interest. Further, in the resonant experiments the phonons only at critical points take part whereas in the transport processes all phonons of the short wavelength region are involved even though the frequency of the two-phonons are selected at $\omega = XX$ in view of the flatness of the TA branch.

In conclusion, we note that in semiconductor such as n-InSb, the electron two-phonon mechanism contributes to energy loss process at low temperatures besides the one-phonon processes viz., acoustic and polar optical modes.

It is also found that the electron two-phonon interaction plays equally important role in case of GaSb /78/ for the energy loss process, as in case of n-InSb, at temperatures below 25K. Magnetophonon experiment in InP shows the electron scattering by two-phonons /79/ which can be tested by studying the electrical transport properties. The formulation carried out by us for two-phonon process can also be used for the scattering by $2T_0$ (zone edge) when one wants to work at higher temperatures.
PART II
2.6 Many-Valley Model with Ellipsoidal Energy Surface

It is well known that Ge and Si are typical non-polar semiconductors with many-valley band model i.e., with several set of band extrema in k-space and $E_k$ vs $k$ is typically of the form given by (1.1.9). The constant energy surfaces are ellipsoidal of revolution in nature. In what follows we shall describe the method of calculating the transport properties for the above model.

In thermal equilibrium all the valleys, in a given set, are equally populated and the electron distribution is governed by the equilibrium distribution. In the presence of an electric field the population of the valleys changes from its equilibrium value due to intervalley scattering process and accordingly the contribution from the other valleys to the given valley arises. Hence it is essential to solve the Boltzmann transport equation for a given valley taking into account the rate of change of distribution due to intervalley process besides intravalley process.

As was done in (2.1), we shall assume the displaced Maxwellian distribution to be the solution of the Boltzmann transport equation in each valley. The distribution function for the $i$-th valley may, then, be written as
where $A_i$ is the normalization constant such that

$$
\sum_{k} f^i_k = A_i \sum_{k} e^{\frac{E^i_k}{k_B T}}, \quad (2.6.2)
$$

where $n_i$ is the $i$-th valley electron density. The electron density $n$ of the material is related to valley electron density through the relation

$$
\sum_i n_i = n. \quad (2.6.3)
$$

Now following the procedure outlined in (2.1), we set up the Boltzmann equation for electrons in $i$-th valley in the steady state as

$$
\left( \frac{\partial f^i_k}{\partial t} \right)_C + \left( \frac{\partial f^i_k}{\partial t} \right)_F = 0, \quad (2.6.4)
$$

where

$$
\left( \frac{\partial f^i_k}{\partial t} \right)_C = \left( \frac{\partial f^i_k}{\partial t} \right)_{\text{intra}} + \left( \frac{\partial f^i_k}{\partial t} \right)_{\text{inter}}. \quad .... (2.6.5)
$$

In (2.6.5) the first term on r.h.s. represents the rate of

---

* In view of the later application of the development of the present section to non-degenerate, pure Ge and Si at elevated temperatures, the contribution of the impurity scattering term in (2.6.5) has been dropped.
change of $i$-th valley distribution due to intravalley scattering and the second term is due to intervalley scattering. The intravalley scattering includes scattering by the lattice and interelectronic collisions. The terms due to interelectronic collisions in the intravalley scattering does not contribute to average momentum and energy losses as shown in (2.1). In an intervalley scattering the wave vector difference between initial and final states are large and at such large wave vectors the Coulomb matrix element of interelectronic process falls off rapidly; hence we neglect the contribution of interelectronic scattering in intervalley scattering also. Thus we consider only phonon induced intra and intervalley scattering. Then from (2.6.5), we can write the momentum and energy balance equations, for the electrons in the $i$-th valley as

$$\sum_{k} \hbar k \left\{ \left( \frac{\partial f_{ik}}{\partial t} \right)_{\text{intra}} + \left( \frac{\partial f_{ik}}{\partial t} \right)_{\text{inter}} + \left( \frac{\partial f_{ik}}{\partial t} \right)_{F} \right\} = 0,$$

\[ \text{(2.6.6)} \]

and

$$\sum_{k} \hbar k \left\{ \left( \frac{\partial f_{ik}}{\partial t} \right)_{\text{intra}} + \left( \frac{\partial f_{ik}}{\partial t} \right)_{\text{inter}} + \left( \frac{\partial f_{ik}}{\partial t} \right)_{F} \right\} = 0.$$

\[ \text{(2.6.7)} \]

Further, we make use of the fact that the number of electrons is conserved i.e.
The summation over \( k \) in (2.6.6) to (2.6.8) is complicated in view of the ellipsoidal nature of the energy surfaces. To overcome this difficulty we invoke the well known Herring and Vogt transformation /80/ which is as follows. This transformation is essentially a co-ordinate transformation on wave vectors such that in the new co-ordinate system the constant energy surfaces will be spherical in nature so that the procedure developed in section (2.1) may be extended to the present case. The new co-ordinate system is usually termed as 'starred system'. In the starred system the vector quantities \( k, q, F \) and \( v_d \) have the following transformations:

\[
\begin{pmatrix}
    k^* \\
    q^* \\
    F^*
\end{pmatrix} = \alpha^\frac{1}{2}
\begin{pmatrix}
    k \\
    q \\
    F
\end{pmatrix}
\quad (2.6.9)
\]

and

\[
v_d = \alpha^\frac{1}{2} v_d^*
\quad (2.6.10)
\]

where \( \alpha \) is diagonal tensor in the principal axes system of each valley and is given by
\[ \mathbf{a} = \begin{bmatrix} 0 & 0 & 0 \\ m_0/m_t & 0 & 0 \\ 0 & m_0/m_t & 0 \end{bmatrix} \]  
\hspace{1cm} (2.6.11)\]

Z-axis being the longitudinal axis. In the starred system it follows that

\[ E_{k*} = \frac{h^2 k^*^2}{2m_0} \]

\[ \hat{\mathbf{e}}_{k*} = \mathbf{e}_{k*} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \]

\[ \mathbf{e}_{k*} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \]

and

\[ \int d^3 k \mathcal{O}(k) \rightarrow \left( \frac{t m^{1/2}}{m_0^{3/2}} \right) \int_{k* = 0}^{\infty} \mathcal{O}(k*) k*^2 dk* \]

\[ \times \left( \frac{t}{2} \right) \sum_{0}^{2\pi} \sin \gamma * d\gamma * \int_{0}^{2\pi} d\psi * \]

where \( \mathcal{O}(k) \) is some function of \( k \); \( \gamma* \) and \( \psi* \) are the polar and azimuthal angles, respectively, of \( k* \) w.r.t. \( \mathbf{F*} \). Making use of these transformations the field terms in (2.6.6) and (2.6.7) give, respectively, \( \mathbf{e}_{F*} n_1 \) and \( \mathbf{e}_{F*} \mathbf{v}^* n_1 \); thus we get

\[ \mathbf{e}_{F*} n_1 = - \int nk* \left\{ \left( \frac{\partial e_{F*}}{\partial t} \right)_{\text{intra}} + \left( \frac{\partial e_{F*}}{\partial t} \right)_{\text{inter}} \right\} d^3 k* = 0 \]

\hspace{1cm} (2.6.13)\]

and

\[ \mathbf{e}_{F*} \mathbf{v}^* n_1 = - \int nk* \left\{ \left( \frac{\partial e_{F*}}{\partial t} \right)_{\text{intra}} + \left( \frac{\partial e_{F*}}{\partial t} \right)_{\text{inter}} \right\} d^3 k* = 0, \]

\hspace{1cm} (2.6.14)\]
where $v_d^*$ is the electron drift velocity pertaining to the $i$-th valley. The equations (2.6.13) and (2.6.14) are the extension of F-P approach to the many-valley semiconductors of ellipsoidal energy surfaces /81/.

As has been discussed earlier in section (2.1), one can use in place of (2.6.13) and (2.6.14), respectively,

$$ eF^* n_1 = -\int \left( \frac{\partial h k^*}{\partial t} \right)^i \frac{f_i^*}{k} d^3 k^* \quad (2.6.15) $$

and

$$ eF^* \cdot v_d^* n_1 = -\int \left( \frac{dE_k^*}{dt} \right)^i \frac{f_i^*}{k} d^3 k^* \quad (2.6.16) $$

In what follows we will calculate the average momentum and energy losses due to intra and intervalley processes wherein the scattering due to one-phonon and two phonons are involved i.e., we calculate

$$ \left< \frac{\partial h k^*}{\partial t} \right> \quad \text{or intra} \quad \text{or inter} = \frac{1}{n_i} \int (-\frac{\partial h k^*}{\partial t})^i \frac{f_i^*}{k} d^3 k^* = \left< \frac{\partial h k^*}{\partial t} \right>_{1p} + \left< \frac{\partial h k^*}{\partial t} \right>_{2p} \quad \ldots (2.6.17) $$

and

$$ \left< \frac{dE_k^*}{dt} \right> \quad \text{or intra} \quad \text{or inter} = \frac{1}{n_i} \int (-\frac{dE_k^*}{dt})^i \frac{f_i^*}{k} d^3 k^* = \left< \frac{dE_k^*}{dt} \right>_{1p} + \left< \frac{dE_k^*}{dt} \right>_{2p} \quad \ldots (2.6.18) $$
A. One-Phonon Processes

In non-polar semiconductors the possible one-phonon processes are acoustic deformation and non-polar optical mode types. These are further classified as intra or intervalley scattering mechanisms and will be considered in the following:

(a) Intravalley Scattering /17,81/

(i) Acoustic-Phonon Scattering

In the acoustic phonon scattering the energy and wave vector of the phonons are small and the scattering may be regarded approximately as elastic; consequently only intravalley scattering is possible. Interaction of electrons with acoustic modes in non-polar semiconductors of ellipsoidal energy surface are given by (1.3.17) and (1.3.18). Now we shall calculate r.h.s. of (2.6.15) and (2.6.16) for acoustic mode intravalley scattering process. The momentum loss rate \( \frac{d\mathbf{k}^*}{dt} \) and energy loss rate \( \frac{dE_{\mathbf{k}^*}}{dt} \), respectively, assume the forms given by (2.2.5) and 2.2.6. Next we substitute the absolute square of the matrix elements (1.3.17) and (1.3.18) in these forms and make use of the transformation properties (2.6.12). Following Conwell /17/ we first integrate over \( q^* \). The order of integration is first on \( q^* \) and then \( \theta^* \) and \( \phi^* \); this is inview
of the dependence of $s_{u,d}$ and $q^2$ on $e^*$. Also we assume equipartition of energy for acoustic modes (i.e., $N = k_B T/\hbar \omega_q$). We make use of the property of the Dirac-delta function in the integration. It may be noted that $(dhk*/dt)_{ac}$ and $(dE_k*/dt)_{ac}$ are complicated for arbitrary direction of $k*$; hence it is advisable to calculate these quantities for $k*$ parallel and perpendicular to $Z$; then average is taken over the distribution function $f_{k*}^{i}$, which is expanded in the manner similar to (2.1.4). The average momentum and energy loss rates due to acoustic mode scattering so obtained are, respectively, given by

$$
\left\langle \frac{dhk^*}{dt} \right\rangle_{ac}^{i} = - A \frac{2}{10} T \frac{T^{1/2}}{\epsilon_i} \frac{v^*_i}{\epsilon_i} \tag{2.5.19}
$$

and

$$
\left\langle \frac{dE_k^*}{dt} \right\rangle_{ac}^{i} = - A' \frac{2}{10} (\epsilon_i - T) \frac{T^{1/2}}{\epsilon_i} \tag{2.5.20}
$$

where

$$
A = \frac{2^{9/2} (m_m^{1/2})_1 k_B^{3/2}}{27 m_o^{3/2} \hbar^4 s^2 \rho} \tag{2.6.21}
$$

$$
A' = \frac{2^{9/2} (m_k^{1/2})_1 k_B^{3/2}}{3 m^*_2 \hbar^4 \rho} \tag{2.6.22}
$$

and

$$
E_{10}^{2} = \frac{3 \pi}{2^9} \left( \xi_{d}^2 + \eta_{d}^2 \xi_{u}^2 \xi_{d}^2 + \eta_{d}^2 \xi_{u}^2 \right), \tag{2.6.23}
$$
where \( \xi, \eta, \text{ and } \zeta \) are dimensionless coefficients and depend on the elastic constants, the ratio \((m_e/m_1)\) and the orientations of valley.

(ii) Non-Polar Optical Mode Scattering

For optical modes the dispersion may be neglected; then the absolute square of the matrix element \((1,3.11)\) will be independent of \(\theta\) and \(\phi\). We make use of this matrix element in the momentum and energy loss rate equations, for non-polar optical modes, of the forms \((2.2,5)\) and \((2.2,6)\). We use the transformation equations \((2.6,12)\) in these equations. Then integrations over \(q^*, \theta^*\) and \(\phi^*\) are carried out and later the average is taken over the distribution function of the form \((2.1.4)\). This results in

\[
\langle \frac{d\mathbf{k}^*}{dt} \rangle_{npo} = - \frac{B(DK)^2}{\epsilon^{1/2}} \frac{N}{v_{di} G_1(x_e/2)} \tag{2.6.24}
\]

and

\[
\langle \frac{dE^*}{dt} \rangle_{npo} = - B' (DK)^2 \frac{N}{\epsilon^{1/2}} G_2(\frac{x_e}{2}) \tag{2.6.25}
\]

where

\[
B = \frac{2(m_m^{1/2})^{1}m_0}{3 \frac{\hbar^2}{m_0} \frac{1}{2} k_B^{1/2}} \tag{2.6.26}
\]
(ii) Intervalley Scattering /17, 45, 82, 93/

In this case we have two possibilities (1) equivalent intervalley and (2) non-equivalent intervalley scattering. In the former type the electronic transitions occur between equivalent valleys of a given set; for e.g., (111) set of valleys in Ge for applied field along [100] direction. If the applied field direction is such that the valleys are differently oriented with respect to it, then one has latter-type of intervalley scattering. It should be noted that non-equivalent intervalley scattering also arises if a transition takes place between i-th valley of a given set to j-th valley of another set; for e.g., transition from (111) set of valleys to (100) set in Ge.

Here we briefly mention the method of finding the contribution of intervalley scattering to the momentum and energy balance equations following F-P approach. There it is required to find \( \frac{\partial E}{\partial t} \). Let us write \( E = f_0 + f_1 \). Then

\[
\frac{\partial E}{\partial t} = \frac{\partial E_0}{\partial t} + \frac{\partial E_1}{\partial t},
\]

\[ (2.6.28) \]
where the subscript iv denotes intervalley. Following [17,82], recalling the discussion in (1.3) that the matrix element of intervalley scattering is independent of initial and final states of the electrons in their respective valleys, the integration over $q^*$ space gives

\[ \frac{\partial f_{ij}}{\partial t}_{iv} = N_j \left( \frac{(DK)^2_{ij} (m_e m_l^{1/2})_j}{2^{1/2} h^3 p W_{ij}} \right) \]

\[ \times \left\{ (E - \Delta E_{ij} + \hbar W_{ij})^{1/2} \left[ (N_{ij} + 1) f_{ij} (E + \hbar W_{ij}) - N_{ij} f_{ij} (E) \right] \right\} \]

\[ + (E - \Delta E_{ij} - \hbar W_{ij})^{1/2} \left[ N_{ij} f_{ij} (E - \hbar W_{ij}) - (N_{ij} + 1) f_{ij} (E) \right] \}

\[ = \frac{2^{1/2} h^3 p W_{ij} \{ N_{ij} (E - \Delta E_{ij} + \hbar W_{ij})^{1/2} + (N_{ij} + 1) (E - \Delta E_{ij} - \hbar W_{ij})^{1/2} \}}{ (DK)^2_{ij} (m_e m_l^{1/2})_j} \}

\[ \text{(2.6.29)} \]

and

\[ \frac{\partial f_{ij}}{\partial t}_{iv} = - f_{i1} N_j \left( \frac{(DK)^2_{ij} (m_e m_l^{1/2})_j}{2^{1/2} h^3 p W_{ij}} \right) \]

\[ \times \left\{ N_{ij} (E - \Delta E_{ij} + \hbar W_{ij})^{1/2} + (N_{ij} + 1) (E - \Delta E_{ij} - \hbar W_{ij})^{1/2} \right\} \}

\[ \text{(2.6.30)} \]

where $N_{ij} = (e^{x_{ij}} - 1)^{-1}$, $x_{ij} = \hbar W_{ij} / k_B T$ ($\hbar W_{ij}$ is the intervalley phonon energy) and $\Delta E_{ij}$ is the separation between $i$-th and $j$-th valley. The prime on summation in (2.6.29) and (2.6.30) refers to $j \neq i$. Now we make use of (2.6.29) and (2.6.30) in (2.6.13) and (2.6.14) then integrate over $k^*$. This gives us, for equivalent intervalley scattering (i.e. for $\Delta E_{ij} = 0$, $T_{ei} = T_{ej}$, $n_i = n_j$, $V_{di} = V_{dj}$),
\[ \left\langle \frac{d\mathbf{k}^*}{dt} \right\rangle_{iv} = -B \epsilon_j \left( \frac{\partial}{\partial e_{ij}} \right)^2_{ij} N_{ij} V^*_{di} G_1(x_{ei}/2) \]

and

\[ \left\langle \frac{d\mathbf{k}^*}{dt} \right\rangle_{iv} = -B \epsilon_j \left( \frac{\partial}{\partial e_{ij}} \right)^2_{ij} N_{ij} e_{ij}^{1/2} G_2(x_{ei}/2), \]

where \( \epsilon_{ij} = h^2 n_{ij}/k_B \). For consistency we have used the notation on l.h.s. of (2.6.31) and (2.6.32), as in the acoustic intravalley case, even though we have used (2.6.13) and (2.6.14).

For non-equivalent intervalley scattering (i.e. \( \Delta E_{ij} \) may or may not be zero, \( T_{ei} \neq T_{ej} \), \( n_i \neq n_j \) and \( V_{dj} \neq V_{di} \)), making use of definitions \( \Delta_i = \Delta E_{ij}/k_B T_{ei} \), \( \Delta_j = \Delta E_{ij}/k_B T_{ej} \), \( y_i = E/k_B T_{ei} \) and \( y_j = E/k_B T_{ej} \), we get

\[ \left\langle \frac{d\mathbf{k}^*}{dt} \right\rangle_{iv} = - \xi_j \frac{2^{3/2} (DK)^2_{ij} (m_{ei} m_{lj})^{1/2}}{3 \pi^{3/2} \rho n^2 k_B \epsilon_{ij}} \]

\[ x e^{-\Delta_i} \left\{ I_1(\Delta_i, x_{ei}) + (e^{-x_{ei}}) I_2(\Delta_i, x_{ei}) \right\} \]

\[ \ldots \quad (2.6.33) \]

and
\[
\left( \frac{\partial \mathbf{e}_k^i}{\partial t} \right)_{iv} = -N_j \sum_{ij} \frac{2^{1/2} (D_K^2)^2}{m_i^3} \left[ \frac{(m_m^{1/2})_{ij} k_B^{1/2} T_e_{ij} N_{ij}}{\pi^{3/2} n^2 \rho_{e_{ij}}} \right] \left[ I_1 (\Delta_i, x_{e_i}) + e^{-x_{e_i}} I_2 (\Delta_i, x_{e_i}) \right] - \frac{n_j T^{3/2}_e}{n_i T^{3/2}_e} \sum_{ij} \frac{(m_m^{1/2})_{ij}}{(m_m^{1/2})_{ij}} \left[ I_1 (\Delta_j, x_{e_j}) + e^{-x_{e_j}} I_2 (\Delta_j, x_{e_j}) \right]
\]

where

\[
I_1 (\Delta_i, x_{e_i}) = \int_0^\infty e^{-y_i} (y_i + \Delta_i)^{3/2} (y_i + x_{e_i})^{1/2} dy_i
\]

and

\[
I_2 (\Delta_i, x_{e_i}) = \int_0^\infty e^{-y_i} (y_i + \Delta_i + x_{e_i})^{3/2} y_i^{1/2} dy_i.
\]

Next we obtain the valley population using (2.6.29) in the equation for the conservation of electron number viz.

\[
\int \left( \frac{\partial \mathbf{e}_k^i}{\partial t} \right)_{iv} \ d^3k = 0,
\]

which yields, after integration over \( k \\) and utilising starred system transformation,

\[
\frac{n_i}{n_j} = \frac{T^{1/2}_e (m_m^{1/2})_i \left\{ I_0 (\Delta_j, x_{e_j}) + e^{-x_{e_j}} I_0' (\Delta_j, x_{e_j}) \right\}}{T^{1/2}_e (m_m^{1/2})_j \left\{ I_0 (\Delta_i, x_{e_i}) + e^{-x_{e_i}} I_0' (\Delta_i, x_{e_i}) \right\} e^{\Delta_i}}
\]

.... (2.6.36)
where

\[ I_o(\Delta_i, x_{e_1}) = \int_0^\infty e^{-y_i} (y_i + \Delta_i)^{1/2} (y_i + x_{e_1})^{1/2} dy_i \]

and

\[ I_o'(\Delta_i, x_{e_1}) = \int_0^\infty e^{-y_i} (y_i + \Delta_i + x_{e_1})^{1/2} y_i^{1/2} dy_i \]

\[ \ldots \quad (2.6.36a) \]

B. Two-Phonon Processes /84/

In this section we wish to obtain the average momentum and energy loss rates due to two-phonon process for electrons in the \( i \)-th valley. The two-phonon process is regarded as intravalley process in view of the very small value of the \( Q = q + q' \) involved in the scattering process. The method is similar to the case of spherical energy surface except that we have to work in starred space. We apply the Herring and Vogt transformation to (2.22) and (2.23), then we write

\[
\left[ \frac{d(h_k, E_k)}{dt} \right]_{2p}^i = \left[ \frac{m_{1} m_{2}^{1/2}}{m_{o}^{3/2}} \right]^{2} \frac{G_{*}, G_{*}^{*}}{G_{*}^{*}, G_{*}^{*}} \left\{ \left[ n(g+g')_{k}, n(W_{a} + W_{a}')_{k} \right] \right. \\
\left. \times \left[ p_{aa}(k \rightarrow k+g+g') - p_{ee}(k \rightarrow k-g-g') \right] \right. \\
+ \left[ h(g-g')_{k}, n(W_{a} - W_{a}')_{k} \right] \\
\left. \times \left[ p_{ae}(k \rightarrow k+g-g') - p_{ea}(k \rightarrow k-g+g') \right] \right\} \\
\ldots \quad (2.6.37,38)
where the star on the curly bracket indicates that the quantities within it should be taken in the starred sense.

We now substitute for the transition probabilities $P_{aa}$, $P_{ee}$, and $P_{ea}$ from equations (2.2.18) to (2.2.21) and change the summation over $q^*$ and $q'^*$ to integration. Further we represent $(q + q')^* = Q^*$, where + and - sign indicate, respectively, first and last two terms in (2.6.37) and (2.6.38).

Then we get

$$\left[ \frac{d}{dt} (h_k, E_k)^* \right]_{2p}^1 = \frac{2\pi}{\hbar} \left( \frac{1}{8\pi^3} \right)^2 \frac{m_1}{m_0} \int d^3q^* \int d^3q^*$$

$$x \left\{ \left| V_2(g, Q-q) \right|^2 \left[ h_{Q-k}, h(W_g + W_{Q-q}) \right] \right. + \left. \left[ N_g (N_g + 1) \delta(E_k - E_k + h(W_g + W_{Q-q})) \right] \right. + \left. \left[ N_g (N_g + 1) \delta(E_k - E_k + h(W_g - W_{Q+g})) \right] \right. + \left. \left[ N_g (N_g + 1) \delta(E_k - E_k + h(W_g - W_{Q+g})) \right] \right. \right\} .$$

We now substitute for the matrix element $|V_2(g, Q+q)|$ from (1.3.23) in (2.6.39,40). Since the matrix element is independent of $Q$ and $q$ we can take it
outside the integrals. Let us fix $k^*$ as the polar axis and integrate over $q^*$ which yields, as in (2.2) section,

$$\int d^3q^* \approx \left( \frac{m_o^{3/2}}{m_t^{1/2}} \right) \frac{4 \pi q_z^3}{3}.$$  \hspace{1cm} (2.6.41)

Now we shall integrate over $q^*$ with $k^*$ as polar axis. Integration limits over $Q^*$ are the same as those given by (2.2.34) to (2.2.36) with $k$ and $m$ replaced by $k^*$ and $m_o$, respectively. We get

$$\left[ \frac{\partial h_{k^*}}{\partial t} \right]_{2P} = - \frac{\left( m_t m_1^{1/2} \right)_1 m_o^{1/2} D_s^2 q_z^3 N N^* \hat{k^*}}{3 \pi^3 \rho^2 a^4 k_B^2 \Theta_s^2}$$

$$x \left\{ E^{1/2}(E+k_B \Theta_s)_{1/2} + e^{\Theta_s/\tau} E^{1/2}(E-k_B \Theta_s)_{1/2} \right\} + 2 E e^{\Theta_s/2\tau} \} \hspace{1cm} (2.6.42)$$

and

$$\left[ \frac{\partial E_k^*}{\partial t} \right]_{2P} = - \frac{D_s^2 q_z^3 N N^* \left( m_t m_1^{1/2} \right)_1}{2^{1/2} \pi^{3/2} \rho^2 a^4 k_B \Theta_s}$$

$$x \left\{ (E+k_B \Theta_s)_{1/2} - e^{\Theta_s/\tau} (E-k_B \Theta_s)_{1/2} \right\}.$$

$$... \hspace{1cm} (2.6.43)$$

As in section (2.2) we have made use of the assumption that $W$'s and $N$'s are independent of wave vectors. Also the definitions for $W$ and $\Theta$ are same as defined there.
Now we calculate the average momentum and energy loss rates, as in (2.2.39) and (2.2.40), making use of the displaced Maxwellian distribution function given in (2.6.12) in the form (2.1.4) for the i-th valley. Working in the starred space we get

\[
\left\langle \frac{dh_{k,*}}{dt} \right\rangle_{2p} = -\frac{2(m_{\perp}m_{1}^{1/2})_{i} m_{\perp} D_{s}^{2} q_{z}^{3} N N'}{9 \pi^{7/2} \rho^{2} a^{4} (k_{B} T_{s})^{3/2}} v_{id}^{*} \left\{ G_{1}\left(\frac{r_{e}}{2}\right) + G_{3}\left(\frac{r_{e}}{2}\right) \right\}
\]

and

\[
\left\langle \frac{dE_{k,*}}{dt} \right\rangle_{2p} = -\frac{(m_{\perp}m_{1}^{1/2})_{i} D_{s}^{2} q_{z}^{3} N N'}{3 \pi^{7/2} \rho^{2} a^{4} (k_{B} T_{s})^{1/2}} G_{2}\left(\frac{r_{e}}{2}\right),
\]

... (2.6.44)

\[
\left\langle \frac{dE_{k,*}}{dt} \right\rangle_{2p} = -\frac{(m_{\perp}m_{1}^{1/2})_{i} D_{s}^{2} q_{z}^{3} N N'}{3 \pi^{7/2} \rho^{2} a^{4} (k_{B} T_{s})^{1/2}} G_{2}\left(\frac{r_{e}}{2}\right),
\]

... (2.6.45),

where \( G_{1}\left(\frac{r_{e}}{2}\right) \), \( G_{2}\left(\frac{r_{e}}{2}\right) \) and \( G_{3}\left(\frac{r_{e}}{2}\right) \) are of the form given by equations (2.2.16a), (2.2.17a) and (2.2.43a), respectively.
2.7 Method of Obtaining the $\nu_0$, $\tau_\beta$, $\beta$, $V_{di}$ and $T_e$

The average momentum and energy loss rates, obtained in the foregoing subsections, due to individual scattering mechanisms are added to give the total loss rates and are equated to field terms to give the energy and momentum balance equations. Of course these will be transformed back from the starred space to normal space. These equations may be formally expressed as

$$F/V_{di} = M_i(T_{ei}) \quad (2.7.1)$$

and

$$F V_{di} = E_i(T_{ei}, T_{ej}, n_i, n_j). \quad (2.7.2)$$

The expression for the valley population may be written as

$$n_i/n_j = N_i(T_{ei}, T_{ej}). \quad (2.7.3)$$

In the low field region electrons will be in only lower set of valleys. All the valleys will be equally populated ($n_i = n_j$) and electron temperature in all the valleys will be same ($T_{ei} = T_{ej}$). Then the calculations of $\nu_0$, $\tau_\beta$, and $\beta$ closely follow those described in (2.3). The procedure described there may be followed to calculate high field properties $V_{di}$ and $T_{ei}$ when the scattering is only among the equivalent valleys.
Now we shall describe the method to calculate high field properties when the non-equivalent intervalley scattering are possible. First we fix $T_{ei}$ and $T_{ej}$ and find $n_i/n_j$ from (2.7.3); this is made use of in (2.7.1) and (2.7.2). Now eliminate once $F$ and once $V_{di}$ in these equations, which respectively yield $V_{di}$ as a function of $T_{ei}/T_{ej}$ and $F$ as a function of $T_{ei}/T_{ej}$. The average drift velocity of the electrons is obtained by making use of the expression

$$n V_d = \sum_i n_i V_{di} \quad (2.7.4)$$

In the next section we shall seek the application of the transport theory developed in the present sections to non-degenerate n-Ge and n-Si.
2.8 **Application to n-Germanium**

Electrical transport properties of Germanium have been extensively studied both experimentally and theoretically /41,45,85,86/. In the present section first we shall briefly summarize the experimental observations together with the existing explanations in n-Ge and then we shall compare our calculations with the experimental data of the quantities $\mu_0$, $\gamma$, $\beta$, $V_d$ and $T_e$.

2.8a **Comparison between Experimental Observations and the Existing Theoretical Calculations**

From the existing one-phonon theories /87/, the known scattering mechanisms in Ge are acoustic (deformation type), non-polar optical intravalley and intervalley (equivalent and non-equivalent). The inadequacy of these mechanisms in Ge becomes clear in what follows.

(i) **Zero Field Mobility**

Zero field mobility in n-Ge exhibits a variation with temperature of the form $T^\delta$ where $\delta$ has a value -1.66 in the temperature range 30 to 300K /87-89/; at low temperatures ($\leq$70K) $\delta$ is -1.5.

McLean and Paige /90/ have compared experimental and theoretical lattice limited mobility at low
temperatures (\( \sim 77.7 \text{K} \)) and found good agreement indicating that the scattering is due to the acoustic phonons. Morin and Maita /88/ have explained \( T^{-1.66} \) law for \( \mu_0 \), by considering a simple band model within the relaxation time approximation taking into account combinations of acoustic and non-polar optical modes (i.e. \( \mu_0^{-1} = \mu_{ac}^{-1} + \mu_{np}^{-1} \)) in the temperature range 250K to 1000K. It may be noted that by a proper choice of the ratio of coupling constants of optical to acoustic phonon scattering mechanisms, it is possible to account for the observed \( \mu_0 \) variation with temperature even with a simple band model.

Herring and Vogt /80/ have applied the deformation potential method in the relaxation time approximation to ellipsoidal energy surfaces of many valley semiconductors and obtained \( \mu_0 \) as

\[
\mu_0 = \frac{e}{3} \left\{ \frac{2 \langle T_T \rangle}{m_T} + \langle T_L \rangle \frac{1}{m_L} \right\}, \tag{2.3.1}
\]

where \( T_T \) and \( T_L \) are, respectively, the transverse and longitudinal relaxation times. This was followed later in most of the calculations by many authors /85,86/.

Recently Costato et al. /39/ have calculated \( \mu_0 \) from momentum balance equation and obtained reasonable agreement with experimental observation taking optical
intravalley scattering constant \((DK)_{ii} = 6 \times 10^8 \text{ eV cm}^{-1}\)
besides the usual acoustic deformation potential type scattering. Their calculation took into account the nonparabolicity of the conduction band and mixing of Bloch states.

Rode /91/, using an iterative procedure, has shown that \(\mu_0 \propto T^{-1.63}\) using \((DK)_{ii} = 3 \times 10^8 \text{ eV cm}^{-3}\) and equivalent phonon temperature \(\theta = 382\text{K}\).

(ii) Energy Relaxation Time

In the warm electron region, the energy relaxation time \(\tau_e\) is of particular interest as it provides the information on the energy loss processes. Measurement of \(\tau_e\) has been carried out by many authors /92-97/. It has been found that the observed magnitudes and the temperature dependence of energy relaxation time are markedly different from those calculated theoretically with one phonon scattering mechanisms (see ref. /39/ and curve 2 of figure 8 of our work), which were successful in explaining the \(\mu_0\) variation with \(T\). In view of this it is clear that the scattering mechanisms are not well set to explain energy loss and mobility, with the same set of coupling constants and phonon equivalent temperature.
(iii) Warm Electron Coefficient

In the warm electron range the mobility is a field dependent quantity and it exhibits a quadratic law \( \psi \propto F \). As expected from (2.3.6), the warm electron coefficient \( \beta \) defined by (2.3.6) is very sensitive to scattering mechanisms. Attention has been focussed on measurements of \( \beta \) dependence on temperature \( /40,98/ \) and the observed values of \( \beta \) are typically \( 2 \times 10^{-5} \) and \( 3 \times 10^{-7} \) cm\(^2\) V\(^{-2}\) at 100 and 300K, respectively. Moreover, \( \beta \) takes negative and positive values for pure and impure samples, respectively \( /41/ \).

Gunn \( /41/ \) has compared the experimental and theoretical values of \( \beta \) at 90K and found that the experimental values \( (\beta_{\text{expt}}) \) were less by a factor 10 than those calculated \( (\beta_{\text{cal}}) \). Using momentum and energy balance approach Costato et al. \( /39/ \) have calculated \( \beta \) and compared with the experimental observations \( /40,98/ \). They find that \( \beta_{\text{cal}} \) is more steeper at low temperatures and less steeper at higher temperatures than \( \beta_{\text{expt}} \); moreover \( \beta_{\text{cal}} < \beta_{\text{expt}} \) over the temperature range 70 to 300K (see curve 2 of Fig. 9). The scattering mechanisms and coupling constants used for the calculations of \( \beta \) are same as those used in their calculation of \( \mu_{\Omega} \). As pointed out in (1.4), they have also shown by varying \( (DK)_{ii} \) from \( 3 \times 10^8 \) to \( 9 \times 10^8 \) eV cm\(^{-1}\) (since the coupling constants for acoustic case can be fixed by fitting
the low temperature $\mu_0$ and equivalent intervalley scattering contributes insignificantly) that existing one-phonon theories are inadequate to account for $\beta_{\text{expt}}$.

Allredge and Blatt /30/ have pointed out the need for two-phonon process as an energy loss mechanism but the phonons, they have treated, were of long wavelength acoustic type; whereas we will consider scattering by two-short wave phonons. The latter is supported by large two-phonon deformation potential coupling constants deduced both experimentally /99/ and theoretically /100/.

(iv) Electron drift Velocity in High Field

In the high field region deviation of the mobility from Ohmic value is noticed experimentally /41,101-103/. At room temperature $V_d$ vs $F$ measurements have shown that the slope of the curve varies slowly from one to zero, i.e., drift velocity saturates at higher fields ($F > 3 \times 10^3 \text{ V cm}^{-1}$). However, for lattice temperatures less than 150K, $V_d$ is found to decrease with $F$ at higher fields /104,105/. Furthermore, the anisotropic behaviour of the drift velocity with field is observed /85/.

Considering the many-valley nature of Ge theoretical work has been done by many authors /81,82,106-111/. Reik and Riskin's /82,110/ work is the most detailed one and it incorporates intervalley scattering among (111)
valleys besides intravalley acoustic and optical phonon scattering. The early hot electron theories \(81,111\) have shown that if \(\langle111\rangle\) valleys are parabolic and energy loss through both acoustic and optical phonons are included the drift velocity would not show any saturation at higher fields. Moreover the electron temperatures deduced are too high, and as a result electrons will be in non-parabolic region. The saturation of \(V_d\) has been explained /111-113/, for a parabolic band structure, by considering the additional intervalley scattering from \(\langle111\rangle\) valleys to \(\langle100\rangle\) 'silicon-like' minima (non equivalent intervalley scattering). Calculations have also been carried out including non-parabolicity of conduction band /114/. The coupling constants used in the calculation /114/ for the optical intravalley scattering and non equivalent intervalley scattering are \(6 \times 10^8\) and \(5 \times 10^7\) eV cm\(^{-1}\), respectively. It is to be noted that non equivalent intervalley scattering occurs only in high field region and hence can be neglected in the calculations of \(\mu_0\), \(T_e\) and \(\beta\).

In short we realise that:

1. There is no consistent explanation of transport characteristics with one set of coupling constants and equivalent phonon temperatures in all the three regions of field i.e. low, warm and high fields.
The existing theoretical calculations mentioned are all one-phonon theories and do not consider the role of two-phonon mechanisms.

2.8b Comparison between Present Work and Experimental Observations

The relevant lattice scattering mechanisms which control transport properties in Ge are the following. (i) One-phonon processes /23/: acoustic intravalley, optical intravalley, and equivalent intervalley scattering; (ii) Two-phonon processes /115/: scattering by 2TA (at \( \Xi = XX \)) and 2TO (at \( \Xi = LL \)), where X and L are high symmetry points in the Brillouin zone. The coupling constants and phonon equivalent temperatures for these scattering mechanisms and other material parameters which are essential for the estimation of transport properties are given in Table 2.

Following the procedure outlined in (2.7) we have numerically calculated \( \mu_0, T_e \), and \( \beta \) in the temperature range 30 to 300K. Further, we have calculated \( V_d \) and \( T_e \) as a function of applied electric field \( F \) at lattice temperature 300K.

We have taken value for \( e_s \) in the short wavelength region at points \( \Xi = XX \) and \( LL \) for 2TA and 2TO processes,
TABLE 2
Scattering mechanisms and the material parameters used in the present work in n-Ge.

<table>
<thead>
<tr>
<th>Scattering mechanism</th>
<th>Phonon equivalent constant*</th>
<th>Coupling constant*</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>temperature in K /8/</td>
<td></td>
</tr>
</tbody>
</table>

A One-phonon processes

(i) Intravalley scattering:

<table>
<thead>
<tr>
<th>Acoustic phonon</th>
<th>( g_u = 19 \text{ eV} )</th>
<th>( g_d = -8.5 \text{ eV} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-polar optical</td>
<td>430</td>
<td>((DK) = 3 \times 10^8 \text{ eV cm}^{-1})</td>
</tr>
</tbody>
</table>

(ii) Intervalley scattering:

| Non-polar optical     | 315                         | \((DK) = 6 \times 10^7 \text{ eV cm}^{-1}\) |

B Two-phonon processes

<table>
<thead>
<tr>
<th>2TA (at ( \Xi = XX ))</th>
<th>240</th>
<th>( 5 \times 10^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2TO (at ( \Xi = LL ))</td>
<td>802</td>
<td>( 11.5 \times 10^3 )</td>
</tr>
</tbody>
</table>

\( m_t = 0.082m_o, m_1 = 1.6m_o, S = 5.4 \times 10^5 \text{ cm s}^{-1}, \)
\( \rho = 5.32 \text{ gm cm}^{-3}, a = 5.66 \text{ A}, \frac{\gamma}{\gamma_0} = 1.31, \frac{\gamma_1}{\gamma} = 1.61, \frac{\gamma_1}{\gamma} = 1.01 \)

* The parameters selected in the present work.
Figure 6

\[ \mu_0 (\text{cm}^2/\text{V}\cdot\text{sec}) \]

vs.

\[ T (\text{K}) \]
respectively. However, we denote simply $D_0$ by $D_{\infty}$ even though $D_0$ value selected here is for the entire short wavelength region as in (2.4).

(i) Zero Field Mobility

In figure 6, we have shown the temperature variation of $\mu_0$ in the range 30 to 300K. The solid line is due to the present work. It is obtained by adding the contributions due to various lattice scattering mechanisms, shown in Table 2, according to Matthiessen's rule. The experimental data, for non-degenerate samples, of $\mu_0$ are also shown /89,116-118/. We observe that for temperatures below 100K, $\mu_0$ is proportional to $T^{-1.5}$ which is clearly due to acoustic phonon deformation type scattering. In the temperature region 30 to 300K the temperature dependence turns out to be $T^{-1.53}$ which is in good agreement with experimental observation /89/ viz. $T^{-1.66}$. The calculated values of mobility at 77 and 300K are, respectively, 3.6 x $10^4$ and 3.85 x $10^3$ cm$^2$/Vs as against the observed values 3.3 to 4.1 x $10^4$ cm$^2$/Vs and 3.8 to 4.2 x $10^3$ cm$^2$/Vs.

(ii) Energy Relaxation Time

We have shown in Fig. 7 the temperature dependence of energy relaxation time (i.e. $T_{\epsilon}^{-1}$ vs $T$), in the warm electron region, which is obtainable by differentiating
Inverse energy relaxation time vs lattice temperature, in n-Ge, for different processes given in Table 2. (1) acoustic, (2) TA (240K), (3) 315K, (4) 430K, (5) TO (803K) and (6) total due to (1) to (5).
Figure 8

Inverse energy relaxation time vs lattice temperature in n-Ge. Theoretical curve (1) is due to all processes given in Table 2; curve (2) is due to all one-phonon processes given in Table 2 but with $(DK) (430K) = 6.6 \times 10^5 \text{eV cm}^{-1}$ in place of $J x 10^5 \text{eV cm}^{-1}$. Experimental points: $\circ$ /92-94/, $\ast$ /97/, and $\square$ /96/.
the power loss with respect to electron temperature $T_e$ for each scattering process (see 2.3). The curve 1 is due to acoustic phonon scattering which is the most dominant energy loss process, in the temperature range 30 to 600K, over the other one-phonon and two-phonon processes (curves 2 to 5). However, contributions of these latter processes are also significant especially above 160K. The variation of energy relaxation time with temperature for optical and two-phonon processes is essentially \( \left( \frac{1}{T^2} \right) \exp \left( -e/T \right) \) for \( e \gg T \). Consequently these mechanisms contribute considerably in higher temperature range, provided coupling constants are reasonably fixed. Curve 6 in Fig. 7 represents the total inverse energy relaxation time obtained by adding the inverse energy relaxation times due to all individual mechanisms.

We have compared the calculated total inverse energy relaxation time with experimental observations /92-94, 96, 97/ in figure 8. Curve 1 is due to present work which includes all processes given in Table 2. Curve 2 is due to only one-phonon processes wherein we have used the value for $D_K$ (intravalley) = $6.6 \times 10^8$ eV cm$^{-1}$, a value used to fit $\mu_0$ with one-phonon mechanisms. We notice that curve 1 is in better agreement with the experimental data than curve 2 both in temperature dependence and magnitude. The experimental value of inverse energy relaxation time
at 77K ranges from $2.75 \times 10^{10}$ to $3.5 \times 10^{10} \text{s}^{-1}$ /92,96/ and at 200K it is $1.6 \times 10^{11} \text{s}^{-1}$ /97/. Our calculated values, which include two-phonon processes, at these temperatures are $6 \times 10^{10} \text{s}^{-1}$ and $1.9 \times 10^{11} \text{s}^{-1}$, respectively; whereas the values due to one-phonon processes (curve 2) are $9 \times 10^{10} \text{s}^{-1}$ and $3.5 \times 10^{11} \text{s}^{-1}$. Thus we see that the inclusion of two-phonon scattering, particularly ZTO, has helped us to obtain low power loss at low temperatures (<150K) and hence makes the $\tau_{\varepsilon}^{-1}$ less steeper at low temperatures, as was expected. If one-phonon processes alone are to be used in fitting $\mu_0$, the optical intravalley coupling constant (DK) required is $6.6 \times 10^8 \text{eV cm}^{-1}$. Then this value of DK would lead to contribution to energy loss at low temperatures itself and, as we can see from curve 2, this makes $\tau_{\varepsilon}^{-1}$ larger and more steeper than that in curve 1. However, the inclusion of two-phonon processes necessitates us to use $\text{DK} = 3 \times 10^8 \text{eV cm}^{-1}$ in fitting $\mu_0$ and contribution to energy loss process, due to these high energy phonons, comes in the higher temperature region (>150K).

Thus we point out that our calculations have improved the agreement between $\tau_{\varepsilon}(\text{expt.})$ and $\tau_{\varepsilon}(\text{cal.})$.

(iv) Warm Electron Coefficient /115/

The calculation of $\beta$ is a straightforward matter as it is proportional to the product $\mu_0 \tau_{\varepsilon}$ (see 2.3.8).
Harm electron coefficient vs lattice temperature in n-Qs.

Theoretical calculations: curve (1) is due to all processes given in Table 2; curve (2) is due to all one-phonon processes given in Table 2 but with $(DK)_{430K} = 6.6 \times 10^8$ eV cm$^{-1}$ in place of $3 \times 10^8$ eV cm$^{-1}$. Experimental points: O /41/, O /45/ and X /48/. 
Making use of the calculated values of $\mu_0$ and $\tau_0$ due to all processes given in Table 2, in (2.3,8), we have obtained $\beta$ at various lattice temperatures and shown in figure 9 by curve 1. Curve 2 is due to only one-phonon processes with intravalley coupling constant $(DK) = 6.6 \times 10^8 \text{ eV cm}^{-1}$. The experimental data /40,41,98/ are also shown in the figure 9 for the purpose of comparison. The curve 1 (present work) is in very good agreement with the experimental data. We see from curve 2 that, eventhough the calculated $\mu_0$, using optical intravalley coupling constant $6.6 \times 10^8 \text{ eV cm}^{-1}$, is in agreement with $\mu_0$ experimental, the $\beta$ calculated with the same coupling constant is not in good agreement with $\beta$ observed (see curve 2). In our present work with the same set of coupling constants (Table 2) both $\mu_0$ and $\beta$ are very well explained and this we attribute to the improved agreement between $\tau_0$ (exp) and $\tau_0$ (cal) due to two-phonon processes considered in the present work.

We see that $\beta$ decreases with increasing temperature because scattering mechanisms are lattice limited as we are working with purer samples of Ge. The values of $\beta$ of our work at 100K and 300K are, respectively, $2.2 \times 10^{-5}$ and $3.3 \times 10^{-6} \text{ cm}^2 \text{ V}^{-2}$ as against the experimental values of $2 \times 10^{-5}$ and $3.2 \times 10^{-6} \text{ cm}^2 \text{ V}^{-2}$/41/.
(v) Electron Drift Velocity and Temperature

To calculate these high field properties, as we have pointed earlier, it is essential to take into consideration the non-equivalent intervalley scattering i.e. scattering from (111) set of valleys to (100) valleys besides the mechanisms shown in Table 2. We have assumed that electrons in (100) valleys are at lattice temperature i.e. $T_e = T$ in (2.6.33), (2.6.34) and (2.6.36) /112/. This is justifiable since these valleys are situated at a height of 0.18 eV from (111) minima, moreover electrons in (100) valleys are assigned the effective mass values of electrons in silicon i.e. $m_c = 0.15m_o$ and $m_l = 0.9m_o$ which are higher than those for electrons in (111) valleys of Ge. The electron mobility for (100) valleys has been taken to be 700 cm$^2$/Vs /112/ and is assumed to be independent of field in the range of interest i.e. $F = 0$ to 6KV.

We have taken the coupling constant for this non-equivalent intervalley scattering to be $5 \times 10^7$ eV cm$^{-1}$ and phonon equivalent temperature $\Theta = 315K$. Following the procedure outlined in (2,7) we have calculated the valley population and the electron drift velocity at lattice temperature 300K for various fields. The calculated $V_d$ vs $F$ is plotted in figure 10 (curve 1). We have also shown the experimental data of Smith /103/. Curve 2 is obtained
FIGURE 30

\[ V_d \times 10^6 \text{ Cm/S} \]

\[ F \text{ (KV/Cm)} \]

\[ \frac{1}{T} \]

\[ \frac{1}{T} \]

\[ 0 \]

\[ 1 \]

\[ 2 \]

\[ 3 \]

\[ 4 \]

\[ 5 \]

\[ 6 \]

\[ 7 \]

\[ 8 \]

\[ 9 \]

\[ 0 \]

\[ 1 \]

\[ 2 \]

\[ 3 \]

\[ 4 \]

\[ 5 \]

\[ 6 \]

\[ 7 \]

\[ 8 \]

\[ 9 \]

\[ 0 \]

\[ 1 \]

\[ 2 \]

\[ 3 \]

\[ 4 \]

\[ 5 \]

\[ 6 \]

\[ 7 \]

\[ 8 \]

\[ 9 \]

FIGURE 10
by leaving the contributions of non-equivalent intervalley scattering. Curve 3 is obtained by considering only one phonon processes with optical intravalley coupling constant \((\Delta K) = 6.6 \times 10^8\) eV cm\(^{-1}\) and without non-equivalent intervalley scattering. We see that inclusion of scattering to higher set of valleys is quite essential whether the scattering due to two-phonon is considered or not. But our present calculations (curve 1) show that including two-phonon processes also one can explain the field dependence of drift velocity.

We have also shown the variation of \(T_e\) with electric field in the figure 10.

Thus we wish to emphasize here that with inclusion of two-phonon processes we have been able to explain the transport properties in all the region of the electric field unlike the case with one-phonon processes.
2.9 Application to n-Silicon

In silicon, there are six equivalent valleys situated along (100) crystallographic directions with conduction band minima at 0.85 $\bar{X}$ of the Brillouin zone /21/. The energy surfaces are prolate ellipsoids of revolution around (100) with $m_{\parallel} > m_{\perp}$. For $F$ along [111], the valleys are all equivalent. From these considerations the method developed in (2,6) is applicable to silicon. Now we briefly summarize the various possible scattering mechanisms in Si and then present our calculations based on (2,6) for the configuration in which the valleys are equivalent.

2.9a Scattering Mechanisms in Silicon

As in the case of Ge, both intra and intervalley scattering are possible in Si. The intravalley scattering is known to arise from the acoustic phonon scattering. The intervalley scattering are of two distinct types, viz., $i$ and $g$. The $f$-type arises as a consequence of electronic transition between perpendicular valleys in [100] direction; $g$-type intervalley scattering arises due to electronic transition between parallel valleys. The accepted intervalley scattering, by selection rules in silicon due to one-phonon processes are: LO $g$-type (at 0.34 $\bar{X}$), LA and TO $f$-type (at $S$ on the Brillouin zone face) /119,120/.
However, TA $f$-type seems to be present in weak amount as is evident from the investigations of various authors (see ref./121/). Strong experimental evidence exists /121-124/ in favour of other processes which are otherwise forbidden by the selection rules. Besides, it may be noted that what is forbidden in one-phonon process may be an allowed process when the same phonons are involved in a multiphonon process. This is evident by two-phonon second-order Raman scattering /125,126/ and magnetophonon /124/ experiments. The intervalley scattering has been investigated from the experimental point of view by many authors in order to gain knowledge of the type and magnitude of scattering. A good account of the subject is given by Norton et al. /121/. It is evident from such studies that several models exist viz. Dumke's /127/, Long's /128/ and that of Asche et al. /129/. All the three models would lead to opposite conclusions regarding the dominance of $f$ or $g$-type scattering over one another. The calculations of Costato et al. /39/ in the low field region show that all the above mentioned models keep close to one another, since the low field properties cannot distinguish the type of scattering. Marked differences among these models and more information about the type of scattering have been found in hot electron region /130-132/.

We wish to point out that all the above mentioned
TABLE 3
Scattering mechanisms and physical parameters used in the present work, in n-Si.

<table>
<thead>
<tr>
<th>Scattering mechanism</th>
<th>Phonon equivalent temperature in K</th>
<th>Coupling constant*</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>A. One-phonon processes</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(i) Intravalley process</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Acoustic phonon</td>
<td>-</td>
<td>$\Xi_u = 8.6$ eV</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\Xi_d = -0.4$ eV</td>
</tr>
<tr>
<td>(ii) Intervalley processes</td>
<td>$\Theta/124/_{/2}$ (DK) in eV cm⁻¹</td>
<td></td>
</tr>
<tr>
<td>g-type</td>
<td>130</td>
<td>$5 \times 10^7$</td>
</tr>
<tr>
<td>f-type</td>
<td>530</td>
<td>$1 \times 10^8$</td>
</tr>
<tr>
<td>f-type</td>
<td>580</td>
<td>$1 \times 10^8$</td>
</tr>
<tr>
<td>f-type</td>
<td>690</td>
<td>$4 \times 10^8$</td>
</tr>
<tr>
<td><strong>B. Two-phonon processes</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$2TA$ (at $\Xi = \Xi X$)</td>
<td>$\Theta/9/_{/2}$</td>
<td>$D_{\Xi}$ in eV</td>
</tr>
<tr>
<td></td>
<td>420</td>
<td>$8.5 \times 10^2$</td>
</tr>
<tr>
<td>$2TO$ (at $\Xi = \Xi X$)</td>
<td>1340</td>
<td>$7.9 \times 10^3$</td>
</tr>
</tbody>
</table>

$m_e = 0.1905m_0$, $m_1 = 0.9163m_0$, $S = 9.037 \times 10^5$ cm s⁻¹,

$\rho = 2.33$ gm cm⁻³, $a = 5.4307$ Å, $\ell = 1.33$, $\eta_1 = 1.15$

$\ell_1 = 1.07$

* The parameter selected in the present work.
one-phonon models are inadequate to explain the observed warm electron properties such as $\beta$ and $T_s$ (see for e.g., figure 14 and calculations of Costato et al. /39/). However, $\mu_o$ vs $T$ and field dependence of the drift velocity by taking the effect of non-parabolicity in higher fields are properly explained /128,133,134/. In view of the above mentioned inadequacy of the scattering mechanism and because of the evidences for the strong electron-two-phonon interactions we would like to reexamine the above said transport properties considering two-phonon processes.

2.9b Comparison Between Experimental Data and Present Work /84/

Following the procedure outlined in (2.7) we have calculated numerically, $\mu_o$, $T_s$, $\beta$, $V_d$ and $T_e$ in a wide range of temperature for field along [111] direction. For our calculations in the present work we have used the scattering mechanisms, coupling constants and equivalent phonon temperatures given in Table 3. The calculated transport properties are compared with experimental results in the following.

(i) Zero Field Mobility

In figure 11, the variation of $\mu_o$ with lattice temperature $T$ is shown together with experimental data
$\mu_0$ (Cm$^2$/Vs)

$T$ (K)

FIGURE 11
Inverse zero field mobility vs lattice temperature in n-Si due to various independent processes given in Table 3: (1) acoustic, (2) 130K, (3) 420K (2TA), (4) 690K, (5) 1340K (2TO) and (6) total. The curves due to 520K and 580K phonons are less than $10^{-5}$ vs cm$^{-2}$. 

FIGURE 12

Inverse zero field mobility vs lattice temperature in n-Si due to various independent processes given in Table 3: (1) acoustic, (2) 130K, (3) 420K (2TA), (4) 690K, (5) 1340K (2TO) and (6) total. The curves due to 520K and 580K phonons are less than $10^{-5}$ vs cm$^{-2}$. 

FIGURE 12
of various authors /121,128,135-137/ in the temperature range of 30 to 300K. It is to be noted that the agreement between our calculations and the experimental data of Long /128/ is good. Infact, our calculations indicate that $\mu_o$ is proportional to $T^{-1.92}$ and Long's data exhibits $T^{-2.0}$ dependence. The agreement is understandable, since the Long's data corresponds to lattice limited zero field mobility. The discrepancy between our calculations and the experimental data of others /121,135-137/ at low temperatures is understandable for the following reason. In this low temperature region the observed mobilities are influenced by impurity scattering which is not considered in our calculations. It is to be noted that there is spread in the experimental results itself. For example at 300K observed $\mu_o$ ranges from 1200 to 1750 cm$^2$/Vs as against the calculated value $15.60 \times 10^3$ cm$^2$/Vs. Below 80K the lattice limited mobility is mostly governed by acoustic intravalley scattering. Therefore coupling constants $\Xi_u$ and $\Xi_d$ for this mechanism are fixed by fitting $\mu_o$ at low temperatures, say 30K.

In figure 12, the inverse zero field mobility as a function of temperature for all independent processes as well as the total inverse mobility due to all the processes, given in Table 3, are shown. We see that contribution of high energy phonon scattering to mobility comes above 100K. We notice from curves 3 and 5 that there is
Inverse energy relaxation time vs lattice temperature in n-Si due to different processes given in Table 3. (1) acoustic, (2) 130K, (3) 420K (ZTA), (4) 510K, (5) 580K, (6) 690K, (7) 1340K (ZST) and (8) total due to (1) to (7).
Inverse energy relaxation time vs lattice temperature in n-Si. Theoretical curves are due to (1) all processes shown in Table 3, (2) Long's model /128/, and (3) Costa and Reggiani model. Experimental data: O /93/, X /138/, □ , ○ , △ /96/.

FIGURE 14
significant contribution from 2TA and 2TO phonon processes. The values for \( \mu_0^{-1} \) (530K) and \( \mu_0^{-1} \) (580K) are less than \( 10^{-5} \) Vs/cm\(^2\) for all over the temperature range.

(ii) **Energy Relaxation Time**

In figure 13, we have shown the temperature dependence of inverse energy relaxation time in the temperature range 30 to 300K in the warm electron region for each scattering process (curves 1-7) given in Table 3 as well as the total energy relaxation time (curve 8). It may be noted that the two-phonon processes like 2TA (curve 3) and 2TO (curve 7) and the one-phonon process viz., f-type (\( \Theta = 690K \), curve 6) are the dominant processes contributing to the total energy relaxation time. The temperature dependence of energy relaxation time for all the mechanisms except acoustic intravalley scattering, is given by

\[
\frac{1}{T^2} N,
\]

where \( N \) being phonon equilibrium distribution function, as in the case of Ge.

We have compared the calculated total \( \tau_T^{-1} \) (curve 1 in figure 1) with experimental data /93,96,138/. We observe that at 77K the calculated value of \( \tau_T^{-1} \) due to our work is \( 5.5 \times 10^{10} \) s\(^{-1}\); the corresponding values due to Long's /128/ and Costato and Reggianis /133/ models are respectively, \( 1.6 \times 10^{11} \) s\(^{-1}\) and \( 2.8 \times 10^{11} \) s\(^{-1}\).
FIGURE 15

\( T (K) \)

\[ \beta \,(Cm^2/V^2) \]

-4
-5
-6
-7
-8
10
100
200
300
The latter values of \( \tau_e^{-1} \) are higher than our calculated value. Furthermore, our \( \tau_e^{-1} \) values, in the temperature range shown in Figure 14, are closer to the Hess and Seeger's experimental data /93/ than those due to other models (curves 2 and 3).

(iii) Warm Electron Coefficient

In figure 15, the calculated \( \beta \) along with experimental data /98,40/ is shown in the temperature range 70 to 300K. In calculating \( \beta \), we have made use of calculated values of \( \mu_o \) (Fig. 11) and \( \tau_e \) (Fig. 14, curve 1). There is good agreement between experimental data and present calculations except at low temperatures. The deviation at low temperatures is attributed again to impurity scattering.

(iv) Electron Drift Velocity and Temperature

In figure 16, we have shown the calculated drift velocity and electron temperature as a function of electric field in the field range 0 to \( 6 \times 10^4 \text{ V cm}^{-1} \) at lattice temperature 300K. We notice that no saturation seems to occur for drift velocity in high fields, where it is expected to occur. Recently, Canali et al /132/ have also shown, with one-phonon processes, that theoretically no saturation would be obtained within the parabolic band model for silicon. However, Jacoboni et al. /134/ have demonstrated that the inclusion of non-parabolicity in the
Electron drift velocity ($V_d$) and reduced electron temperature ($T_e/T$) vs electric field, taken along [111], at lattice temperature 300K.
calculations leads to saturation of $V_d$ and the effect of non-parabolicity on $V_d$ at the highest field ($\approx 6 \times 10^4 \text{ V cm}^{-1}$) is to reduce $V_d$ by 30%. From Fig. 16 our calculated value of $V_d$ is $1.47 \times 10^7 \text{ cm/s}$ for $F = 6 \times 10^4 \text{ V cm}^{-1}$.

If we reduce it by 30%, attributing it to non-parabolicity for the purpose of comparison, we get $V_d = 10^7 \text{ cm s}^{-1}$ which is same as the experimentally observed saturation value /134, 139/. Therefore, it may be pointed out that in the hot electron region the non-parabolic effect should be included for quantitative experimental comparison.
2.10 Discussions and Conclusions

The transport theory of many-valley semiconductors, developed in section (2.6) taking into consideration carrier-two-phonon (short wavelength) scattering besides the usual one-phonon mechanisms, has been applied to n-Ge and n-Si. In such developments the displaced Maxwellian distribution function for electrons has been assumed as a solution of Boltzmann transport equation for simplicity. However, we wish to point out that it is a reasonable approach in view of the following points.

It is well known that if the interelectronic collisions are dominant over the lattice scattering mechanisms then the displaced Maxwellian distribution function would be enforced \(^{48}\). This requires a large carrier concentration and a critical value \(n_p\), above which the displaced Maxwellian distribution would result, may be calculated by equating the rate of change of momentum due to e-e collision to that due to lattice scattering. In Ge at room temperature \(n_p = 10^{17} \text{ cm}^{-3} \) \(^{140}\). But the samples, with which we have compared our transport calculations, are having the carrier concentrations two orders of magnitude less than that required to achieve displaced Maxwellian. Nevertheless, it has been found that the transport properties, such as \(\mu_0\) and \(V_d\), calculated by other methods
are not significantly different from those calculated by using the displaced Maxwellian distribution function in Ge. Further, we have used the symmetric part of the displaced Maxwellian distribution function which is Maxwellian at electron temperatures. This results owing to the energy randomisation of the electrons. Dumke /142/ has calculated the distribution function and has shown that it is nearly Maxwellian.

In silicon, it has been observed that in the field range 0 to $10^5$ V cm$^{-1}$ the velocity distribution is well randomised /131/ in view of the fact that $\frac{V_d}{V_{rms}}^2 \ll 1$, where $V_{rms}$ is the root mean square value of the carrier velocity. This would justify the comparison of experimental data of sample having $n = 10^{15}$ cm$^{-3}$ with our calculation eventhough our calculations require $n \sim 10^{17}$ cm$^{-3}$.

The phonon equivalent temperatures in Ge for the one-phonon processes have been selected in accordance with the dispersion relation of Brockhouse and Iyengar /8/ and these are the values widely used in the literature /17/. The two-phonon equivalent temperatures are also read from Brockhouse and Iyengar /8/ for $2TA$ and $2TO$ at critical points $XX$ and $LL$, respectively. We have selected the two-phonon equivalent temperatures for $2TA$ and $2TO$ at $XX$ and $LL$, respectively, because the interaction of electrons with
these phonons is evidenced by second-order Raman scattering experiments /99/.

In silicon the one-phonon mechanisms and phonon equivalent temperatures have been selected in accordance with the recent magnetophonon experiments /124/. The two-phonon interactions by $2\text{TA}$ and $2\text{TO}$ at $XX$ are evidenced from second-order Raman experiment /125/ and the two-phonon equivalent temperatures, for these, are read from neutron scattering data of Brockhouse /9/.

We shall now consider the various coupling constants used in the present work for Ge and Si. For acoustic modes the deformation potential coupling constants $\Xi_d$ and $\Xi_u$ for Ge, are $-8.5$ and $19$ eV, respectively, and for Si the corresponding values are $-0.4$ and $8.6$ eV. These values are very nearly the same as the ones available in literature /17,39/. For Ge the optical intravalley coupling constant has range of values from $3$ to $9 \times 10^8$ eV cm$^{-1}$ in the literature /17/ and our selection of $3 \times 10^8$ eV cm$^{-1}$ for the same is reasonable. In Ge, we have fitted $V_d$ vs $F$ by selecting non-equivalent intervalley coupling constant to be $5 \times 10^7$ eV cm$^{-1}$. This value agrees with that of Chattopadyay and Nag /112/. In Si also one-phonon coupling constants used by us (see Table 3) are in reasonable agreement with those quoted in the literature (see for e.g., /39/).
The two-phonon deformation potential constants of semiconductors have been deduced in the literature /34/. In Ge the available values of \( D_\Xi \) are only from the second-order resonant Raman scattering experiments /99/. For 2TA and 2TO they are, respectively, 170 and 2534 eV whereas the values for the same used by us are, respectively, 500 and 11500 eV. In case of silicon the values for the two-phonon deformation potential constants used by us for 2TA and 2TO are, respectively, 850 and 7900 eV. These are the same as those found from second-order non-resonant Raman scattering experiment /143/. The second order resonant Raman scattering experiment /125/ gives the values an order of magnitude less than the ones we have used. Magneto-phonon experiment /124/ gives 1750 eV for 2TA. The differences in the values of \( D_\Xi \) deduced from different sources are understandable, as pointed out in (2.3).

Now, we shall discuss the possible effect of non-parabolicity on the calculations we have carried out. Costa et al. /39/ have shown, in Si and Ge, that in low fields the effect of non-parabolicity is negligibly small and thus we are justified in using parabolic band model in our calculations of \( \mu_o, \tau'_e \), and \( \beta \). However, in high fields in silicon, as discussed earlier, non-parabolicity of the band structure need to be considered. In Ge the comparison of our calculations with experimental data shows that really
there is no necessity of inclusion of non-parabolicity. This is supported by the work of Fawcett and Paige /113/ who have shown that the non-parabolicity of the conduction band has least effect on the high field properties when one includes scattering of electrons from (111) valleys to (100) valleys.

In conclusion we wish to point out that by including the scattering due to two-phonons in the short wavelength region, besides the scattering by one-phonon, we have been able to explain low and high field electrical transport properties in Ge and Si. It is to be emphasized that the properties in the warm electron range are better explained by including two-phonon processes than only due to one-phonon processes. Further these electron-two-phonon interactions are supported from the mageto-phonon and second order Raman scattering experiments.