Non-stationary modeling of III-V compound semiconductor materials and devices

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S.C. van Someren Gréve

NON-STATIONARY MODELING
OF III-V COMPOUND
SEMICONDUCTOR MATERIALS AND DEVICES
THIS WORK WAS SUPERVISED BY DR. T.G. VAN DE ROER.
List of errata for the thesis of S.C. van someren Greve.

On page 19 equation (III-9) should read:

\[ A_{nm} = \frac{2n+1}{2} \int_{-1}^{+1} X_n(s)P_m(s) ds \quad (n,m = 0,1,2, \ldots) \]  

On page 20 expression (III-12) should read

\[ B_{nm} = \begin{cases} \frac{(n+1)(n+2)}{(2n+3)} & m = n+1 \\ \frac{n(n-1)}{(2n-1)} & m = n-1 \\ 0 & m \neq n \pm 1 \end{cases} \]  

On page 23 the sentence after (III-26) and equation (III-27) should read:

> With this function inserted equation (III-25) becomes 

\[
\frac{d}{dk} f^{(i+1)}(k) + \frac{1}{k} A^{-1} B f^{(i+1)}(k) + \frac{\gamma}{eE} A^{-1} f^{(i+1)}(k) = \frac{\gamma}{eE} A^{-1} \phi(k)
\]  

On page 26 equation (III-34) should read:

\[ \Psi(s) = \frac{-1}{(s)} \frac{\hbar}{eE} A^{-1} \]  

On page 37 the equations (III-55) and (III-56) should read:

\[ \tilde{\nu}(t) = \frac{1}{3n(t)} \frac{\hbar}{m} G_{10}(t) \]  
\[ \tilde{\varepsilon}(t) = \frac{1}{2n(t)} \frac{\hbar}{m} G_{01}(t) \]  

On page 38 the equations (III-59) and (III-60) should read:

\[ \tilde{\nu}(t) = \frac{\hbar}{nm} (\alpha_0 G_{10}(t) + \alpha_1 G_{11}(t) + \alpha_2 G_{12}(t) + \ldots) \]  
\[ \tilde{\varepsilon}(t) = \frac{\hbar^2}{2nm} (\beta_1 G_{01}(t) + \beta_2 G_{02}(t) + \beta_3 G_{03}(t) + \ldots) \]  

On page 39 equation (III-65) should read:
\[
\frac{3G_{nm}}{\partial t} = 4\pi \int_{0}^{\infty} k^{2+n+2m} dk \left[ \frac{V}{(2\pi)^{3}} \int_{0}^{\infty} k'^{2} dk' S_{n}(k',k)f_{n}(k') - v(k)f_{n}(k) \right]
\]

(III-65)

On page 40 the equations (III-66) and (III-67) should read:

\[
\frac{3G_{nm}}{\partial t} = 4\pi \int_{0}^{\infty} k^{2} \Omega_{n}(k)f_{n}(k)dk
\]

\[
\Omega_{n}(k) = k^{n} (\gamma_{0} + \gamma_{1}k^{2} + \gamma_{2}k^{4} + \ldots)
\]

(III-66) (III-67)

On page 45 equation (III-76) should read:

\[
\phi_{\text{ns}p} = \frac{1}{k} \int_{0}^{2\pi} \frac{H_{2m}(\xi)}{\xi^{n}} \left\{ A_{ns} \frac{d}{d\xi} + B_{ns} \xi \right\} \xi^{m} H_{2p}(\xi) \exp(-\xi^{2}) d\xi
\]

(III-76)

On page 46 equation (III-80) should read:

\[
\nu = \frac{4\pi}{3} \int_{0}^{\infty} \xi^{3} v(\mu) \frac{d}{d\xi} F_{l_{m}} H_{2m}(\xi) \exp(-\xi^{2}) d\xi = \sum_{m} \alpha_{m} F_{l_{m}}
\]

(III-80)

The end of page 49 should read:

= number of Hermite polynomials is 8. Eq. (III-90) would give ...

On page 60 the equations (IV-9), (IV-10) and (IV-11) should read:

\[
v(k) \frac{\partial}{\partial x} h(x,k)^{(n)} + e_{h} \frac{\partial}{\partial k} h(x,k)^{(n)} = \frac{e_{h}}{\hbar} (k;\theta)^{n-1}(x,k)
\]

(IV-9)

\[
k = k_{0} + \frac{e_{h}}{\hbar} t
\]

\[
x = x_{0} + \int_{0}^{t} v(k_{0}+t) dt = x^{+}(x_{0},t)
\]

(IV-10)

\[
k = k_{0} + \frac{e_{h}}{\hbar} t
\]

\[
x = x_{0} - \int_{0}^{t} v(k_{0}-t) dt = x^{-}(x_{0},t)
\]

(IV-11)

On page 61 equation (IV-16) should read:
\[
\int_0^{n+2+2m} v(k)f_{n+1} dk = \sum_{r=0}^{\infty} V_1 G_{n+1,m+r} \quad (n=0,1,2,\ldots)
\]

(IV-16)

\[
\int_0^{n+2+2m} v(k)f_{n-1} dk = \sum_{r=0}^{\infty} V_2 G_{n-1,m+r}
\]

On page 62 equation (IV-17) should read:

\[
\frac{\partial G}{\partial t} = \frac{eE}{h} \left\{ \frac{(2m+2n+1)n}{(2n-1)} G_{n-1,m} + \frac{2m(n+1)}{(2n+3)} G_{n+1,m-1} + \right.
\]

\[
\left. \frac{3}{2^m} \sum_{p} V_2 G_{n,m-1,m+p+1} + \frac{n+1}{(2n+3)} \sum_{p} V_1 G_{n,m,n+1,m+p} \right\} = \left( \frac{\partial G}{\partial t} \right)_{\text{coll}}.
\]

(IV-17)

In the middle of page 74 it should read:

step (IV-43) or (IV-46) is then replaced by:

On page 78 fig.V-1 and the figures on page 80, 81, 82, 90, 91, 92 and 93 the device dimensions should be:

-------- 0.5----------1.5-----

\[x(\mu m)\]
NON-STATIONARY MODELING OF III-V COMPOUND SEMICONDUCTOR MATERIALS AND DEVICES

PROEFSCHRIFT

ter verkrijging van de graad van doctor in de technische wetenschappen aan de Technische Hogeschool Eindhoven, op gezag van de rector magnificus, prof.dr. S.T.M. Ackermans, voor een commissie aangewezen door het college van dekaten in het openbaar te verdedigen op 9 november 1984 te 16.00 uur

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## CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>References</td>
<td>7</td>
</tr>
<tr>
<td>II. BASIC EQUATIONS</td>
<td>8</td>
</tr>
<tr>
<td>II-1. Transport equations.</td>
<td>11</td>
</tr>
<tr>
<td>II-2. Scattering mechanisms.</td>
<td>17</td>
</tr>
<tr>
<td>III. THE SPACE-INDEPENDENT PROBLEM</td>
<td>18</td>
</tr>
<tr>
<td>III-1. Legendre polynomial expansion of Boltzmann equation</td>
<td>23</td>
</tr>
<tr>
<td>III-2. The method of Hammar.</td>
<td>25</td>
</tr>
<tr>
<td>III-3. Transforming to an integral form.</td>
<td>29</td>
</tr>
<tr>
<td>III-4. Numerical implementation and results.</td>
<td>36</td>
</tr>
<tr>
<td>III-5. The method of Generalized Transport Quantities</td>
<td>44</td>
</tr>
<tr>
<td>III-6. The method of Hermite polynomials.</td>
<td>49</td>
</tr>
<tr>
<td>III-7. Numerical results.</td>
<td>57</td>
</tr>
<tr>
<td>References</td>
<td>58</td>
</tr>
<tr>
<td>IV. THE SPACE DEPENDENT PROBLEM</td>
<td>58</td>
</tr>
<tr>
<td>IV-1. Discussion previous methods.</td>
<td>63</td>
</tr>
<tr>
<td>IV-2. The LHE method.</td>
<td>65</td>
</tr>
<tr>
<td>IV-3. Numerical solutions.</td>
<td>76</td>
</tr>
<tr>
<td>References</td>
<td>77</td>
</tr>
<tr>
<td>V. RESULTS ON ONE-DIMENSIONAL DEVICES</td>
<td>77</td>
</tr>
<tr>
<td>References</td>
<td>96</td>
</tr>
<tr>
<td>VI. THE TWO-DIMENSIONAL PROBLEM</td>
<td>97</td>
</tr>
<tr>
<td>References</td>
<td>114</td>
</tr>
</tbody>
</table>
I. INTRODUCTION

In recent years considerable interest has developed in the calculation of carrier distribution functions in semiconductors. With the short dimensions and time scales in which modern devices operate, the macroscopic quantities like the averaged carrier velocity and energy do not attain instantaneously the stationary values corresponding to a given field. In modern materials like GaAs these quantities can even considerably exceed to a great extent their stationary values.

It is clear that in the simulation of these small devices transport equations, which make use of field dependent mobility and diffusivity are no longer adequate. More sophisticated methods are needed which give more information about the distribution function (D.F.).

The most rigorous method is to simulate the entire D.F. in phase space either as a continuous function in the fluid approximation (Iterative method) or as a collection of points in the Monte Carlo (M.C.) method.

Of the iterative methods the best known is the method of Rees [1] in which the time dependent D.F. is calculated by converting Boltzmann's equation to an integral equation which is iteratively solved. The D.F. is approximated by points in a $k$-space grid. According to Rees their number should be around 1000 for realistic calculation of a high field D.F. for GaAs.

To simulate time and space-dependent situations the iterative method will be too costly in computer memory and time.

To reduce these Rees [2] used a set of steady state functions as a basis to represent the time-space dependent D.F. In this way he formulated a matrix representation of the microscopic transport properties of the free carriers.

The Monte Carlo (M.C.) method [3] which is based on simulation of
the motion of one or a number of carriers allows complicated band structures and complicated scattering mechanisms to be taken into account. The method has the advantage of being free from approximations other than the models of bandstructure and scattering rates. The disadvantage is that the simultaneous simulation of a large number of carriers will become costly in memory and time just as the iterative method. Especially when a device has great variations in doping concentration the space and time-dependent simulation will suffer from large fluctuations unless a very large number of carriers is taken into account. This is often beyond the capacity of a medium-sized computer.

Different methods are based on the assumption that not all the details of the D.F. have to be known in order to get accurate knowledge of the macroscopic quantities. The space and time-dependent method of Rees mentioned before is an example of this. The simplest way is to include in the macroscopic transport equations, apart from the averaged velocity and density, also the averaged energy of the carriers. In this way the averaged velocity and energy do not need to be single valued functions of the electric field but relax to the stationary values with properly defined energy dependent relaxation times.

This method, proposed by Bløtekjær [4] and applied by Shur [5] is simple and gives satisfactory results in the space-independent problem. Defining diffusion in this model is not straightforward, especially in III-V compounds like GaAs. Despite the fact that this method may not be really justified, it is the most practical and surely the fastest one to get some insight in the behaviour of GaAs devices.

Many analyses have been made assuming that the D.F. evolves through the different states as a displaced Maxwellian. It has been shown and will be also in this work that the D.F., although in some cases behaving as a displaced Maxwellian, most of the time doesn't come
near such a shape. In GaAs such a proposition is certainly not justified.

An extended definition of a displaced Maxwellian has been proposed by Grubin [6]. This model allows for more general shapes of the D.F. A lot of assumptions have to be made however and the scattering rates have to be adapted to this method.

Another method has been introduced by Hammar [7]. In the case that the electric field forms an axis of symmetry the angular dependence of the D.F. can be expanded in Legendre polynomials. This leads to an infinite set of differential equations which, after truncation, can be solved iteratively. The difficulty with this method is that the equations have homogeneous solutions which explode either at zero momentum or at infinity. Hammar found a clever method to subtract the unwanted solutions during numerical integration. The method however becomes very complicated when a large number of equations is taken into account. With a small number of equations the details of the D.F. are lost but Hammar has demonstrated that averages like velocity and energy are still obtained with good accuracy. Hammar applied his method to obtain stationary values for the macroscopic quantities but his method can easily be modified to simulate time-dependent problems. Compared to the method of Rees there is a reduction of points in k-space when a small number of equations is taken into account. Including space dependence into this method may be possible, but then it will also be costly in memory and time.

For the space-dependent problem the present situation is that we have two extremes. On one hand accurate but very costly methods like M.C. and the iterative methods, on the other hand very simplified macroscopic equations which are far less costly but whose justification is questionable in the treatment of III–V compounds. The peculiar properties of the latter result from the fact that being in the lowest energy minimum the carriers lose far less momentum and energy than in the higher lying minima. All knowledge
of occupation number of the carriers in these "valleys" is lost. Especially in the case of the transferred electron devices which can only be understood from the fact that the carriers are scattered to higher lying minima (satellite valleys) one would like to have information about the macroscopic averages in each minimum.

In this work we try to bridge the gap by developing a method that is less costly than the M.C. or iterative ones but more accurate than the relaxation time approach. We limit ourselves to the one-dimensional problem. The electric field has only one component in real space.

In Chapter II the basic equations and scattering mechanisms which are used throughout this work will be given. In Chapter III the Boltzmann Transport Equation will be developed in a expansion of Legendre polynomials. The method of Hammar which is based upon this expansion will shortly be discussed. In paragraph 3, we will improve the method of Hammar by transforming the equations into an integral form. Although Hammar subtracted unwanted solutions, instabilities could occur after many iterations unless a number of precautions was taken. This transformation removes this tendency. Moreover each iteration step is now equivalent to a physical time step. Furthermore the method is not more difficult to implement numerically for a large number of equations then for a small number. We will show that this method is very successful for the time-dependent problem of GaAs.

The results obtained form a basis for constructing more efficient methods.

In Chapter III, paragraph 5, a method is constructed based on moments which can deal with each valley separately. To do this more parameters appear to be necessary compared to the energy relaxation method which does not deal with each valley separately. Only by including many more moments, each being important, velocity overshoot can be described accurately enough. Scattering has to be
incorporated in a far more sophisticated way than by simply using energy-dependent relaxation times. This method is successful for the time-dependent problem of GaAs.

The use of Legendre polynomials showed that when the macroscopic quantities depend only on the first two expansion coefficients already a limited number of these (e.g. four) will give these averages already quite accurately. This property is fully exploited in Chapter III, paragraph 6. Here the radial part of the D.F. will be expanded in Hermite polynomials. The D.F. is now represented by a number of expansion coefficients which are functions of space and time. In this Chapter only the space-independent problem will be treated. Not only is this method far more efficient than the M.C. or iterative method but it is nearly as accurate for the cases of interest. The strength of this method is that all the transport and scattering parameters can be obtained directly by numerical means. No assumptions or expensive preliminary calculations are needed.

In Chapter IV the time and space-dependent problem is discussed. Only the LHE method (Legendre - Hermite Expansion) is fully investigated for reasons mentioned there. Algorithms will be given and discussed with which the time and space dependent problem can successfully be handled. Results on one-dimensional devices will be given in chapter V.

The LHE method can also be extended to the two-dimensional problem. The resulting equations will be given in Chapter VI. Unfortunately any numerical evaluation of this problem was beyond the capacity of the available numerical facility.

Nearly all the work was done for GaAs. The methods outlined can however easily be adopted for Si. In this case the dimensions of future devices will make more accurate simulations necessary. The
LHE method may be ideal for this.
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ITERATIVE METHOD FOR CALCULATING HOT CARRIER DISTRIBUTIONS IN SEMICONDUCTORS.
II. BASIC EQUATIONS

II-1. Transport equations.

In this work we are concerned with the transport of charge carriers in semiconductors. The basic equation which describes the phenomena is the Boltzmann equation:

\[
\frac{\partial}{\partial t} f(k, x, t) + \frac{d k}{d t} \cdot \nabla f(k, x, t) + v \cdot \nabla f(k, x, t) = Sf(k, x, t) \quad (II-1)
\]

were the D.F. \( f(k, x, t) \) denotes the probability that a charge carrier occupies a state at time \( t \) described by the wavevector \( k \) and positionvector \( x \).

In this work we consider the electric field \( E \) as the only external force acting on a carrier. The rate of change of the wavevector is therefore given by:

\[
\frac{d k}{d t} = \frac{e}{h} E(x, t) \quad (II-2)
\]

e and \( h \) being the charge of the electron and Planck's constant respectively. \( v \) is the velocity of a charge carrier

\[
v(k) = \frac{1}{h} \frac{\partial}{\partial k} \varepsilon(k) \quad (II-3)
\]

\( \varepsilon(k) \) describes the energy of a carrier in state \( k \) as a function of \( k \). The scattering operator \( S \) describes the rate of change of the D.F. due to scattering.

In this work we are not going into too much detail about the bandstructure given by the function \( \varepsilon(k) \) or in the examination of the different expressions of the scatteroperators. We take the expressions given in the litterature [1] for granted.

For the bandstructure we assume that for the cases of interest to us
the Kane model [2] is sufficiently accurate. The different states are treated as a continuous function and the relationship between the energy and state \( k \) is approximated by:

\[
\varepsilon(1+\alpha) = \frac{\hbar k^2}{2m} \equiv \gamma(k)
\]

(II-4)

\( \alpha \) and \( m^* \) being the non-parabolicity parameter and effective mass at zero \( k \) of the carriers respectively. In the materials of interest to us the bandstructure has different minima. Equation (II-4) can be applied to each minimum having its own different values for the non-parabolicity parameter and effective mass. In Appendix A more details of the numerical values of the parameters are given.

We shall deal only with the situation that the semiconductor is non-degenerate. This means that any state to which a carrier can be scattered is assumed to be unoccupied.

The rate of change of the D.F. due to scattering is then given by:

\[
\tilde{S} f(k, \mathbf{r}, t) = \sum_{k'} \left[ S(k', k)f(k', \mathbf{r}, t) - S(k, k')f(k, \mathbf{r}, t) \right]
\]

(II-5)

were \( S(k', k) \) is the probability per unit time of scattering of a carrier from state \( k' \) to state \( k \). In practice we will replace the summation in equation (II-5) by an integral over \( k \)-space.

\[
\sum_{k} \rightarrow \frac{V}{(2\pi)^3} \int dk
\]

(II-6)

were \( V \) is the volume of a cell in which all the states are considered. We define the following functions:

\[
g(k, \mathbf{r}, t) = \frac{V}{(2\pi)^3} \int S(k', k)f(k', \mathbf{r}, t)dk'
\]

(II-7)
and
\[ v(k) = \frac{V}{(2\pi)^3} \int S(k, k') dk' \] (II-8)

If one introduces polar coordinates and take the polar axis in the direction of \( k \) expression (II-8) transforms into:
\[ v(k) = \frac{V}{(2\pi)^3} \int k' dk' \int \sin \theta' d\theta' \int S(k, k') d\phi' \] (II-9)

The rate of change of the D.F. due to scattering can then be written as:
\[ \tilde{S}f(k_0, r, t) = g(k_0, r, t) - v(k) f(k, r, t) \] (II-10)

The scattering probabilities of interest to us will be discussed in the next paragraph.
Once the D.F. \( f(k, r, t) \) has been calculated the macroscopic quantities can be found. The carrier concentration:
\[ n(r, t) = \int f(k, r, t) dk \] (II-11)

The averaged velocity of the carriers:
\[ \tilde{v}(r, t) = \frac{1}{n(r, t)} \int v(k) f(k, r, t) dk \] (II-12)

and the mean energy:
\[ \tilde{\varepsilon}(r, t) = \frac{1}{n(r, t)} \int \varepsilon(k) f(k, r, t) dk \] (II-13)
I-2 Scattering mechanisms.

The total scattering rate \( S_{\mathbf{k}, \mathbf{k}'} \) is a sum of scattering rates due to different processes. The probability of each process is calculated by means of Fermi's golden rule:

\[
S_p(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} \left| \left< \mathbf{k} \left| H_{\text{int}, p} \right| \mathbf{k}' \right> \right|^2 \delta(\varepsilon_{\text{final}} - \varepsilon_{\text{initial}}) \quad (II-14)
\]

where \( H_{\text{int}, t} \) is the Hamiltonian describing the interaction of conducting carriers with disturbances of the perfect periodicity of the crystal lattice, e.g. phonons or impurities.

\( \varepsilon_{\text{initial}} \) and \( \varepsilon_{\text{final}} \) are the energies of the electron before and after scattering. Applying perturbation theory restricts us to cases where the interaction Hamiltonian is small, i.e. to cases where scattering events are seldom. This condition is well fulfilled in high mobility semiconductors like the III-V compounds.

We consider the following processes:

1. **Scattering by acoustic phonons.**

If the crystal temperature is above 20 K the energy exchanged in a collision is much smaller than \( k_B T \). Therefore this scattering process may be treated as being elastic [3]. The scattering rate from state \( \mathbf{k} \) to state \( \mathbf{k}' \) is then given by [4]:

\[
S_a(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} \frac{\hbar}{2 \rho_0 \nu S} \frac{2}{\nu_0 \nu S} G(k, k') \delta(\varepsilon(k') - \varepsilon(k)) \quad (II-15)
\]

where \( \bar{\varepsilon} \) is the acoustic deformation potential constant, \( \rho_0 \) the specific mass of the crystal, \( \nu S \) the (longitudinal) sound velocity and \( V \) the volume of the crystal. The function \( G(k, k') \) is the overlap
integral of the cell periodic parts of the electron wave functions. This integral is approximately equal to (see [4]):

\[ G(k,k') = (a_k^* a_{k'} + c_k c_{k'} \cos \beta)^2 \]  \hspace{1cm} (II-16)

where:

\[ a_k = \sqrt{\frac{1+\alpha \varepsilon(k)}{1+2\alpha \varepsilon(k)}} \quad ; \quad c_k = \sqrt{\frac{\alpha \varepsilon(k)}{1+2\alpha \varepsilon(k)}} \]  \hspace{1cm} (II-17)

and \( \beta \) is the angle between \( k \) and \( k' \). To determine the probability that an electron is scattered out of state \( k \) by acoustic phonon scattering we have to sum over the final states and over absorption and emission. Replacing the summation by an integral according to (II-6) and integrating according to (II-9) we arrive at:

\[ v_a(k) = \frac{\xi^2 k_B T}{4 \pi^2 p_0^2 v_s h} \rho(E) \frac{(1 + \alpha \varepsilon)^2 + (\alpha \varepsilon)/3}{(1 + 2\alpha \varepsilon)^2} \]  \hspace{1cm} (II-18)

where the density of states

\[ \rho(E) = \frac{4 \pi}{h^3} \sqrt{2m^* \varepsilon(1 + \alpha \varepsilon)(1 + 2\alpha \varepsilon)} \]  \hspace{1cm} (II-19)

2. Scattering by polar optical phonons.
In compounds the unit cell is occupied by different ions. The change in electric field between the ions when an ion is displaced relative to the other, can scatter the electrons. The scattering rate from state \( k \) to state \( k' \) is given by [4]:

\[ S_{po}(k,k') = \frac{\pi}{\hbar} \frac{\varepsilon^2 n_{po}}{2 V \varepsilon_0} \left( \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0} \right) \frac{1}{|k - k'|} G(k,k') \left( N_{po} + \frac{1}{2} \pm \frac{1}{2} \right) \delta(\varepsilon(k') - \varepsilon(k) \pm \hbar \omega_{po}) \]  \hspace{1cm} (II-20)
where \(h \omega_{p0}\) is the energy of the polar optical phonon. \(\varepsilon_0\) and \(\varepsilon_\infty\) are the relative static and "infinite" frequency dielectric constants respectively. \(G(k,k')\) is the overlap integral of the electron wave functions given by (II-16)

\[
N_{p0} = \left[ \exp\left( \frac{\hbar \omega_{p0}}{k_B T} \right) - 1 \right]^{-1}
\]

(II-21)

is the phonon number. The scattering rate out of state \(k\) is given by:

\[
v_{p0}(k) = \frac{\varepsilon_0^2 \omega_{p0}^2}{8 \pi^2 m \varepsilon_0} \left( \frac{N_{p0}}{\varepsilon_\infty - \varepsilon_0} \right) \left( N_{p0} + \frac{1}{2} \right) \frac{\rho(\varepsilon')}{kk'}
\]

\[
\left[ (a_k a_{k'} + c_k c_{k'}) \frac{k^2 + k'^2}{2kk'} \right]^{2} \left| \frac{k + k'}{k - k'} \right|^2 \ln \left( \frac{k + k'}{k - k'} \right) - c_k c_{k'} \left( 2a_k a_{k'} + \frac{k^2 + k'^2}{2kk'} \right) c_k c_{k'}
\]

(II-22)

where

\[
\varepsilon' = \varepsilon \pm h \omega_{p0} \quad ; k' = \sqrt{2m \gamma(\varepsilon')/\hbar}
\]

and

\[
\rho(\varepsilon') = \begin{cases} \\
\frac{4\pi}{\hbar^3} \sqrt{2m \varepsilon'(1 + \alpha \varepsilon')(1 + 2\alpha \varepsilon')} & \text{if } \varepsilon' > 0 \\
\frac{4\pi}{\hbar^3} \sqrt{\varepsilon'(1 + \alpha \varepsilon')(1 + 2\alpha \varepsilon')} & \text{if } \varepsilon' < 0
\end{cases}
\]

(II-23)

3. Equivalent and non-equivalent intervalley scattering.

The scattering of an electron from one valley to another equivalent
or non-equivalent valley is accompanied by the emission or absorption of a phonon. This process can only take place if the energy of an electron exceeds the energy of the bottom of the valley to which it is scattered. The scattering rate from state $k$ to state $k'$ is given by [4]:

$$ S_{i,j}^{(k,k')} = \left( Z_j - \delta_{ij} \right) \frac{2\pi D_{ij}^2}{\hbar} \frac{\hbar^2}{2\rho_0 \omega_{1j}} G_{ij}^{(k,k')} $$

where $D_{ij}$ is a coupling constant for intervalley scattering. The electron scatters from the valley with the index $i$ to the valley with the index $j$. The minima of the valleys are situated at energies $\Delta_i$ and $\Delta_j$ respectively. $Z_j$ indicates the number of equivalent valleys of type $j$ and $\delta_{ij}$ is the Kronecker delta function. $\hbar \omega_{1j}$ is the energy of the phonon involved. The overlap integral is given by:

$$ G_{ij}^{(k,k')} = \frac{(1 + \alpha_i \varepsilon_i)(1 + \alpha_j \varepsilon'_j)}{(1 + 2\alpha_i \varepsilon_i)(1 + 2\alpha_j \varepsilon'_j)} $$

The expression for the phonon number is similar to (II-23). The scattering rate of state $k$ to another valley is:

$$ \nu_{ij}^{(k)} = \frac{D_{ij}^2}{2\pi \rho_0 \hbar \omega_{1j}} \frac{1}{Z_j - \delta_{ij} - \rho \left( \varepsilon_i + \Delta_i - \Delta_j \pm \hbar \omega_{1j} \right)} $$

where
\[
\rho_j(\varepsilon) = \begin{cases} 
\frac{4\pi}{\hbar^3} \sqrt{2m_j^*(1 + \alpha_j \varepsilon)} (1 + 2\alpha_j \varepsilon) & \text{if } \varepsilon > 0 \\
0 & \text{if } \varepsilon < 0
\end{cases}
\] 

(II-27)

4. Scattering by optical phonons.

This process does not occur in all the valleys of compound materials. Using the three-valley model for GaAs this scattering process occurs only in the L valley. There its effect is masked by other processes. Its description is the same as for equivalent intervalley scattering if one replaces:

\[ Z_j = \delta_{ij} + 1 \]

5. Impurity Scattering.

This scattering process is elastic. We adopt the Brooks-Herring model. Positive or negative charged atoms in the crystal lattice form point-like charges which are surrounded by a space charge created by the surrounding electrons. These charges create a field which scatters the electrons. The potential is assumed to be a Yukawa potential. The scattering rate from state \( k \) to state \( k' \) is:

\[
S_{imp}(k, k') = \frac{4}{(2\pi \varepsilon_0 \varepsilon_s)^2} \frac{G(k, k')}{2\hbar} \frac{\delta[\varepsilon(k) - \varepsilon(k')]}{(|k-k'|^2 + \zeta^2)^2} 
\]

(II-28)

where

\[
\zeta^2 = \frac{2n_e}{\varepsilon_0 \varepsilon_s k_B T_e} 
\]

(II-29)

\( n_e \) and \( T_e \), being the electron density and electron temperature
respectively.

\[ N_i = N_a + N_d \]

\( N_a \) and \( N_d \) being the ionised acceptor and donor density, respectively. In this model the electron gas is assumed to be in thermodynamic equilibrium. The model will however be applied to situations where this is not true. The parameter \( T_e \) can be adapted to the state of the electron gas. The overlap integral is the same as (II-16). No great errors are introduced if one puts \( G(k,k') = 1 \). This will simplify the calculations considerably. The scattering rate out of state \( k \) is then given by:

\[ v_{imp}(k) = \frac{4 \pi \hbar^2}{\hbar^2 \varepsilon_0} \frac{1}{\hbar^2} \frac{1}{k \left[ 1 + (\zeta/k)^2 \right]} \]  

(II-30)
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MONTE CARLO DETERMINATION OF ELECTRON TRANSPORT PROPERTIES
IN GALLIUM ARSENIDE.
III. THE SPACE-INDEPENDENT PROBLEM

III-1. Legendre polynomial expansion of Boltzmann's equation.

Boltzmann's equation in its space-independent form reads (see II-1)

$$\frac{3}{\delta t} f(k, t) + \frac{eE}{\hbar} \cdot \nabla_k f(k, t) = g(k, t) - \nu(k)f(k, t)$$  \hspace{1cm} (III-1)

We assume that the scattering processes are isotropic and the bandstructure has spherical symmetry. \(\nu(k)\) and \(\varepsilon(k)\) are then functions of modulus \(k\) alone:

\[ \nu(k) = \nu(k) \text{ and } \varepsilon(k) = \varepsilon(k) \]

When the electric field \(E\) has only one component in real space it can be shown that any deviation of the D.F. from rotational symmetry, with an axis parallel to \(\vec{E}\), dies out in time. We assume this symmetry to be present all the time. We can write the D.F. as:

\[ f(k,t) = f(k,\cos\theta,t) \]  \hspace{1cm} (III-2)

were \(k\) is modulus \(k\) and \(\theta\) the angle between the vector \(k\) and the electric field \(E\). Making the substitution:

\[ s = \cos\theta \]

we can write equation(III-1) as:

$$\frac{3}{\delta t} f(k, s, t) + \frac{eE}{\hbar} \left[ s \frac{3}{3k} + \frac{1-s}{k} \frac{2}{3s} \right] f(k, s, t) =$$

$$g(k, s, t) - \nu(k)f(k, s, t)$$  \hspace{1cm} (III-3)
The next step is to apply a Legendre polynomial expansion to the functions $f$ and $g$:

$$f(k,s,t) = \sum_{n=0}^{\infty} f_n(k,t) P_n(s) \quad g(k,s,t) = \sum_{n=0}^{\infty} g_n(k,t) P_n(s) \quad (III-4)$$

The Legendre polynomials satisfy the orthogonality relation:

$$\int_{-1}^{1} P_m(s) P_n(s) ds = \begin{cases} \frac{2}{2m+1} & m = n \\ 0 & m \neq n \end{cases} \quad (III-5)$$

In the following we will also have use of the recurrence relations:

$$nP_n(s) - (2n-1)sP_{n-1}(s) + (n-1)P_{n-2}(s) = 0 \quad (III-6)$$

$$(1-s^2)P'_n(s) + nsP_n(s) -nP_{n-1}(s) = 0 \quad (III-7)$$

Inserting the expansion (III-4) into (III-3) and applying the orthogonality relation (III-5) we arrive at an infinite set of equations:

$$\frac{\partial}{\partial t} f_n(k,t) + \sum_{m} A_{nm} \frac{\partial}{\partial k} f_m(k,t) + \frac{1}{k} B_{nm} f_n(k,t) = g_n(k,t) - \nu(k)f_n(k,t) \quad (III-8)$$

with:

$$A_{nm} = \frac{2m+1}{2} \int_{-1}^{1} s P_n(s) P_m(s) ds \quad (n,m = 0,1,2,\ldots) \quad (III-9)$$
Using the recurrence relations (III-6) and (III-7) we can evaluate the integrals as:

\[
A_{nm} = \begin{cases} 
\frac{n+1}{2n+3} & m = n+1 \\
\frac{n}{2n-1} & m = n-1 \\
0 & m \neq n \pm 1 
\end{cases} \quad (III-11)
\]

\[
B_{nm} = \begin{cases} 
\frac{(n+1)(n+2)}{(2n+3)} & m = n+1 \\
-\frac{n(n+1)}{(2n-1)} & m = n-1 \\
0 & m \neq n \pm 1 
\end{cases} \quad (III-12)
\]

To solve the set of equations one has to close the system. One way to do this is to truncate it after N terms. Then (III-8) can be written in vector notation as:

\[
\frac{3}{\hbar} \frac{\partial}{\partial t} f(k,t) + \frac{eE}{\hbar} \left\{ A \frac{\partial}{\partial k} + \frac{B}{k} \right\} f(k,t) = g(k,t) - \nu(k)f(k,t) \quad (III-13)
\]

Note that, unlike the usual convention the indices number from zero to N-1, instead of 1 to N. This is done to remain consistent with the numbering of the Legendre polynomials.

Since the D.F. is symmetric around the axis formed by the electric field one can substitute:

\[
\int dk = 2\pi \int_0^\infty k^2 dk \int_0^\pi \sin \theta d\theta = 2\pi^2 \quad (III-14)
\]
The expressions for the macroscopic quantities \( (\text{II-11,12,13}) \) transform using the orthogonality relations \( (\text{III-5}) \) into:

\[
\begin{align*}
n(t) &= 4\pi \int_{0}^{\infty} k^2 f_0(k,t) dk \\
\tau(t) &= \frac{4\pi}{3n} \int_{0}^{\infty} v(k) k^2 f_1(k,t) dk \\
\varepsilon(t) &= \frac{4\pi}{n} \int_{0}^{\infty} \varepsilon(k) k^2 f_0(k,t) dk
\end{align*}
\]  

(III-15)  
(III-16)  
(III-17)

One pleasant property of the expansion in Legendre polynomials is that the calculation of the components of the function \( g(k,t) \) is particularly simple. The scattering processes we deal with have transition probabilities which only depend on the angle between \( k' \) and \( k \) and on their position in \( k \)-space. Therefore we can make the expansion:

\[
S(k',k,\cos \beta) = \sum_{m=0}^{\infty} S(k',k) P_m(\cos \beta)
\]  

(III-18)

where \( \beta \) is the angle between \( k' \) and \( k \). The angular coordinates of \( k' \) are \( \theta', \phi' \) and of \( k \) are \( \theta, \phi \) so

\[
\cos \beta = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos(\phi - \phi')
\]  

(III-19)

The addition theorem (cf Wittaker & Watson p.395 [1]) for Legendre polynomials states that if \( \cos \beta \) is given by equation (III-19) then:

\[
\begin{align*}
P_m(\cos \beta) &= P_m(\cos \theta)P_m(\cos \theta') + \\
&\quad \quad \quad 2 \sum_{k=1}^{m} \frac{(m-k)!}{(m+k)!} P_k(\cos \theta)P_k(\cos \theta') \cos(k(\phi - \phi'))
\end{align*}
\]  

(III-20)
Inserting the expansions (III-4) and (III-18) in the equation for the function $g(k)$ given by (II-7) one finds:

$$g(k) = \frac{V}{(2\pi)^3} \int_0^\infty k'^2 \int_0^{2\pi} \int_0^\pi \sum_{n,m} \delta(k',k) f_n(k')$$

$$\int \sin \theta' \theta' \delta \rho_n^m (\cos \theta') [2\pi \rho^m_n (\cos \theta) \rho^m_m (\cos \theta') +$$

$$+ \sum_{k=1}^{m} \frac{(m-k)!}{(m+k)!} \rho^m_n (\cos \theta) \rho^m_m (\cos \theta') \int_0^{2\pi} \cos k(\phi - \phi') d\phi']$$

Equation (III-21)

which because of the orthogonality of the Legendre functions can be reduced to:

$$g(k,\cos \theta) = \frac{V}{(2\pi)^3} \sum_{n=0}^{\infty} \frac{4\pi}{(2n+1)} \rho_n^m (\cos \theta) \int_0^{2\pi} k'^2 \int_0^\pi S_n(k',k) f_n(k')$$

Equation (III-22)

Equation (III-22) shows that the function $g(k)$ can also be expanded in Legendre polynomials. The $n$'th coefficient is given by:

$$g_n(k) = \frac{V}{(2\pi)^3} \frac{4\pi}{(2n+1)} \int_0^{2\pi} k'^2 \int_0^\pi S_n(k',k) f_n(k')$$

Equation (III-23)

To calculate $g_n(k)$ one has only to operate on the corresponding function $f_n(k)$.

Our purpose is now to solve (III-13). We shall do so in the next Chapters.

In its time-independent form equation (III-13) reads:

$$\frac{eE}{h} \left[ A \frac{d}{dk} f(k) + \frac{B}{k} f(k) \right] = g(k) - \nu(k)f(k)$$

(III-24)

which can be transformed into:

$$\frac{d}{dk} f(k) + \frac{1}{k} A^{-1} B f(k) = \frac{h}{eE} A^{-1} \left[ g(k) - \nu(k)f(k) \right]$$

(III-25)

The set (III-25) is the original form derived by Hammar [2] where he used the notation $A$ for $A^{-1}$ and $B$ for $A^{-1}B$. The transformation can only be performed if the matrix $A$ has an inverse. This is only the case if the number of expansion coefficients is even.

An iteration scheme can now be set up. With the approximation of $f(k)$ obtained in the $i$'th step the function $g(k)$ can be calculated.

$$g_m^{(i)}(k) = \frac{V}{(2\pi)^3} \frac{4\pi}{(2m+1)} \int_0^\infty S_m(k',k)f_m^{(i)}(k')dk'$$

(III-26)

With this function inserted equation (III-23) becomes a linear differential equation which gives a new $f(k)$.

$$\frac{d}{dk} f^{(i+1)}(k) + \frac{1}{k} A^{-1} B f^{(i+1)}(k) + \frac{h}{eE} A^{-1} f^{(i+1)}(k) = \frac{h}{eE} A^{-1} g^{(i)}(k)$$

(III-27)

The coupled differential equations (III-27) cannot be integrated in a straightforward manner. The homogeneous solutions obtained when $g(k) = 0$ explode either at zero momentum or at infinity. Hammar devised a clever method to subtract these unwanted solutions during numerical integration. It amounts to integrating a modified
function from \( k = 0 \) to \( k = \infty \). Then working back from \( k = \infty \) to \( k = 0 \) the correct D.F. can be reconstructed from the modified function by subtracting corresponding amounts of the unwanted homogeneous solutions. If one takes more than two equations this method becomes very complicated. Moreover unwanted solutions may enter at \( k = \infty \) after many iterations. With a modification of (III-25) there is a far more elegant way to remove the unwanted solutions. This will be discussed in the next paragraph.
III-3. Transforming the Legendre Expansion to integral-form.

We start again from the Boltzmann equation in its time-independent form:

\[ A \frac{d}{dk} f(k) + \frac{1}{k} B f(k) = \frac{\hbar}{eE} \left[ g(k) - v(k) f(k) \right] \]  \hspace{2cm} (III-28)

Following Rees [3], we can introduce a "self scattering" rate, describing fictitious scattering from state \( k \) to \( k \). This rate is chosen such that the total scattering rate out of state \( k \) becomes constant at a value \( \Gamma \). The time independent equation then reads:

\[ \{ A \frac{d}{dk} + \frac{1}{k} B \} f(k) + \frac{\hbar \Gamma}{eE} f(k) = \frac{\hbar}{eE} \left[ g(k) + (\Gamma - v(k)) f(k) \right] = \frac{\hbar}{eE} \Gamma \]  \hspace{2cm} (III-29)

As was argued by Rees this process of "self-scattering", although it does not change the state vector \( k \), must be physical in the sense that, in a positive increment of time, there must be a positive probability that an electron in an initial state \( k \) is scattered to a final state \( k \). This is only the case if:

\[ \Gamma > v(k) \text{ for all } k \]  \hspace{2cm} (III-30)

Then each iteration step is equivalent to a physical time step \( 1/\Gamma \) provided \( \Gamma \) is large enough. This is easily shown as follows: in the \( i \)'th iteration step we have:

\[ \{ A \frac{d}{dk} + \frac{1}{k} B \} f^{(i)}(k) + \frac{\hbar \Gamma}{eE} f^{(i)}(k) = \frac{\hbar \Gamma}{eE} \star (i-1) \]  \hspace{2cm} (III-31)

However, when the time dependence is included we must have:

\[ \frac{\partial}{\partial t} f^{(i-1)} + \frac{eE}{\hbar} \left[ A \frac{\partial}{\partial k} + \frac{B}{k} \right] f^{(i-1)} + \Gamma f^{(i-1)} = \star (i-1) \]
Subtracting the last two equations we find:

\[ \frac{\partial}{\partial t} f(t-1) = \Gamma [f(t) - f(t-1)] + \frac{eE}{h} \left[ A \frac{\partial}{\partial k} + \frac{B}{k} \right] (f(t) - f(t-1)) \]

When we put \( \Gamma = 1/\Delta t \) then in the limit \( \Delta t \to 0 \) the second term on the right vanishes and the expected result follows.

The homogeneous part of equation (III-29) allows \( N \) independent solutions \( \Phi(k) \) which are the column vectors of the fundamental matrix \( \Phi(k) \):

\[ \frac{\partial}{\partial k} \Phi(k) = -A^{-1} \left( \frac{h\Gamma}{eE} + \frac{B}{k} \right) \Phi(k) \quad \text{(III-32)} \]

If the fundamental matrix is known the particular solution of the inhomogeneous set can be written as:

\[ f(k) = \Phi(k)\psi(k_0) + \Phi(k) \int_{k_0}^{k} \psi(s) \Phi^*(s) ds \quad \text{(III-33)} \]

where

\[ \psi(s) = \Phi^{-1}(s) \frac{h}{eE} A \quad \text{(III-34)} \]

An analytical method has been found to calculate the matrices \( \Phi \) and \( \psi \) for arbitrary rank \( N \). Full details have been published in an EUT report [4]. Only the results will be given here. For the matrices \( \Phi \) and \( \psi \) we have

\[ \Phi_{ij}(k) = \tilde{\Phi}_{ij}(k) \exp(\lambda_j k) = \exp(\lambda_j k) \sum_{m=0}^{N-1} \frac{eE(2i + 1)\lambda_j Q_{ij}}{\frac{h\Gamma(\lambda_j)^{m+1}}{eE}} \frac{\exp(-h\Gamma)}{eE\lambda_j} \quad \text{(III-35)} \]
and

\[ \tilde{\psi}_j(k) = \tilde{\psi}_j(k) \exp(-\lambda_j k) = (III-36) \]

\[
\exp(-\lambda_j k) \frac{P_j \left( \frac{h \Gamma}{eE \lambda_i} \right) (-1)^j}{\left[ 2N \frac{h \Gamma}{eE \lambda_i} \right]^2 \left( \frac{2eE}{h \Gamma \lambda_i} \right)^2 - 1} \sum_{m=0}^{N-1} \frac{Q_{im}}{(\lambda_j k)^{m-1}}
\]

where

\[ Q_{im} = \frac{(i + m)!}{(-2)^m (i + m)! m!} \quad (m \leq i) \]  

\[ Q_{im} = 0 \quad (m > i) \]  

(III-37)

The \( \lambda_i \) are the roots of the equation:

\[ P_j \left( \frac{h \Gamma}{eE \lambda_i} \right) = 0 ; \quad P_j \] is the \( N \)th Legendre polynomial

(III-38)

Since \( N \) is even, the \( \lambda_i \) occur in pairs with opposite sign. The ordering of the homogeneous solutions is such that:

\[ \lambda_{2n} > 0 ; \quad \lambda_{2n+1} = -\lambda_{2n} \quad (n = 0, 1, 2, \ldots, \frac{N-1}{2}) \]

The particular solution (III-33) has to obey the boundary conditions

\[ \lim_{k \to 0} f_0(k) = f_0(0) \quad (III-39a) \]

\[ \lim_{k \to 0} f_n(k) = 0 \quad (n > 0) \quad (III-39b) \]

\[ \lim_{k \to \infty} f_n(k) = 0 \quad \text{all } n \quad (III-39c) \]
The condition (III-39a) is fulfilled if the components of the vector \( \mathbf{v}(k_0) \) obey the relation at \( k_0 = 0 \):

\[
v_{2n+1}(0) = -v_{2n}(0)
\]  

(III-40)

It turns out that condition (III-39b) is then fulfilled automatically. The condition (III-39c) can be fulfilled if the components \( v_{2n}(0) \) are chosen in the following way (see ref. [4] page 17):

\[
v_{2n}(0) = \int_0^\infty \sum_{i=0}^{N-1} \mathcal{v}_{2n,1}(s)g_i^*(s)ds
\]  

(III-41)

Defining:

\[
g_n^*(-k) = (-1)^n g_n^*(k)
\]  

(III-42)

the components \( v_{2n+1}(0) \) take the form:

\[
v_{2n+1}(0) = \int_0^\infty \sum_{i=0}^{N-1} \mathcal{v}_{2n+1,1}(s)g_i^*(s)ds
\]  

(III-43)

The particular solution can then be expressed as:

\[
f_j(k) = \sum_{n=0}^{N-1} \left\{ -\mathcal{v}_{j,2n}(k)I_{2n}(k) + \mathcal{v}_{j,2n+1}(k)I_{2n+1}(k) \right\}
\]  

(III-44)

where:

\[
I_{2n}(k) = \int_0^\infty \exp(-\lambda_{2n} t) \sum_{i=0}^{N-1} \mathcal{v}_{2n,1}(k+t)g_i^*(k+t)dt
\]  

(III-45)

\[
I_{2n+1}(k) = \int_0^\infty \exp(-\lambda_{2n+1} t) \sum_{i=0}^{N-1} \mathcal{v}_{2n+1,1}(k-t)g_i^*(k-t)dt
\]  

(III-46)
III-4. Numerical implementation and results.

The integrals given by (III-45) and (III-46) can be evaluated very efficiently. By expressing them as:

\[
I_{2n}(k) = \exp(-\lambda_{2n} \Delta k) I_{2n}(k + \Delta k) + \\
\Delta k \int_{0}^{\frac{N-1}{2}} \exp(-\lambda_{2n} t) \sum_{i=0}^{\frac{N-1}{2}} \widehat{\mathcal{L}}_{2n,i}^{*}(k+t) g_i(k+t) dt
\]  

(III-47)

\[
I_{2n+1}(k) = \exp(-\lambda_{2n} \Delta k) I_{2n+1}(k - \Delta k) + \\
\Delta k \int_{0}^{\frac{N-1}{2}} \exp(-\lambda_{2n} t) \sum_{i=0}^{\frac{N-1}{2}} \widehat{\mathcal{L}}_{2n+1,i}^{*}(k-t) g_i(k-t) dt
\]  

(III-48)

One can see that a double sweep gives both the integrals. First one integrates from \( k \) sufficiently large to \( k = 0 \) to obtain \( I_{2n} \). No growing errors are introduced by putting in the first step \( I_{2n}(k+\Delta k) = 0 \). A useful property of the integrals is:

\[
I_{2n}(0) = I_{2n+1}(0)
\]  

(III-49)

Having obtained \( I_{2n} \) one can integrate from \( k = 0 \) to \( k \) is sufficiently large, making use of (III-49) in the first step, to obtain \( I_{2n+1} \). For the largest \( k \) involved condition (III-30) must be obeyed. If one includes impurity scattering using the Brooks-Herring model (see II-30) the function \( v(k) \) may be very large for very small values of \( k \). If condition (III-30) is violated for these small values of \( k \) immediately instabilities are observed. Choosing \( \Gamma \) large enough may result in a timestep which is to small to be practical. The best is to modify \( v_{\text{imp}}(k) \). The number of electrons involved with this modification is so small that the
Fig. III-1. Response of the average velocity to a field step of 10 and 20 kV/cm. Dotted line shows the results of a two term expansion, the dashed dotted line of a four term expansion and the solid line of a six term expansion.

Fig. III-2. Comparison with the results of a Monte Carlo calculation (ragged curve).
macroscopic quantities hardly suffer from this. To test this method we chose as a material intrinsic GaAs. Using the "three valley model" [5] the third valley can be omitted for fields up to 20 kV/cm.

Hammar found that at room temperature a two-term expansion already gives quite good results for the macroscopic quantities. From our work we conclude that this is only true for the time-dependent macroscopic quantities if the electric field is not too high. (E < 10 kV/cm) This is shown in fig. III-1 where the response of the averaged velocity to a field step from zero to 10 resp. 20 kV/cm is plotted vs. time using a two, four and six-term expansion.

Only a four and six-term expansion show good agreement with a M.C. simulation as is shown in fig. III-2. It was found that in the transient regime the functions $f_2(k)$ and $f_3(k)$ belonging to the central valley are of equal magnitude as $f_0(k)$ and $f_1(k)$.

Approaching the stationary state the functions $f_0(k)$ and $f_1(k)$ begin to exceed the higher expansion functions. In the satellite valleys the functions $f_3(k)$ and with higher index are never very important. In fig. III-3a, b, c the stationary averaged velocity fraction of carriers in the central valley and averaged energy is shown using a two, four and six term expansion. The difference between a four and six-term expansion is very small but using a two-term expansion there is an error for all fields. The apparent good values for higher fields are due to compensating errors.

The averaged velocity, energy and carrier density are functions of $f_0(k)$ and $f_1(k)$ alone. Using macroscopic transport equations which take only into account only these quantities, it should at its best approach the results of a two-term expansion. This puts some question to the accuracy claimed by some authors using this method. Although using a six-term expansion the reconstruction of the D.F. using (III-4) is poor, it gives nevertheless a good estimate of the expected form. The reconstructed D.F. at different field strengths is shown in fig. III-4a, b, c, d. These figures show that for high fields the form is complicated and certainly not a shifted Maxwellian.
Fig. III-3a. Steady state average velocity as a function of the electric field. Dotted line the results of a two term expansion, solid line the results of four and six term expansions.

Fig. III-3b. As fig. III-3a. Fraction of carriers in the central valley as a function of the electric field.
Fig. III-3e. Average energy of the carrier as function of the electric field. Six term expansion.
Fig. III-4a. Steady state central valley Distribution Function as function of the wave vector $k$. The electric field is zero. The arrows indicate those values of $k$ where intervalley scattering occurs.

Fig. III-4b. As fig. III-4a. $E = 5 \text{ kV/cm.}$
Fig. III-4a. As fig. III-4a. $E = 10 \text{ kV/cm}$.

Fig. III-4b. As fig. III-4a. $E = 20 \text{ kV/cm}$.
III-5. The method of generalized transport coefficients.

We will now try to find methods to reduce the information needed to represent the distribution function. In the previous paragraph the angular dependence of the D.F. was developed in Legendre polynomials. For each function \( f_n(k) \) about 200 points in k-space were needed. So when representing the distribution function by 6 Legendre polynomials about 1200 points are needed for each valley. Including space dependence the number of points needed in k- and x-space will be increased drastically.

We will therefore in this paragraph try to represent the D.F. accurately enough for our purposes using a smaller number of parameters than the number of points in k-space.

We start with the set of equations obtained by the expansion of the Boltzmann equation in Legendre polynomials:

\[
\frac{\partial}{\partial t} f(k,t) + \frac{eE}{\hbar} \frac{3}{k} [A \frac{\partial}{\partial k} + B] f(k,t) = g(k,t) - \nu(k)f(k,t) \quad (III-50)
\]

We define the following integrals:

\[
G_{nm} = 4\pi \int_0^\infty f_n(k)k^{2+n+2m}dk \quad (m=0,1,2, \ldots) \quad (III-51)
\]

If we multiply equation (III-50) with the different powers of \( k \) we can obtain a coupled set of equations for the quantities \( G_{nm} \).

We find:

\[
\frac{3}{\partial t} G_{nm} - \frac{eE}{\hbar} \frac{n(2m+2n+1)}{(2n-1)} G_{n-1,m} + \frac{2m(n+1)}{(2n+3)} G_{n+1,m-1} = (\frac{\partial}{\partial t} G_{nm})_{coll.} \quad (III-52)
\]

Where we have defined:
\[
\left(\frac{\partial}{\partial t} G_{nm}\right)_{\text{coll.}} = 4\pi \int_0^\infty \left[g_n(k) - v(k)f_n(k)\right]k^{2n+2m}dk
\]  
(III-53)

We assume for the moment that we can find good expressions for these collision integrals. The carrier density can be recovered immediately from the quantities \(G_{nm}\) (see III-15)

\[
n(t) = G_{00}(t)
\]  
(III-54)

If the bandstructure is parabolic, i.e.

\[
v(k) = \frac{\hbar}{m} k \quad \text{and} \quad \varepsilon(k) = \frac{\hbar^2 k^2}{2m}
\]

the averaged velocity and mean energy can also easily be recovered

\[
\tilde{v}(t) = \frac{1}{n(t)} \frac{\hbar}{m} G_{10}(t)
\]  
(III-55)

and

\[
\tilde{\varepsilon}(t) = \frac{1}{n(t)} \frac{\hbar^2}{m} G_{01}(t)
\]  
(III-56)

Suppose that in the non-parabolic case the following power series form good approximations up to a certain value of \(k\):

\[
v(k) = \frac{\hbar}{m} (\alpha_0 k + \alpha_1 k^3 + \alpha_2 k^5 + \ldots)\]  
(III-57)

\[
\varepsilon(k) = \frac{\hbar^2}{2m} (\beta_1 k^2 + \beta_2 k^4 + \beta_3 k^6 + \ldots)\]  
(III-58)

Then using definition (III-51) good approximations for the averaged velocity and mean energy follow:
Both the series (III-57) and (III-58) do not converge. However forming the integrals the functions \( f_n \) serve as a kind of weight function. For large \( k \) the functions \( f_n \) drop off very rapidly. Therefore the series (III-59) and (III-60) will give accurate results. The averaged velocity and mean energy can thus be recovered from the quantities \( G_{nm} \). For \( G_{00} \) we find:

\[
G_{00}(t+\Delta t) = G_{00}(t) + \Delta t \left( \frac{\partial G_{00}}{\partial t} \right)_{\text{coll}}. \tag{III-61}
\]

The collision term describes the change of the particle density due to scattering. In case of one valley this term vanishes. In case of more valleys this term describes the change of particle density in each valley due to intervalley scattering. One condition for stability is of course that our time step has to be small in order that:

\[
\Delta t \left( \frac{\partial G_{00}^i}{\partial t} \right)_{\text{coll.}} \cong \Delta t \left( \frac{\partial n^i}{\partial t} \right)_{\text{coll.}} \leq n^i(t). \tag{III-62}
\]

where superscript \( i \) refers to the valley taken into consideration. Equation (III-61) gives the solution for \( G_{00}(t+\Delta t) \). With this solution we can solve:

\[
G_{10}(t+\Delta t) = G_{10}(t) + \frac{3\Delta t}{\hbar} G_{00}(t+\Delta t) + \Delta t \left( \frac{\partial G_{10}}{\partial t} \right)_{\text{coll}}. \tag{III-63}
\]

With \( G_{10}(t+\Delta t) \) we can solve \( G_{01}(t+\Delta t) \) and \( G_{20}(t+\Delta t) \).
Following the scheme shown in fig.III-5, we can solve all the quantities $G_{nm}$ provided we have expressions for the collision terms.

\[ \begin{align*}
G_{00} & \quad \rightarrow \quad G_{10} \\
G_{01} & \quad \rightarrow \quad G_{11} \\
G_{02} & \quad \rightarrow \quad G_{12} \\
G_{03} & \quad \rightarrow \quad G_{13} \\
\vdots & \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \ quadratic equations provided we have expressions for the collision terms.

\[ G_{00} \rightarrow G_{10} \]
\[ G_{01} \rightarrow G_{11} \]
\[ G_{02} \rightarrow G_{12} \]
\[ G_{03} \rightarrow G_{13} \]
\[ \vdots \]

Fig.III-5 suggests a truncation of the form:

\[ n = 0,1,2,3,\ldots,N \]
\[ m = 0,1,\ldots,N-n \]  \hspace{1cm} (III-64)

The question now arises if there can be found adequate expressions for the scattering terms. For a coefficient $G_{nm}$ the scattering term is formed from an operation on the corresponding function $f_n$ (see III-23)

\[ \left( \frac{\partial G_{nm}}{\partial t} \right)_{\text{coll}} = 4\pi \int_0^\infty k^{2+n+2m} dk \left[ \frac{V}{(2\pi)^3} \frac{4\pi}{(2n+1)} \int_0^\infty k'^3 S_n(k',k)f_n(k') \right] \]

\[ -\nu(k)f_n(k') \]  \hspace{1cm} (III-65)

Since the integrations over $k'$ involve in our approximation only delta functions it is always possible to find a function $Q_n(k)$.
which makes the right hand side of (III-65) equivalent with:

\[
\left(\frac{\partial G_{nm}}{\partial t}\right)_{\text{coll}} = 4\pi \int_0^\infty \Omega_n(k) f_n(k) dk
\]  

(III-66)

It will not be proved here but the function \(\Omega_n(k)\) is an even (odd) function of \(k\) when \(n\) is even (odd). Also \(\Omega_n(k)\) is of the order \(k^n\). This means that \(\Omega_n(k)\) can be expanded as:

\[
4\pi \Omega_n(k) = k^n (\gamma_0^n + \gamma_1^n k^2 + \gamma_2^n k^4 + \ldots)
\]  

(III-67)

Again such an expansion is not valid for the whole interval \(0 - \infty\).

The function \(f_n\) serves as a sort of weightfunction. Suppose the expansion is accurate for the largest \(k\) of interest. Then by definition (III-53) we have:

\[
\left(\frac{\partial G_{nm}}{\partial t}\right)_{\text{coll}} = \gamma_{0n}^n + \gamma_{1n}^n + \gamma_{2n}^n + \ldots
\]  

(III-68)

The above shows that under the assumption of an accurate expansion the relaxation of for instance the averaged velocity is a function of the coefficients \(G_{1m}\) and not of the mean energy (which is equivalent or near equivalent to \(G_{01}\)) as is often assumed in relaxation-time approaches.

The method described here delivered very good results. We choose as a material intrinsic GaAs, where two valleys are considered. We truncated as follows: put \(N = 3\) (see III-64) for both valleys. Each valley is now represented by ten coefficients. First, stationary values for the macroscopic quantities, the coefficients \(G_{nm}\) and the scattering terms (see III-65) were calculated for different values of the electric field using the method of the previous paragraph. Then we tried to find the best fitting functional
relationship between the coefficients to describe the scattering rate:

\[
\frac{\partial G_{nm}}{\partial t}_{\text{coll}} = F(G_{00}, G_{n1}, \ldots, G_{nm}) \quad \text{(III-69)}
\]

A functional relationship was guessed. Then a least square method was used to get the best fit with the stationary values. Then this functional relationship was tested. With the method described in the previous paragraph the response of the D.F. on a step of the electric field (E = 0-10kV/cm and E = 0-20kV/cm) was calculated with the coefficients \( G_{nm} \) and the scattering terms. These time dependent coefficients \( G_{nm} \) were inserted in the optimized guessed function to obtain the time dependent scattering rates. These could then be compared with the exact calculated time dependent scattering rates.

It was found that a functional relationship of the form (III-68) is the only one that could give good results in the transient regime. This supported the reasoning from which (III-68) was derived. More complicated relationships always gave poor results. Not always is it possible to arrive at such a simple expression covering all the situations if one varies the electric field from zero to let's say 30kV/cm. All the intravalley scattering processes and scattering processes describing the transfer of carriers from the satellite valley to the central valley could, some even with very high precision be expressed like III-68. This depends on how good an expansion like (III-67) approximates the function \( \Omega_n(k) \). For processes like the transfer of carriers and energy from the central valley to the satellite valley it was best to find such a linear relationship for different regimes. Then one uses one of the coefficients \( G_{0m} \) as a measure to shift from one description of the scattering rate to another. This has to be done carefully in order to avoid that with a slight difference of the coefficients \( G_{0m} \) not a sudden difference in scattering occurs. This construction of the
Fig. III-6a. Velocity overshoot calculated with the GTQ method (solid line) compared with the method of the preceding paragraph (dotted line).

Fig. III-6b. As fig. III-6a. Fraction of carriers in the central valley.
scattering rates is laborious and also a bit of an art to get the best results. An advantage is however that it has to be done only once. If done properly the results are very good. In the same way the coefficients $a_i$ and $b_i$ for reconstructing the average velocity and energy can be found. A single set of coefficients give these macroscopic quantities with high precision.

In fig.III-6 the results are shown. Fig.III-6b shows the good description of the particle density of each valley obtained with this method. Only the inclusion of the coefficients $G_{2m}$ and $G_{3m}$ can give good results. This stresses again that the macroscopic quantities corresponding to $f_2$ and $f_3$ are important in the central valley. Since the electric field is incorporated in a far less complicated way as in the method of the previous paragraph there is no loss of computation time if the electric field is made an arbitrary function of time. This makes this method an excellent tool for studying the non-stationary electron dynamics at high microwave frequencies.
III-6. The method of Hermite polynomials.

In the previous paragraph we demonstrated a successful way to construct a system which represents the D.F. in each valley separately. The construction of the functions which represent the scattering was difficult however and needed expensive preliminary calculations. As will be discussed in the next chapter there also arise difficulties when one tries to extend this method to include space dependence.

The expansion of the angular dependence of the D.F. in Legendre polynomials showed that the macroscopic quantities which depend on the first two expansion coefficients, come out very accurate using only a limited number of these. We will now try to do exactly the same for the radial dependence of the D.F. We start again with the set of equations obtained by the expansion of the space-independent Boltzmann equation in Legendre polynomials:

\[
\frac{3}{5t} f(k,t) + \frac{e}{h} E \left\{ A \frac{3}{3k} + \frac{B}{k} \right\} f(k,t) = g(k,t) - v(k)f(k,t)
\]  

(III-70)

The infinite set had to be truncated after \( N \) terms. (\( N = 4 \) or 6 gave already a good approximation of the macroscopic quantities).

We expand the functions \( f(k) \) in the following way:

\[
f_n(k) = \xi^n \sum_{m=0}^{\infty} F_{nm} H_m(\xi) \exp(-\xi^2)
\]  

(III-71)

With:

\[
\xi = k/\kappa
\]  

(III-72)

Here \( \kappa \) is a parameter whose value still has to be determined. The reason for this expansion is that \( f_n(k) \) is an even (odd) function when \( n \) is even (odd) and around \( k = 0 \) \( f_n(k) \) is of the order \( k^n \).
Each function $f_u(k)$ is now approximated by a sum of orthogonal Hermite polynomials. Later we will determine a suitable value of $M$, the number of functions at which the series has to be truncated. The entire distribution function is now replaced by a system consisting of $N^M$ quantities.

We normalise the Hermite polynomials so that:

$$\int_{-\infty}^{+\infty} H_m(\xi) H_n(\xi) \exp(-\xi^2) d\xi = 2\delta_{mn}$$  \hspace{1cm} (III-73)

From the definition (III-71) we find for the coefficients $F_{nm}$:

$$F_{nm} = \int_{0}^{+\infty} \frac{f_n(\kappa \xi)}{\xi^n} H_{2m}(\xi) d\xi$$  \hspace{1cm} (III-74)

By inserting expression (III-71) in the set of equations (III-70), multiplying left and right with $H_{2m}$ and integrating one obtains the following set of equations for the coefficients $F_{nm}$:

$$\frac{d}{dt} F_{nm}(t) + \frac{\phi E}{\hbar k} \sum_s \sum_p \phi_{nmsp} F_{sp}(t) = S_{nm} F_{np}(t)$$  \hspace{1cm} (III-75)

Where:

$$\phi_{nmsp} = \frac{1}{\kappa} \int_{0}^{+\infty} \frac{H_{2m}(\xi)}{\xi^n} \left[ A_{ns} \frac{d}{d\xi} + B_{ns} \frac{1}{\xi} \right] H_{2p}(\xi) \exp(-\xi^2) d\xi$$  \hspace{1cm} (III-76)

Inserting the Hermite polynomials and integrating one obtains the following non-zero elements of $\phi$.
The scattering matrix $S$ is defined as follows:

$$S_{nm} = \int_0^\infty d\xi \frac{2m}{\xi^n} \begin{bmatrix} \sum_{k',k} H_{2p}(\xi') \xi' n \exp(-\xi'^2) d\xi' \\
-v(k) H_{2p}(\xi) \xi^n \exp(-\xi^2) \end{bmatrix}$$  \hspace{1cm} (III-78)

The matrix elements of $S$ have to be calculated numerically.

The macroscopic quantities, i.e. the quantities we are interested in, like particle density $n$, average velocity $v$ and energy $\varepsilon$ can be recovered from the quantities $F_{nm}$.

$$n = 4\pi k^3 \int_0^\infty \xi^2 \sum_{m} F_{0m} H_{2m}(\xi) \exp(-\xi^2) d\xi = k^3 V^{1/4} (F_{00} + \sqrt{2} F_{01})$$ \hspace{1cm} (III-79)

$$nv = 4\pi k^3 \int_0^\infty \xi^3 v(\mu) \sum_{m} F_{1m} H_{2m}(\xi) \exp(-\xi^2) d\xi = \sum_{m} \alpha_m F_{1m}$$ \hspace{1cm} (III-80)

$$ne = 4\pi k^3 \int_0^\infty \xi^2 \sum_{m} F_{0m} H_{2m}(\xi) \exp(-\xi^2) d\xi = \sum_{m} \beta_m F_{0m}$$ \hspace{1cm} (III-81)

In case of a parabolic bandstructure only the coefficients $\alpha_m$ and $\beta_m$ with $m \leq 3$ are non-zero and can be found analytically. For the non-parabolic situation $\alpha_m$ and $\beta_m$ can be calculated numerically. Usually only the first four terms are important.

Instead of using the matrix $F$ one can construct a vector $\psi(t)$ with the components:

$$\phi_{n,m,n+1,m} = \frac{2(n+1)}{(2n+3)} (m-n-1)$$

$$\phi_{n,m,n+1,m-1} = \frac{2(n+1)}{(2n+3)} \frac{1}{\sqrt{m(m-1)}}$$  \hspace{1cm} (III-77)

$$\phi_{n+1,m-s,n,m} = \frac{(n+1)}{(2n+1)} (-1)^s s+1 \frac{m! \sqrt{(2m-2s)!}}{(m-s)! \sqrt{2m!}}$$
The matrices $\Phi$ and $S$ will then transform into 2-dimensional matrices. Equation (III-75) will then transform into:

$$\frac{d}{dt} \underline{w}(t) + \frac{eE}{\hbar c} \Phi \underline{w}(t) = S \underline{w}(t)$$ (III-83)

It is well-known [6] that the evolution of the system (III-83) from $t$ to $t+\Delta t$ is given by:

$$\underline{w}(t+\Delta t) = \exp\left\{\Delta t \left( - \frac{eE}{\hbar c} \Phi + S \right) \right\} \underline{w}(t)$$ (III-84)

Where the exponential of a matrix is defined as:

$$\exp A = I + \frac{A}{1!} + \frac{A \cdot A}{2!} + \ldots$$

Equation (III-83) can also be generalized in case we have to deal with different valleys. For this situation the solution (III-84) is not very practical. If we assume, as we have done so far, that the scattering occurs at fixed time-intervals we can construct a very simple iteration scheme. In absence of an electrical field $E$ the evolution of the system will be:

$$\underline{w}(t+\Delta t) = \exp(S\Delta t)\underline{w}(t) = \left\{I + \Delta t S + \frac{1}{2!} (\Delta t S)^2 + \ldots \right\} \underline{w}(t)$$ (III-85)

If we choose our timestep small enough (III-85) can be approximated by:

$$\underline{w}(t+\Delta t) = \left\{I + \Delta t S \right\} \underline{w}(t)$$ (III-86)
This means that the particles are scattered only once. When we have to deal with a system consisting of two valleys (c=central valley; s=satellite valley) eq. (III-86) reads:

\[
\begin{align*}
\bar{\Psi}^c(t+\Delta t) &= (I+\Delta t S^c c - \Delta t S^c s)\bar{\Psi}^c(t) + \Delta t S^c s \bar{\Psi}^s(t) \\
\bar{\Psi}^s(t+\Delta t) &= (I+\Delta t S^s s - \Delta t S^s c)\bar{\Psi}^s(t) + \Delta t S^s c \bar{\Psi}^c(t)
\end{align*}
\]  

(III-87)

In case there is an electric field we can take the left hand side of eq. (III-86) as the starting values of \( \bar{\Psi}(t) \). \( \bar{\Psi}(t) \) is then scattered at time \( t \) and only transported by the electric field from \( t \) to \( t+\Delta t \).

The evolution of \( \bar{\Psi}(t) \) from \( t \) to \( t+\Delta t \) is then:

\[
\begin{align*}
\bar{\Psi}^c(t+\Delta t) &= \exp(-\Delta t \frac{eE}{\hbar k} c^c) \left\{ (I+\Delta t S^c c - \Delta t S^c s)\bar{\Psi}^c(t) + \Delta t S^c s \bar{\Psi}^s(t) \right\} \\
\bar{\Psi}^s(t+\Delta t) &= \exp(-\Delta t \frac{eE}{\hbar k} s^s) \left\{ (I+\Delta t S^s s - \Delta t S^s c)\bar{\Psi}^s(t) + \Delta t S^s c \bar{\Psi}^c(t) \right\}
\end{align*}
\]  

(III-88)

We can approximate \( \exp(-\Delta t E\Phi) \) by the serie:

\[
\exp(-\Delta t E\Phi) = \sum_{n=0}^{\infty} (-\Delta t \frac{eE}{\hbar k} \Phi)^n \frac{1}{n!}
\]  

(III-89)

The number of terms depends on the value of \( \kappa \), \( \Delta t \) and the electric field \( E \). Using \( \Delta t = 10^{-14} \) sec. and \( \kappa \) around \( 3.10^{+8} \) m\(^{-1}\) only three terms are necessary for fields up to 20 kV/cm. For higher fields more terms are needed.

Similar expressions can be obtained for systems consisting of three or more valleys.

To obtain accurate numerical results some care must be taken with the choice of the weightfactor $\kappa$ (see III-72). For a Maxwellian distribution function at temperature $T$ the most natural choice would be:

$$\kappa = \frac{1}{n} \sqrt{(2m^*kT)}$$  \hspace{1cm} (III-90)

Then in case of a parabolic band and absence of an electric field, only the coefficient $P_{00}$ (see III-71) will be non-zero. When the deviations from the equilibrium distribution function are not too large this choice is good. When the deviations increase it will be necessary to choose a larger value of $\kappa$. The example chosen for numerical computation is the time-dependent behaviour of GaAs.

The bandstructure and scattering mechanisms were taken according to the model of M.A. Littlejohn [5] et al. For simplicity the third valley has been omitted. For the satellite valleys the choice of the weightfactor according to (III-90) is always good since the deviations of the D.F. from the zero-field stationary state are never great. For the central valley the situation is different. A large portion of the carriers can acquire an energy up to the value where intervalley scattering can occur. An expansion of the central valley D.F. in Hermite polynomials must therefore be able to peak around $\epsilon = 0.3$ eV (the energy necessary to scatter to the satellite valley).

To test this method the ballistic transport of carriers in the central valley was calculated, omitting the scattering. Fig.III-7a,b and c, this ballistic transport when an electric field of 20kV/cm is switched on at $t=0$. The number of Legendre polynomials is 6, the number of Hermite polynomials is 8. Eq.(III-91) would give a value $\kappa = 2.068 \times 10^8$ m$^{-1}$. In this example the value $\kappa = 3.883 \times 10^8$ m$^{-1}$ was
Fig. III-7a. $t = 0$ sec.

Fig. III-7b. $t = 10^{-13}$ sec.

Fig. III-7c. $t = 2 \cdot 10^{-13}$ sec.
chosen. In fig. III-7a we see the zero-field D.F. reconstructed from the coefficients \( F_{nm} \). In fig. III-7b we see how the D.F. has moved in the direction of the electric field at \( t=10^{-13} \) sec. In fig. III-7c we see the displacement at \( t=2\times10^{-13} \) sec. We see an increasing deterioration of the original shape. The limited number of Legendre polynomials accounts for the ripples that are appearing. Increasing their number would improve the picture. Nevertheless it is interesting to note that the macroscopic quantities in this case are still calculated very accurately using not only a limited number of Legendre polynomials but also a limited number of Hermite polynomials. The situation in fig. III-7c is already the limit to where the D.F. can move. The peak has reached the point were a considerable amount of carriers will be scattered to the satellite valley. This has the effect that the anisotropy is strongly reduced. In the following figures all the scattering processes and the satellite valley have been included. Some care now has to be taken. If one chooses a somewhat smaller value for \( k \) in the central valley, for instance \( k = 2.857\times10^{8} \) m\(^{-1}\) no problems arise for fields up to 20 kV/cm. For fields less then 10 kV/cm 6 Hermite polynomials will give already an excellent result and using more gives no improvement. If the field is 20 kV/cm more Hermite polynomials will give better results as can be seen in fig. III-8. For fields exceeding 20 kV/cm the results will diverge if not some precautions are taken. The first thing one can do is to choose the largest acceptable value for \( k \) in the central valley. Making \( k \) larger one can obtain better results for higher fields if one takes care that the transport of particles and energy from the central valley to the satellite valley is well described by the matrix elements \( S_{mp}^{cs} \).

The right hand side of the expression:

\[
G_{mm}^{s} = \sum_{p=0}^{M} S_{mp}^{cs} F_{0p}^{s} \quad (III-91)
\]
Fig. III-8. Response of the average velocity to a field step of 10 and 20 kV/cm calculated with the LHE method. $\kappa = 2.85 \cdot 10^8 \text{ m}^{-1}$.

(Compare with fig. III-1 and III-2)

- 6 Hermite polynomials
- 7 Hermite polynomials
- 8 Hermite polynomials

will converge rapidly after the first two or three terms and can be truncated if $m < 4$. For $m > 4$ a truncation of the series will give either a too large or a too small result. Since we know from other considerations that $G_0^c$ must be very small if $m > 4$ there is hardly no error if one puts:

$$S_{mp}^{cs} = 0 \quad \text{for } m > 4$$

By choosing $\kappa$ too large the description of the system will become inaccurate for low fields. Again it is the expression (III-91) which is the source of the difficulties. The results of the calculation show that it will not converge to accurate values if $m < 3$, resulting in a too large or even negative fraction of carriers in the satellite valley. A good compromise seems to be to choose $\kappa_c = 3.333 \cdot 10^8$. Still there remains a difficulty at high fields. For increasing $k$ the scattering rate increases. Now, at a given field the energy gained through the electric field will be balanced by the loss of energy due to scattering. The same is true of course for the velocity.
This behaviour should be reflected in the matrix representation of the D.F. Let us consider the matrix elements defined in (III-78):

$$ S_{m}^{\alpha} = \oint d\xi \, H_{2m}(\xi) \, \nu(\xi) \, H_{2p}(\xi) \, \exp(-\xi^2) \quad (III-92) $$

These matrix elements represent the scattering out of state $k$ to all states $k'$. From these matrix elements the expansion coefficients $\beta$ of the following function can be recovered:

$$ \xi^{2p-2} \nu(\xi) = \sum_{m=0}^{M} \beta_{2m} \, H_{2m}(\xi) \quad (III-93) $$

For $p = 0$ one has the expansion of $\nu(k)$ in Hermite polynomials. The result of the approximation of $\nu(k)$ by a limited number of terms may look like fig.III-9.

![Fig.III-9. The approximation of $\nu(k)$ by two, three and four Hermite polynomials.](image-url)
If one adds more terms the approximation will become more accurate but only up to a certain value of $k$. Beyond this value the approximation will deviate strongly. This effect will become more pronounced if one adds more terms to the expansion. A larger value of $k$ will move this point to larger $k$. Consequently the scattering will be badly described if the last terms of the expansion of the D.F. become too large with respect to those with a low index. Adding more terms to the expansion will not help.

If $v(k)$ resembles a function of the form of $k^n$ ($n < M$) this bad behaviour of the approximation at large $k$ will not occur. It is therefore advantageous if $v(k)$ behaves like a power of $k$. In GaAs one can include the scattering to the X-valley (Three valley model).

The shape of $v(k)$ in the $\Gamma$ and L valleys will then give much better conditioned numbers in the scattering matrix. As can be seen in fig.III-10a,b and c, one obtains satisfactory results for fields which are much higher than 20 kV/cm using a value for $k$ of $3.33 \times 10^8$ m$^{-1}$ which gives also very good results for very low fields.
Fig.III-10a. Steady state average velocity as a function of the electric field calculated with the LHE method. $\kappa = 3.33 \times 10^8 \text{ m}^{-1}$.

Fig.III-10b. Fraction of carriers in the different valleys as a function of the electric field calculated with the LHE method.
Fig. III-10a. The average energy as a function of the electric field calculated with the LHE method.
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IV. THE SPACE-DEPENDENT PROBLEM.

IV-1. Introduction. Discussion of previous methods.

We will now consider the space-dependent situation. In this chapter we will restrict ourselves to one-dimensional problems in which the D.F. has only a gradient in the direction of the electric field. The methods described previously, i.e. the method of Legendre polynomials, the GTQ method and the LHE method, will now be applied to this situation in consecutive order and their feasibility will be discussed. If one takes the electric field along the x-axis the B.T.E. reads:

\[ \frac{\partial}{\partial t} f(k,x,t) + \frac{q}{\hbar} E(x,t) \frac{\partial}{\partial k_x} f(k,x,t) + v(k) \frac{\partial}{\partial x} f(k,x,t) = g(k,x,t) - v(k) f(k,x,t) \]  

(IV-1)

The electric field follows from Poisson's equation

\[ \frac{\partial}{\partial x} E(x,t) = \frac{q}{\varepsilon} \left( N_d - n(x,t) \right) \]  

(IV-2)

where \( N_d \) is the ionised donor concentration and \( n \) the electron density. Equation (IV-1) can also be expanded in Legendre polynomials. Since the band structure is assumed to have spherical symmetry the velocity is a function of modulus \( k \) alone:

\[ v_x(k) = v(k) \cos \theta ; v(k) = \left| v(k) \right| \]

where \( \theta \) is the angle between \( k \) and the electric field \( E \). The expansion in Legendre polynomials then reads:
where the symbols have the same meaning as in (III-1). As has been mentioned in Chapter III the matrix \( A \) has real eigenvalues. This means that the set of equations (IV-3) is hyperbolic. Because of the boundary conditions at \( k = 0 \) and \( k = \infty \) the set (IV-3) will be difficult to solve.

One possible method would be to introduce "self-scattering" as was done in Chapter III, paragraph 3. This is equivalent to replacing the time derivate by:

\[
\frac{\partial}{\partial t} f(x,k,t) = \frac{f(x,k,t+\Delta t) - f(x,k,t)}{\Delta t} = \Gamma [f(x,k,t+\Gamma t) - f(x,k,t)] \quad (IV-4)
\]

where:

\[
\Gamma = \frac{1}{\Delta t} \quad (IV-5)
\]

Following the same routine as in Chapter III, paragraph 3, the set (IV-3) transforms into the following iteration scheme which approximates the time dependent evolution of the system:

\[
\Gamma f^{(n)} + Av(k) \frac{\partial}{\partial x} f^{(n)} + \frac{e}{\hbar} E \{ A \frac{\partial}{\partial k} + \frac{B}{k} \} f^{(n)} = \phi^{*(n-1)} \quad (IV-6)
\]

where:

\[
\phi^{*(n-1)}(x,k) = \phi^{(n-1)}(x,k) + (\Gamma - \nu(k)) f^{(n-1)}(x,k) \quad (IV-7)
\]

In Chapter III, paragraph 3 the matrices \( \Phi(k;\Gamma) \) and \( \Psi(k;\Gamma) \) were introduced with their properties. By introducing the vector \( h(x,k) \) in the following way:
\( f(x,k) = \phi(k,\Gamma)h(x,k) \)  \( \text{(IV-8)} \)

the system (IV-6) transforms into (see III-34):

\[
v(k) \frac{\partial}{\partial x} h(x,k)(n) + \frac{e}{h} \sum_k \frac{\partial}{\partial k} h(x,k)(n) = \phi(k,\Gamma)^{(n-1)}(x,k) \quad \text{(IV-9)}
\]

If the electric field is constant then the system (IV-9) has the following characteristics:

\[
\begin{align*}
  k &= k_0 + t \\
  x &= x_0 + \frac{h}{eE} \int_0^t v(k_0 + \tau) d\tau = x^+(x_0, t) \\
  & \quad \text{for } t > 0 \quad \text{(IV-10)}
\end{align*}
\]

and:

\[
\begin{align*}
  k &= k_0 + t \\
  x &= x_0 + \frac{h}{eE} \int_0^t v(k_0 - \tau) d\tau = x^-(x_0, t) \\
  & \quad \text{for } t < 0 \quad \text{(IV-11)}
\end{align*}
\]

By taking into account the proper boundary conditions at \( k = 0 \) and \( k = \infty \) the system (IV-9) can be integrated along the characteristics (IV-10) and (IV-11). The solution of (IV-6) can then be written as:

\[
f_j(x,k) = \sum_{n=0}^{N-1} \left[ - \phi_{j,2n}(k) I_{2n}(x,k) + \phi_{j,2n+1}(k) I_{2n+1}(x,k) \right] \quad \text{(IV-12)}
\]

where:

\[
I_{2n}(x,k) = \int_0^{\exp(-\lambda_{2n} t)} \sum_{i=0}^{N-1} \Psi_{2n,i} (k+t) g_1(x^+(t),k+t) dt \quad \text{(IV-13)}
\]

\[
I_{2n+1}(x,k) = \int_0^{\exp(-\lambda_{2n} t)} \sum_{i=0}^{N-1} \Psi_{2n+1,i} (k-t) g_1(x^-(t),k-t) dt \quad \text{(IV-14)}
\]
The evaluation of the integrals (IV-14) is now less simple than it was in the space-independent situation. Moreover the electric field will be a function of the coordinate $x$. This makes the characteristics along which one has to integrate very complicated. Therefore any numerical solution of a space-dependent situation according to the scheme given by (IV-12) will now be very time consuming, so no further effort has been made in this direction.

Another possible solution of the space-dependent problem would be an extension of the GTQ method. In Chapter III, paragraph 5 the GTQ method was outlined as a means to simplify the representation of the D.F. A set of integrals was defined from which a coupled set of equations could be formed. In the space-independent situation this set could be solved successfully.

$$\frac{\partial}{\partial t} G_{nm} = \sum L \left[ \frac{(2m+2n+1)n}{(2n-1)(2n+3)} G_{n-1,m} + \frac{2m(n+1)}{(2n+3) G_{n+1,m-1}} \right] = \left( \frac{\partial}{\partial t} G_{nm} \right)_{\text{coll}}$$

Suppose that the quantities $V_1$ and $V_2$ can be found with which the following integrals can be approximated:

$$\int_{0}^{\infty} k^{n+2+2m} v(k) f_{n+1} dk = \sum_{m=0}^{\infty} V_{n,m} G_{n+1,m} \quad (n=0,1,2,...)$$

$$\int_{0}^{\infty} k^{n+2+2m} v(k) f_{n-1} dk = \sum_{m=0}^{\infty} V_{2,n} G_{n-1,m}$$

These quantities $V_{n,m}$ can be obtained by evaluating the form of $v(k)$ or by curvefitting data from stationary values. The set of eqs. (IV-15) can then be extended to include space-dependence:
\[
\frac{\partial G_{nm}}{\partial t} - \frac{eE}{\hbar} \left\{ \frac{(2m + 2n + 1)n}{(2n-1)} G_{n-1,m} + \frac{2m(n+1)}{(2n+3)} G_{n+1,m-1} + \right.
\]
\[
\frac{3}{2\hbar} \left\{ \frac{n}{2n-1} \sum V_{2n,m} G_{n-1,m} + \frac{n+1}{(2n+3)} \sum V_{1n,m} G_{n+1,m} \right\} = \left( \frac{\partial}{\partial t} G_{nm} \right)_{\text{coll}}.
\]

The difficulty is now how to truncate this system. The left-hand side of (IV-17) will not form now, as it did in the space-independent situation, a closed system. When there is strong scattering the system (IV-17) appears to be stable after truncation. In GaAs the scattering in the central valley was not strong enough to obtain stable results with simple methods. The method was not investigated further, because in the next paragraph a method will be discussed which has a more clear structure.

In materials where the scattering has a more dominant character like Si this method however should be stable, accurate and fast.
IV-2. The LHE method.

The space-dependent problem becomes much clearer if we adopt the method of Hermite polynomials. As we will see the nature of the set of equations obtained will truly form a hyperbolic system. Our starting point will be again the set (IV-3). We will expand the functions \( f(x,k) \) in the same way as in Chapter III, paragraph 6. Now the amplitude coefficients will be functions of \( x \) and \( t \):

\[
f_n(x,k,t) = \sum_{m=0}^{\infty} F_{nm}(x,t) t^n H_{2m}(\xi) \exp(-\xi^2) \quad (n=0,1,2...) \tag{IV-18}
\]

where \( \xi \) is defined as in (III-72).

We define the following matrix elements:

\[
V_{n,m,n+1,k} = \frac{n}{(2n+1)} \int_{0}^{\infty} H_{2m}(\xi) v(k) \xi H_{2k}(\xi) \exp(-\xi^2) d\xi
\]

\[
V_{n,m,n-1,k} = \frac{n-1}{(2n-1)} \int_{0}^{\infty} H_{2m}(\xi) \frac{v(k)}{\xi} H_{2k}(\xi) \exp(-\xi^2) d\xi
\]

The set of equations for the coefficients \( F \) is then given by:

\[
\frac{\partial}{\partial t} F_{nm} + \frac{\epsilon}{\hbar} E \sum_{sp} \phi_{nmsp} F_{sp} + \sum_{sp} \sum_{nm} V_{nmsp} \frac{\partial}{\partial x} F_{sp} = \sum_{p} S_{nmp} F_{np}
\]

Just as in Chapter III paragraph 6 we can consider \( F \) to be elements of a vector \( \bf{w} \). The matrices \( \phi \) and \( V \) will have then only two indices. Equation (IV-20) transforms into:

\[
\frac{\partial}{\partial t} \bf{w}(x,t) + V \frac{\partial}{\partial x} \bf{w}(x,t) + \frac{\epsilon}{\hbar \kappa} E(x,t) \psi(x) \bf{w}(x,t) = S \bf{w}(x,t) \tag{IV-21}
\]

The system (IV-21) is hyperbolic if the eigenvalues of \( V \) are real. Then there exists a matrix \( T \) with the property:
\[ T^{-1}VT = \Lambda \]  
(IV-22)

Where:

\[
\Lambda = \begin{pmatrix}
\lambda_1 & 0 & 0 & \ldots & 0 \\
0 & \lambda_2 & 0 & \ldots & 0 \\
0 & 0 & \lambda_3 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & \lambda_N
\end{pmatrix}
\]
(IV-23)

with all the eigenvalues real. It turns out that the matrix \( V \) can be transformed into the form given by (IV-23). The eigenvalues are real and form pairs of equal magnitude and opposite sign. With proper arrangement of the columns of \( T \) we find:

\[
\Lambda = \begin{pmatrix}
\lambda_1 & 0 & 0 & 0 & \ldots \\
0 & -\lambda_1 & 0 & 0 & \ldots \\
0 & 0 & \lambda_2 & 0 & \ldots \\
0 & 0 & 0 & -\lambda_2 & \ldots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\]
(IV-24)

This is of course what we expect. If the material has an spherical conduction band any initial carrier concentration which is symmetric in \( x \)- and \( k \)-space will evolve while holding this symmetry.

Making use of the matrix \( T \) we define:

\[ \bar{w}(x,t) = \bar{h}(x,t) \]
(IV-25)

Inserting (IV-25) into (IV-21) we obtain the transport equation for \( \bar{h}(x,t) \):

...
\[ \frac{3}{3t} h(x,t) + A \frac{\partial}{\partial x} h(x,t) + \frac{e}{E(x,t)} T^{-1} \Phi h(x,t) = T^{-1} S h(x,t) \] (IV-26)

Each scalar equation has the characteristic:

\[ x = x_0 + \lambda t \] (IV-27)

The evolution of \( h_n(x,t) \) from \( t \) to \( t+\Delta t \) can be obtained by integrating along the characteristic:

\[ h_n(x,t) = h_n(x-\lambda t,0) + \]

\[ \int_0^t \sum m \sum p \sum k T_{nm}^{-1} \left\{ - \frac{e}{h\kappa} E(x-\lambda (t-s),s) \Phi + S \right\} T_{pk} h_k(x-\lambda (t-s),s) ds \] (IV-28)

Transforming back to the vector \( w(x,t) \) we obtain the solution of the system at time \( t \):

\[ w_n(x,t) = \sum m \sum p T_{nm}^{-1} T_{mp} \left\{ - \frac{e}{h\kappa} E(x-\lambda (t-s),s) \Phi + S \right\} w_p(x-\lambda t,0) + \]

\[ \int_0^t \sum m \sum p T_{nm} T_{mp}^{-1} \left\{ - \frac{e}{h\kappa} E(x-\lambda (t-s),s) \Phi + S \right\} w_p(x-\lambda (t-s),s) ds \] (IV-29)


Much has been written about the set of equations (IV-21). See e.g. ref. [1], [2] and [3])

Most in use are implicit schemes, which are complicated but allow large time steps to be taken. In order to properly account for scattering our timestep has to be small anyway so only explicit
schemes which are much simpler will be considered here. When we exclude for a moment the electric field and scattering mechanisms equation (IV-26) becomes:

\[ \frac{\partial}{\partial t} h(x,t) + \Lambda \frac{\partial}{\partial x} h(x,t) = 0 \]  \hspace{1cm} (IV-30)

Or:

\[ \frac{\partial}{\partial t} h_n(x,t) + \lambda_n \frac{\partial}{\partial x} h_n(x,t) = 0 \]  \hspace{1cm} (IV-31)

Each scalar equation has a solution of the form:

\[ h_n(x,t+\Delta t) = h_n(x-\lambda_n \Delta t,t) \]  \hspace{1cm} (IV-32)

If we use a grid as is indicated in fig.IV-1 a difference scheme of first-order accuracy is:

\[ h_n^p = h_n^s + \lambda_n \frac{\Delta t}{\Delta x} (h_n^q - h_n^s) \]  \hspace{1cm} \text{if } \lambda_n > 0 \hspace{1cm} (IV-33)

\[ h_n^r = h_n^s + \lambda_n \frac{\Delta t}{\Delta x} (h_n^r - h_n^s) \]  \hspace{1cm} \text{if } \lambda_n < 0

where \( \Delta x = x_m - x_{m-1} \). The Courant-Friedrichs-Lewy (C.F.L) condition requires the characteristics through P (see fig.IV-1) to intersect the line \( t = t_n \) within the range of points considered by the formula at the level \( t_n \). Equations (IV-33) obey this
condition only if:

\[
\left| \frac{\Delta t}{\Delta x} \lambda_n \right| < 1 \quad \text{(IV-34)}
\]

Knowledge of the eigenvalues of the matrix \( V \) is therefore essential for constructing stable difference schemes.

Following ref. [1] page 238 we split the matrix \( \Lambda \) in two parts:

\[
\Lambda = \Lambda^+ + \Lambda^-
\]

\( \Lambda^+ \) containing only the positive eigenvalues, \( \Lambda^- \) containing only the negative ones. A first-order difference scheme of the set (IV-4) is then given by:

\[
\begin{align*}
\dot{h}(x,t+\Delta t) &= h(x,t) + \frac{\Delta t}{\Delta x} \Lambda^+ [h(x,t)-h(x-\Delta x,t)]^+ \\
&\quad + \frac{\Delta t}{\Delta x} \Lambda^- [h(x+\Delta x,t)-h(x,t)] 
\end{align*}
\]

This can be rewritten as:

\[
\begin{align*}
\dot{h}(x,t+\Delta t) &= h(x,t) - \frac{\Delta t}{\Delta x} \frac{\Lambda^+ - \Lambda^-}{2} [h(x+\Delta x,t)-h(x-\Delta x,t)] \\
&\quad + \frac{\Delta t}{\Delta x} \frac{\Lambda^+ - \Lambda^-}{2} [h(x+\Delta x,t) + h(x-\Delta x,t)-2h(x,t)] 
\end{align*}
\]

(IV-37)

Transforming back to the vector \( \mathbf{w}(x,t) \) one obtains:

\[
\begin{align*}
\dot{\mathbf{w}}(x,t+\Delta t) &= \dot{\mathbf{w}}(x,t) - \frac{\Delta t}{\Delta x} \frac{\mathbf{V}}{2} [f(x+\Delta x,t)-f(x-\Delta x,t)] \\
&\quad + \frac{\Delta t}{\Delta x} \frac{\mathbf{M}}{2} [f(x+\Delta x,t)+f(x-\Delta x,t)-2f(x,t)] 
\end{align*}
\]

(IV-38)
where:

\[ M = T(\Lambda^+ - \Lambda^-)T^{-1} \]  

(IV-39)

The von Neumann condition requires that:

\[ \left| \frac{\Delta t}{\Delta x} \lambda_s \right| \leq 1 \]  

(IV-40)

where \( \lambda_s \) is the eigenvalue which is the largest in magnitude.

We will now construct an iteration scheme. First we have to calculate the electric field at time \( t \). Because we assume a non-stochastic sufficiently smooth carrier density function we can use a simple double sweep method for calculating the potential everywhere. Through numerical differentiation the electric field follows. It can be shown that the system (IV-21) can be solved by iteration (see [2] page 217)

\[ \frac{\partial}{\partial t} w^{(i+1)} + V \frac{\partial}{\partial x} w^{(i+1)} = \left\{ -\frac{e}{\hbar c} E \Phi + S \right\} w^{(i)} \]  

(IV-41)

Another way would be to solve (IV-29) iteratively. Such an iteration would however be very expensive in computertime. We therefore try the following schemes and study their stability by examples. We calculate the function:

\[ u(x) = \exp\left\{ -\Delta t \frac{e}{\hbar c} E(x,t) \Phi \right\} [I + \Delta t S] w(x,t) \]  

(IV-42)

(See chapter III, paragraph 6). This function \( u(x) \) serves as the initial value from which \( w(x,t+\Delta t) \) can be calculated according to (IV-38)

\[ w(x,t+\Delta t) = u(x) - \Delta t \frac{V}{2} \left\{ u(x+\Delta x) - u(x-\Delta x) \right\} + \Delta t \frac{M}{2} \left\{ u(x+\Delta x) + u(x+\Delta x) - 2u(x) \right\} \]  

(IV-43)
The iteration steps given by (IV-42) and (IV-43) will be referred to as scheme I. As in chapter III, paragraph 6 we can make the expansion (see III-89):

\[
\exp\left\{-\Delta t \frac{e}{\hbar k} E(x,t)\phi\right\} = \sum_{n=0}^{N} \frac{1}{n!} \left\{-\Delta t \frac{e}{\hbar k} E(x,t)\phi\right\}^n
\]  

(IV-44)

In a device the electric field can be very high. Even if this happens in a very small region of the device instabilities appear if the value of \( N \) in (IV-44) is not chosen rightly. The minimum value of \( N \) depends on the weightfactor \( \kappa \), \( \Delta t \) and the electric field \( E \) (see III-72). Using \( \Delta t = 10^{-14} \text{ sec.} \) and the value \( \kappa = 3.33 \times 10^8 \text{ m}^{-1} \) in the central valley it appears that for fields less than 1kV/cm \( N \) may be 1. For fields up to 20 kV/cm \( N \) must at least be 2 and the time step has to be halved, otherwise instabilities occur. For higher fields \( N \) must be larger than 2.

To test scheme I we choose a simple device. In Fig.IV-2 the doping concentration of an \( n^+\text{-}n\text{-}n^+ \text{ GaAs diode is shown. The initial D.F. is a zero field Boltzmann distribution with a carrier concentration equal to the donor concentration. As a boundary condition we connect both ends. The potential at both ends is put at zero. It is assumed that the D.F. will evolve from this initial value to a stationary value. The current density and averaged velocity should, under these circumstances, then be zero. In the example we use a mesh width \( \Delta x = 0.5 \times 10^{-8} \text{ m} \) and \( \Delta t = 1 \times 10^{-14} \text{ sec.} \). The weightfactors are \( \kappa_c = 3.33 \times 10^8 \text{ m}^{-1} \) and \( \kappa_s = 3.883 \times 10^8 \text{ m}^{-1} \).

(\( c = \text{central valley}, s = \text{satellite valley, only two valley are taken into consideration}. \) In the central valley 8 Hermite polynomials are used and in the satellite valley 6. The number of Legendre polynomials in the satellite valley is 2 and in the central valley we tried 2 and 4. The largest eigenvalue of the matrix \( V_c \Delta t/\Delta x \) is larger then 1. Therefore we replaced \( \Delta t \) in (IV-43) by \( \Delta t = \Delta t/n \) where \( n \) is an integer. By repeating the step (IV-43) \( n \) times the desired result follows. Using two Legendre polynomials in the central valley we
get stable results. Using four some instability may occur. This can be remedied by a simple smoothing of $F_{3m}$ and $F_{4m}$.

$$F_{3m}(x) = \frac{1}{2} \left[ F_{3m}(x+\Delta x) + F_{3m}(x-\Delta x) \right]$$

$$F_{4m}(x) = \frac{1}{2} \left[ F_{4m}(x+\Delta x) + F_{4m}(x-\Delta x) \right]$$

The averaged velocity after reaching steady state is shown in Fig.IV-3. One can see that it is nearly zero as we wanted.

We can replace step (IV-43) in scheme I by:

$$w(x,t) = \frac{1}{2} \left[ u(x+\Delta x) + u(x-\Delta x) \right] - \frac{\Delta t}{\Delta x} \frac{v}{2} \left[ u(x+\Delta x) - u(x-\Delta x) \right]$$

This will be referred to as scheme II. (See ref[4] page 495) The von Neumann condition has the same requirements as scheme I. This scheme spares the multiplication with the matrix $M$ and is therefore a far more efficient scheme than scheme I. If one calculates the averaged velocity after reaching the steady state the result is not very accurate as is shown in fig.IV-3. If one is interested only in the total current flowing through the device scheme I and II do not differ much.
Fig. IV-3. The average velocity. (ΔV = 0 Volt)

--- scheme I

--- scheme II

Fig. IV-4 shows the total current density as a function of time when a voltage of 0.6 Volt is applied using both schemes.

The total current density is calculated by integrating the local current density over the length of the device, using the Ramo-Shockley theorem.

\[
J(t) = \frac{1}{L} \int_0^L j(x,t) \, dx = \frac{q}{L} \int_0^L n(x,t)v(x,t) \, dx + \frac{\varepsilon_0 \varepsilon_s}{L} \frac{d}{dt} \left[ V(0) - V(L) \right]
\]

(IV-47)

where \( L \) is the length of the device. Applying a voltage step adds a delta function current at \( t = 0 \). This delta function has been omitted in fig. IV-4.
In order to save computer time the two schemes can be mixed. The steps (IV-43) and (IV-46) are equivalent with the following operations on the coefficients $U_{nm}(x,t)$. $U_{nm}(x,t)$ being the matrix representation of the vector $u(x,t)$:

\[ F_{nm}(x,t+\Delta t) = U_{nm}(x,t) - \frac{\Delta t}{2\Delta x} \sum_s \sum_p \left[ V_{nmsp}D_1 - I_{nmsp}D_2 \right] U_{sp}(x,t) \]

\[ F_{nm}(x,t+\Delta t) = U_{nm}(x,t) - \frac{1}{2} \sum_s \sum_p \left[ \frac{\Delta t}{\Delta x} V_{nmsp}D_1 - I_{nmsp}D_2 \right] U_{sp}(x,t) \]

(IV-48)

where $I$ is the identity matrix. The operators $D_1$ and $D_2$ stand for:

\[ D_1 U(x) = U(x+\Delta x) - U(x-\Delta x) \]

\[ D_2 U(x) = U(x+\Delta x) - 2U(x) + U(x-\Delta x) \]

(IV-49)

The macroscopic quantities we are interested in are given by the coefficients $F_{0m}$ and $F_{1m}$. These we want with high precision. We therefore mix (IV-48) and (IV-49) in the following way:
\[ F_{0m}(x,t+\Delta t) = U_{0m}(x,t) - \frac{\Delta t}{2\Delta x} \sum_s \sum_p \left( v_{0msp} D_{1} - M_{0msp} D_{2} \right) U_{sp}(x,t) \]

\[ F_{1m}(x,t+\Delta t) = U_{1m}(x,t) - \frac{\Delta t}{2\Delta x} \sum_s \sum_p \left( v_{1msp} D_{1} - M_{1msp} D_{2} \right) U_{sp}(x,t) \]

\[ F_{2m}(x,t+\Delta t) = U_{2m}(x,t) - \frac{1}{2} \sum_s \sum_p \left( \frac{\Delta t}{\Delta x} v_{2msp} D_{1} - I_{2msp} D_{2} \right) U_{sp}(x,t) \]

\[ F_{3m}(x,t+\Delta t) = U_{3m}(x,t) - \frac{1}{2} \sum_s \sum_p \left( \frac{\Delta t}{\Delta x} v_{3msp} D_{1} - I_{3msp} D_{2} \right) U_{sp}(x,t) \]

etc. \hspace{1cm} (IV-50)

This will be referred to as scheme III. Scheme III appears to be just as accurate as scheme I but has the advantage of being much faster if more than two Legendre polynomials are involved. No smoothing appears to be necessary. Depending on the available software it might be difficult to calculate the matrix \( M \).

\[ \frac{\Delta t}{\Delta x} M = \frac{\Delta t}{\Delta x} T (\Lambda^+ - \Lambda^-)^{-1} \] \hspace{1cm} (IV-51)

From (IV-24) we have the following relationship:

\[ \left( \frac{\Delta t}{\Delta x} \Lambda \right)^2 = \left( \frac{\Delta t}{\Delta x} (\Lambda^+ - \Lambda^-) \right)^2 \] \hspace{1cm} (IV-52)

Therefore:

\[ \frac{\Delta t}{\Delta x} (\Lambda^+ - \Lambda^-) = \sqrt{\frac{\Delta t}{\Delta x} \Lambda^2} \] \hspace{1cm} (IV-52)

Since we must choose \( \Delta t \) and \( \Delta x \) so that:

\[ \frac{\Delta t}{\Delta x} |\lambda_g| \leq 1 \]

where \( \lambda_g \) is the largest element of the matrix \( \Lambda \) we can form the
following expansion:

\[
\frac{\Delta t}{\Delta x} (A^+ - A^-) = \left[ 1 + \left( \frac{\Delta t}{\Delta x} A \right)^2 - 1 \right]^{\frac{1}{2}} = \left[ 1 + B \right]^{\frac{1}{2}} = \\
1 + \frac{1}{2} B - \frac{1}{8} B^2 + \ldots + \frac{\frac{1}{2}(\frac{1}{2}-1) \ldots (\frac{1}{2}-N)}{N!} B^N
\]

Transforming back we find:

\[
\frac{\Delta t}{\Delta x} M = 1 + \frac{1}{2} C - \frac{1}{8} C^2 + \ldots + \frac{\frac{1}{2}(\frac{1}{2}-1) \ldots (\frac{1}{2}-N)}{N!} C^N \quad \text{(IV-53)}
\]

where

\[
C = \left( \frac{\Delta t}{\Delta x} v \right)^2 - 1 \quad \text{(IV-54)}
\]

Taking only one term of the expansion (IV-54) leads to scheme II. By adding more terms one approaches scheme I. It appears that for any number of terms the expansion produces an iteration scheme which gives stable results.

Some other schemes have also been tested. A widely recommended scheme is Lax-Wendroff explicit scheme [2]. The step (IV-41) or (IV-47) is then replaced by:

\[
\omega(x, t+\Delta t) = u(x) - \frac{\Delta t}{\Delta x} \frac{V}{2} \left[ u(x+\Delta x) - u(x-\Delta x) + \\
\frac{1}{2} \left( \frac{\Delta t}{\Delta x} V \right)^2 \left[ u(x+\Delta x) + u(x-\Delta x) - 2u(x) \right] \right]
\]

The von Neumann condition gives the same requirements as scheme I. This second order scheme appears to be unstable even with various kinds of smoothing. Apparently the von Neumann condition is not the only criterion for stability. It may be possible that the combination of transport equations and the equation of Poisson
strongly enhances certain modes generated by an iteration scheme.

Scheme III proved to be the most reliable and efficient scheme. Some results obtained with this scheme will be given in the next Chapter.
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ANALYSIS OF NUMERICAL METHODS.
V RESULTS ON ONE-DIMENSIONAL DEVICES

The LHE method described in the previous chapter can be applied to one-dimensional devices as has been shown there. In this chapter a few results of the simulation of a millimeter-wave Gunn-effect oscillator will be presented. The material is GaAs and the frequency region is around 150 GHz. In this region GaAs is not used because it is inferior to InP. The calculations therefore will not be of much practical use but its main purpose here is to show the effects of a short device length. The results will be more demonstrative than practical.

With this method we can now make not only accurate pictures of the average velocity and energy but also accurate pictures of the particle density in each valley throughout the device at any instant of time. These pictures will greatly help to get a clear insight in the operation of the device.

The device dimensions are shown in fig.V-1. The anode and cathode contact regions are heavily doped \(2 \times 10^{23} \text{ m}^{-3}\). This doping gave no stability problems using a mesh width \(\Delta x=10^{-8} \text{ m}\). The length of the anode contact (0.5 \(\mu\)m) ensures that the heated electron gas has enough time to cool and fall back to the central valley. It appears that nearly the entire length of the contact is needed for this. As a boundary condition we connect both ends. This ensures charge conservation. Since the electrons are cooled down sufficiently no heat is pumped in at the cathode boundary.

In fig.V-2 the current density vs. voltage is given for the device shown in fig.V-1. The crystal temperature was taken at 300 K. As one can see the device shows no negative differential resistance in the regime that was investigated. The \(N_dL\) product is \(2 \times 10^{12}\) but no Gunn type instabilities occur with a constant voltage difference between the contacts. The reason that the critical \(N_dL\) product is higher in short devices has been discussed by Jones and Rees [1]
Fig. V-1. The device dimensions and doping density.

Fig. V-2. The current density as a function of the applied voltage for the device shown in fig. V-1.
and by Bosch and Thim [2]. The carriers need a certain zone in which they are accelerated before they can scatter into the satellite valleys. In this zone the average velocity overshoots the static velocity. This zone has been called by Bosch and Thim the dead zone. Some authors use a different definition of the dead zone. One can define the dead zone as that region where the average energy is below the threshold for intervalley scattering [4]. This allows of course a more exact determination of the length of the dead zone. One can also speak of an acceleration zone. The remaining part of the channel where the carriers exceed the threshold energy is called the active zone. In Fig. V-3a,b,c the total carrier density, the carrier density in each valley, the average velocity and energy are shown for three different applied voltages. These results have been obtained by starting from a zero voltage and then applying a step in voltage. As can be seen from the figures the average velocity near the cathode reaches a value about $2.8 \times 10^5$ m/s. This is higher than the peak of the static velocity-field characteristic. For different voltages the average velocity near the cathode appears to be the same. The electric field also appears to be the same in a region of about 0.5 µm from the cathode. Especially in the region of about 0.25 µm from the anode we see the influence of raising the voltage.

From the evolution to the stationary state a layer of slow moving carriers forms which moves towards the anode. The more this layer moves towards the anode the more the field near the cathode drops and the high field region decreases in width. This is the consequence of Poisson's equation. When the field near the anode drops the lengths of the region where the carriers overshoot the static velocity while remaining in the central valley increases. This in turn makes the accumulation layer narrower and pushes it more towards the anode which again as a consequence of Poisson's equation, makes the field near the cathode drop. Raising the voltage apparently does not result in a significant reduction of
Fig. V-3a. Applied voltage $\Delta V = 1.6$ Volt. "A" shows the total carrier density (solid line) and the doping profile (dotted line). "B" shows the carrier density of the central valley (solid line) and the carrier densities of the satellite valleys (dotted lines).
Fig. V-3b. As fig. V-3a. Applied voltage $\Delta V = 2.0$ Volt.
Fig. V-3c. As fig. V-3a. Applied voltage $\Delta V = 2.4$ Volt.
the length of the dead zone.

We will now study the microwave properties of this device. The theoretical possibility of using this device as a microwave oscillator will be shown. Since the efficiency vs frequency calculations for bulk material submitted to fields uniform in space are not applicable we try to explain the operation of the device using plots obtained during one period of the microwave signal. We consider only the fundamental mode.

We add to the d.c. voltage a sinusoidal component:

\[ V(t) = V_0 + V_1 \sin \omega t \quad (V-1) \]

As a result a current will flow through the device of the form:

\[ J(t) = J_0 + J_1 \sin(\omega t + \psi_1) + J_2 \sin(2\omega t + \psi_2) + \ldots \quad (V-2) \]

For the moment we are only interested in \( J_1 \) and \( \psi_1 \).

If:

\[ 90^0 < \psi_1 < 270^0 \]

the device shows a negative differential resistance at the fundamental frequency. The efficiency is calculated according to:

\[
\eta = \frac{\int_0^T V_1 \sin \omega t \ J(t) \ dt}{\int_0^T V_0 \ J(t) \ dt} \quad (V-3)
\]

where \( T \) is the period. No exhaustive search was done to obtain optimum values for \( V_0 \) and \( V_1 \). \( V_0 \) was put at 2 Volt. For \( V_1 \) the
Fig. V-4a. The current $J_0$ as a function of the frequency.

Fig. V-4b. The current $J_1$ as a function of the frequency.
Fig. V-4c. The phase $\psi$ as a function of the frequency.

Fig. V-4d. The efficiency as a function of the frequency.
values 0.4, 0.6 and 0.8 Volt were chosen. The figures V-4a,b,c,d show the resulting direct current density $J_0$ and amplitude $J_1$, phase $\psi$ and efficiency $\eta$ as function of the frequency $\omega/2\pi$. As one can see the current density amplitude $J_1$ increases with increasing frequency and with increasing amplitude $V_1$. At a certain frequency the phase difference drops below $90^\circ$. The efficiency therefore has a maximum at a certain frequency.

To study the behaviour of the device as an oscillator the diode was placed in a circuit to similar that of Tully [5],

![Circuit Diagram](image)

The circuit is a parallel resonant circuit as shown in fig.V-5. The capacitance $C$ includes both an external capacitance and the device dielectric capacitance. The current $I(t)$ is determined by the capacitance, inductance and load resistance according to the equations:

\[ I(t) = C \frac{dV(t)}{dt} + I_e(t) \quad \text{(V-4)} \]

\[ I(t) = - \frac{V(t)}{R} - \int \frac{V(t)-V_B}{L} \, dt \quad \text{(V-5)} \]

where $I_e(t)$ is the electronic device current calculated according to:
\[ I_e(t) = -\frac{qA}{L} \int_0^L n(x,t) v(x,t) \, dx \tag{V-6} \]

where \( A \) is the device area. From (V-4,5) we can derive a pair of finite difference equations:

\[ V(t+\Delta t) = V(t) + \frac{I(t)-I_e(t)}{C \Delta t} \tag{V-7} \]
\[ I(t+\Delta t) = I(t) - \frac{V(t+\Delta t)-V(t)}{C} - \frac{V(t)-V_B}{L \Delta t} \tag{V-8} \]

Choosing the frequency \( \omega = 175 \text{ GHz} \), \( V_1 = 0.6 \text{ Volt} \) and a device area of \( 10^{-10} \text{ m}^2 \) and choosing \( R, L \) and \( C \) in a manner that:

\[ Z_{\text{device}} = -Z_{\text{circuit}} \]

where \( Z_{\text{device}} \) is the impedance found in the previous calculations, we arrive at the following circuit parameters:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C )</td>
<td>0.113 pF</td>
</tr>
<tr>
<td>( L )</td>
<td>6.22 pH</td>
</tr>
<tr>
<td>( R )</td>
<td>64.7 ( \Omega )</td>
</tr>
<tr>
<td>( F_c = \frac{1}{2\pi \sqrt{LC}} )</td>
<td>190 GHz</td>
</tr>
<tr>
<td>( V_B )</td>
<td>2.0 Volt</td>
</tr>
</tbody>
</table>

With these parameters inserted a simulation was made. As an initial condition the state of the device at zero voltage was calculated. \( I(t) \) and \( V(t) \) were put zero. Then the simulation was started. This is equivalent by assuming a switch between the inductance and the voltage source which is open for \( t<0 \) and is closed at \( t=0 \).
Convergence was observed after about 10 RF cycles. The resulting current and voltage waveforms are shown in fig.V-6.

\[ V(t) = (2.0 + 0.733 \sin 2\pi \omega t + h.h.) \text{Volt} \]
\[ I_e(t) = (0.831 \times 10^{-1} + 0.205 \times 10^{-1} \sin(2\pi \omega t + \psi) + h.h.) \text{Amp.} \]

with \( \omega = 173 \text{ GHz} \) and \( \psi = 112^\circ \). The device operated with an efficiency of 1.69\%. The output power is 5.66 mW. The higher harmonics in the voltage waveform may account for the fact that the device does not operate at the voltage amplitude we expected.

Now we want to have a look inside the device operating in this circuit and try to understand how it works. Therefore we divided one RF cycle in eight equal parts according to fig.V-7. At each instant labelled a,b,...,h snapshots were taken of the total particle density, particle density in each valley, average velocity and electric field inside the device. These are shown in the figures V-8, V-9, V-10 and V-11.

At the instant labelled "a" the voltage \( V(t) \) is at its lowest. The device current is rising. The electric field is about 5 to 6 kV/cm over a range of more than 0.5\( \mu \text{m} \) in the central layer. Only at the anode there is a sharp rise of the electric field. Looking at the averaged velocity we see a velocity overshoot (about \( 2.8 \times 10^5 \) m/s) over a range of 0.75\( \mu \text{m} \). Only in the last 0.25 \( \mu \text{m} \) of the channel the average velocity drops due to scattering to the satellite valleys. As can be seen in Fig.V-9a only close to the anode we find a large fraction of carriers in the satellite valleys. This situation results from the previous cycle. As we come to the end of this series it will become clear how this situation was created.

At instant "b" the voltage is rising. During the time between the instants a and b some accumulated carriers have been absorbed by the anode. Because of the rising of the voltage and the decrease of accumulation near the anode the electric field rises more or
Fig. V-6. The resulting current and voltage wave forms.

Fig. V-7. The division of one RF cycle in eight equal parts.
Fig. V-8. Snapshots of the total carrier density.
Fig. V-9. Snapshots of the carrier densities per valley. Solid line central valley, dotted lines the satellite valleys.
Fig. V-10. Snapshots of the average velocity ($10^5$ m/s).
Fig. V-11. Snapshots of the electric field (kV/cm).
less uniform in the entire channel length. This is the consequence of Poisson's equation. During this instant the higher electric field causes a still greater velocity overshoot. At about 0.25 μm from the cathode the average velocity is about $3.6 \cdot 10^5$ m/s. In the remaining part of the channel one can see that the velocity drops due to intervalley scattering. Because of the higher electric field near the cathode the length needed for the carriers to acquire threshold energy is reduced. At instant "c" we see that the velocity has dropped even more because more carriers have gone to the satellite valleys. As one can see in fig.V-8c,d an accumulation starts at about 0.5 μm from the cathode which causes the field to rise strongly at this point. But there the increasing scattering to the satellite valleys causes the carriers to lose more momentum than they can acquire from the electric field. Combined with the fact that the velocity overshoot becomes much lower due to the lowering of the field near the cathode the electronic current drops even before $V(t)$ passes through the value $V_0$ (This is necessary if $\psi > 90^0$). At the instants "d" and "e" we see the build-up of a layer which moves with saturated velocity ($1 \cdot 10^5$ m/s) in the direction of the anode. At instant "f" the voltage is dropping again. Before the maximum height of the layer the velocity decreases to the saturated value. This causes the layer to pile up. This combined with the fact that the voltage drops causes the electric field just to the left of the layer to become even lower. In the zone before the layer the carriers hardly acquire enough energy to scatter to the satellite valleys. At instant "g" the layer starts to merge with the anode. Despite the lowering of the voltage the loss of accumulated carriers near the anode will cause the rise of the electric field in the dead zone. This we can see at the instants "h" and "a". The channel is swept clean from slow moving carriers. Loosing the accumulation layer the electric field has to rise uniform in the entire channel. The rapid rising of the electric field causes a velocity overshoot in nearly the entire channel length. This is again situation "a". The electronic current will
rise rapidly.

From these pictures we see that the rise and fall of the electric current cannot be understood from the properties of bulk material with electric fields uniform in space alone. The fact that the field drops when the voltage rises and vice versa in some regions of the channel, a fact which can be understood from the consequences of the charge distribution on the equation of poisson, is equally important for the understanding of the operation of this device.
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   THEORETICAL STUDY. OF 100 GHz GaAs TRANSFERRED-ELECTRON
   DEVICES.

   MONTE CARLO SIMULATION OF A MILLIMETER-WAVE GUNN-EFFECT
   RELAXATION OSCILLATOR.
V-I. THE TWO-DIMENSIONAL PROBLEM

In the study of devices of a more complex geometry it is the simplest to assume first that the device is extended along one space-coordinate to infinity. On the assumption of a spherically symmetric bandstructure and scatter operators that can be expanded in Legendre polynomials the gradients in that direction vanish. We express the components of the wave vector and the velocity vector as:

\[
\begin{align*}
    k_x &= k \sin \theta \cos \psi \\
    v(k)_x &= v(k) \sin \theta \cos \psi \\
    k_y &= k \sin \theta \sin \psi \\
    v(k)_y &= v(k) \sin \theta \sin \psi \\
    k_z &= k \cos \theta \\
    v(k)_z &= v(k) \cos \theta
\end{align*}
\]  

(VI-1)

The derivatives in \( k \) space can be expressed as:

\[
\begin{bmatrix}
\frac{2}{\partial k} \\
\frac{2}{k \partial \theta} \\
\frac{2}{k \sin \theta \partial \psi}
\end{bmatrix}
= \begin{bmatrix}
\sin \theta \cos \psi & \sin \theta \sin \psi & \cos \theta \\
\cos \theta \cos \psi & \cos \theta \sin \psi & -\sin \theta \\
-\sin \psi & \cos \psi & 0
\end{bmatrix}
\begin{bmatrix}
\frac{2}{\partial k_x} \\
\frac{2}{\partial k_y} \\
\frac{2}{\partial k_z}
\end{bmatrix}
\]  

(VI-2)

We now put \( E_z = 0 \) and \( \partial f(\mathbf{x})/\partial z = 0 \). Using the coordinates \( k, \theta \) and \( \psi \) the BTE then reads:

\[
\begin{align*}
\frac{3}{\partial t} f + (v \sin \theta \cos \psi \frac{3}{\partial x} + v \sin \theta \sin \psi \frac{3}{\partial y}) f + \\
\frac{e}{\hbar} E_x \{ \sin \theta \cos \psi \frac{3}{\partial k} + \frac{1}{k} \cos \theta \cos \psi \frac{3}{\partial \theta} - \frac{\sin \psi}{k \sin \theta} \frac{3}{\partial \psi} \} f \\
\frac{e}{\hbar} E_y \{ \sin \theta \sin \psi \frac{3}{\partial k} + \frac{1}{k} \cos \theta \sin \psi \frac{3}{\partial \theta} + \frac{\cos \psi}{k \sin \theta} \frac{3}{\partial \psi} \} f = \tilde{S} f
\end{align*}
\]  

(VI-3)

We now expand the angular dependence of the D.F. in spherical
harmonics with amplitude coefficients which are a function of the coordinates $x, y, t$ and $k$:

$$f(\theta, \psi) =$$

$$\sum_{n=0}^{\infty} A_n^0 P_n^0(\cos \theta) + \sum_{n=1}^{\infty} \sum_{m=1}^{n} \left\{ A_{nm} \cos m\psi + B_{nm} \sin m\psi \right\} P_n^m(\cos \theta)$$

(VI-4)

In literature the definitions of the Legendre associated functions differ sometimes in sign. All the material used in this paragraph can be found in Hobson [1] and Robin [2]. All the recurrence relations used in this paragraph can also be found in Sneddon [3]. We follow their definitions. The Legendre associated functions used here can be generated from the Legendre polynomials in the following way:

$$P_n^m(\cos \theta) = (-1)^m \sin^m(\theta) \frac{d^m P_n(\cos \theta)}{(d \cos \theta)^n}$$

(VI-5)

The spherical harmonics satisfy the orthogonality relation:

$$\int_{0}^{\pi} \sin \theta d\theta \int_{0}^{2\pi} \cos m \psi \cos m' \psi d\psi = \begin{cases} 0 & \text{if } m \neq m' \\ \frac{2\pi}{2n+1} \frac{(n+m)!}{(n-m)!} & \text{if } m=m' \neq 0 \\ \frac{4\pi}{2(n+1)} & \text{if } m=m'=0 \end{cases}$$

(VI-6)

For the coefficients $A_{nm}$ and $B_{nm}$ we have:
We can insert the expansion (VI-4) into (VI-3) and recover a coupled set of equations for the coefficients $A_{nm}$ and $B_{nm}$ by using (VI-7).

To do so we need the following relations in order to be able to carry out the integrations over the angles $\theta$ and $\psi$.

We first rewrite the expression:

$$\sin\theta \cos\psi \rho_n^m(\cos\theta) \cos m \psi = \frac{\sin \theta}{2} \left[ \cos((m+1)\psi) + \cos((m-1)\psi) \right] \rho_n^m(\cos\theta)$$

(VI-8)

We can use the recurrence relations:

$$\sin \theta \rho_n^m(\cos\theta) = \frac{1}{2n+1} \left[ \rho_{n+1}^{m+1}(\cos\theta) - \rho_{n-1}^{m+1}(\cos\theta) \right]$$

(VI-9)

and:

$$\sin \theta \rho_n^m(\cos\theta) = \frac{(n+m)(n-m+2)}{(2n+1)} \rho_{n+1}^{m-1}(\cos\theta) - \frac{(n+m)(n+m-1)}{(2n+1)} \rho_{n-1}^{m-1}(\cos\theta)$$

(VI-10)

Using (VI-9) and (VI-10) we can rewrite (VI-8) as
\[ \sin \theta \cos \psi \ P_n^m(\cos \theta) \cos m \psi = \]

\[ \frac{1}{2(2n+1)} \left[ \cos(m+1) \left( P_{n-1}^{m+1} - P_{n+1}^{m+1} \right) \right] + \]

\[ \frac{1}{2(2n+1)} \left[ \cos(m-1) \left( (n-m+1)(n-m+2) P_{n+1}^{m-1} - (n+m)(n+m-1) P_{n-1}^{m-1} \right) \right] \]

\( (VI-11a) \)

If \( m = 0 \) using only \( (VI-9) \) one obtains:

\[ \sin \theta \cos \psi \ P_n^m(\cos \theta) = \frac{\cos \psi}{2n+1} \left[ P_{n-1}^1(\cos \theta) - P_{n+1}^1(\cos \theta) \right] \]  \( (VI-11b) \)

If also \( n = 0 \) we simply get:

\[ \sin \theta \cos \psi \ P_0^0(\cos \theta) = -\cos \psi \ P_1^1(\cos \theta) \]  \( (VI-11c) \)

In a similar way we find:

\[ \sin \theta \cos \psi \ P_n^m(\cos \theta) \sin m \psi = \]

\[ \frac{1}{2(2n+1)} \left[ \sin(m+1) \left( P_{n-1}^{m+1} - P_{n+1}^{m+1} \right) \right] + \]  \( (VI-12) \)

\[ \frac{1}{2(2n+1)} \left[ \sin(m-1) \left( (n-m+1)(n-m+2) P_{n+1}^{m-1} - (n+m)(n+m-1) P_{n-1}^{m-1} \right) \right] \]

If \( m = 0 \) this expression is zero.
\[
\sin \theta \sin \psi \, P_n^m(\cos \theta) \sin \psi =
\]
\[
\frac{-1}{2(2n+1)} \left[ \cos(m+1) \psi \left[ P_{n-1}^{m+1} - P_n^{m+1} \right] \right] + \tag{VI-13}
\]
\[
\frac{1}{2(2n+1)} \left[ \cos(m-1) \psi \left[ (n-m+1)(n-m+2)P_{n+1}^{m-1} - (n+m)(n+m-1)P_{n-1}^{m-1} \right] \right]
\]
If \( m = 0 \) this expression is zero.

\[
\sin \theta \sin \psi \, P_n^m(\cos \theta) \cos \psi =
\]
\[
\frac{-1}{2(2n+1)} \left[ \sin(m+1) \psi \left[ P_{n-1}^{m+1} - P_n^{m+1} \right] \right] + \tag{VI-14a}
\]
\[
\frac{-1}{2(2n+1)} \left[ \sin(m-1) \psi \left[ (n-m+1)(n-m+2)P_{n+1}^{m-1} - (n+m)(n+m-1)P_{n-1}^{m-1} \right] \right]
\]
If \( m = 0 \) using only (VI-9) one obtains:

\[
\sin \theta \sin \psi \, P_n^m(\cos \theta) = \frac{\sin \psi}{2n+1} \left[ P_{n-1}^1(\cos \theta) - P_{n+1}^1(\cos \theta) \right] \tag{VI-14b}
\]
If also \( n = 0 \) we simply get:

\[
\sin \theta \sin \psi \, P_0^0(\cos \theta) = -\sin \psi \, P_1^1(\cos \theta) \tag{VI-14c}
\]

With the expressions (VI-11), (VI-12), (VI-13) and (VI-14) we find:

\[
\frac{(2n+1)}{C_i} \frac{(n-m)!}{(n+m)!} \int_0^{2\pi} \frac{p^n d\theta}{\cos \psi} \int_0^{2\pi} \frac{\cos \psi d\psi}{\cos \psi} \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} A_{pq} \cos q \psi \, d\psi =
\]
\[
\sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \frac{P}{p q} \left[ \Omega_{\text{nmpq}}^{(1)} + \Omega_{\text{nmpq}}^{(2)} + \Omega_{\text{nmpq}}^{(3)} + \Omega_{\text{nmpq}}^{(4)} \right] A_{pq} \tag{VI-15}
\]
\[
\frac{(2n+1)}{c_1} \frac{(n-m)!}{(n+m)!} \int_0^{2\pi} \sin^2 \theta \, p^m d\theta \int_0^{2\pi} \cos \psi \sin m \psi \sum_{p=1}^{r} \sum_{q=1}^{r} B_{pq} \sin q \psi \, d\psi =
\]
\[
\sum_{p=0}^{r} \sum_{q=0}^{r} \left( \Omega^{(1)}_{nmpq} + \Omega^{(2)}_{nmpq} + \Omega^{(3)}_{nmpq} + \Omega^{(4)}_{nmpq} \right) B_{pq}
\]
\[
(\text{VI-16})
\]

\[
\frac{(2n+1)}{c_1} \frac{(n-m)!}{(n+m)!} \int_0^{2\pi} \sin^2 \theta \, p^m d\theta \int_0^{2\pi} \sin \psi \cos m \psi \sum_{p=1}^{r} \sum_{q=1}^{r} B_{pq} \sin q \psi \, d\psi =
\]
\[
\sum_{p=1}^{r} \sum_{q=1}^{r} \left( \Omega^{(1)}_{nmpq} - \Omega^{(2)}_{nmpq} - \Omega^{(3)}_{nmpq} + \Omega^{(4)}_{nmpq} \right) B_{pq}
\]
\[
(\text{VI-17})
\]

\[
\frac{(2n+1)}{c_1} \frac{(n-m)!}{(n+m)!} \int_0^{2\pi} \sin^2 \theta \, p^m d\theta \int_0^{2\pi} \sin \psi \sin m \psi \sum_{p=0}^{r} \sum_{q=0}^{r} A_{pq} \cos q \psi \, d\psi =
\]
\[
\sum_{p=0}^{r} \sum_{q=0}^{r} \left( -\Omega^{(1)}_{nmpq} + \Omega^{(2)}_{nmpq} + \Omega^{(3)}_{nmpq} - \Omega^{(4)}_{nmpq} \right) A_{pq}
\]
\[
(\text{VI-18})
\]

where \( c_1 = 2 \) if \( m = 0 \) otherwise \( c_1 = 1 \). The non-zero elements of \( \Omega(n) \) are:
\[ \Omega^{(1)}_{n,m,n+1,m+1} = -\frac{(n+m+2)(n+m+1)}{2(2n+3)} \]  
\hspace{1cm} (VI-19a)

\[ \Omega^{(2)}_{n,m,n-1,m-1} = -\frac{1}{2(2n-1)} \text{ if } m > 1 \]  
\hspace{1cm} (VI-19b)

\[ \Omega^{(3)}_{n,1,n-1} = \frac{1}{2(2n+3)} \text{ if } m > 1 \]  
\hspace{1cm} (VI-19c)

\[ \Omega^{(3)}_{n,1,n+1,0} = \frac{1}{2n+3} \]  
\hspace{1cm} (VI-19d)

\[ \Omega^{(4)}_{n,m,n-1,m+1} = \frac{(n-m)(n-m-1)}{2(2n-1)} \]  
\hspace{1cm} (VI-19e)

We are now left with expressions like:

\[ \frac{2n+1}{2\pi} \frac{(n-m)!}{(n+m)!} \int_0^{\pi} \sin \theta \, p^m_n \, d\theta \]

\[ \int_0^{2\pi} \cos \psi \left[ \cos \theta \cos \psi \frac{\partial}{\partial \theta} - \sin \theta \frac{\partial}{\partial \psi} \right] \sum_{p=0} A_p^q \rho^q \cos \psi \, d\psi \]

\hspace{1cm} (VI-20)

We first carry out the integration over \( \psi \). If \( m = 0 \) we get:

\[ \frac{2n+1}{4} \int_0^{\pi} \sin \theta \, p_n \, d\theta \left[ \cos \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin \theta} \right] \sum_{p=1} A_p^1 \rho^p_p \]

\hspace{1cm} (VI-21a)

If \( m > 0 \) we get:
\[
\frac{(2n+1)(n-m)!}{4(n+m)!} \int_0^\pi \sin^\theta p^n d\theta \left[ \left( \cos^\theta \frac{\partial}{\partial \theta} + \frac{(m+1)}{\sin^\theta} \right) \sum_{p=1}^{n} A_{p,m+1} p^{m+1} \right. \\
\left. - C_2 \left( \cos^\theta \frac{\partial}{\partial \theta} - \frac{(m-1)}{\sin^\theta} \right) \sum_{p=1}^{n} A_{p,m-1} p^{m-1} \right]
\]

Where \( C_2 = 2 \) if \( m = 1 \) else \( C_2 = 1 \).

We have:

\[
\sin^2\theta \frac{d}{d(\cos^\theta)} p_n^{m}(\cos^\theta) = -\cos^\theta p_n^{m}(\cos^\theta) - \sin^\theta p_{n+1}^{m+1}(\cos^\theta) \tag{VI-22}
\]

Eq. (VI-22) can be transformed into:

\[
\cos^\theta \frac{\partial p_{n+1}^{m+1}(\cos^\theta)}{\partial \theta} = \cos^\theta p_n^{m+2} + (m+1) \frac{\cos^2\theta}{\sin^\theta} p_n^{m+1} \tag{VI-23}
\]

Using the recurrence relations:

\[
p_n^{m+2} + 2(m+1) \cotg^\theta p_n^{m+1} + (n-m)(n+m+1)p_n^m = 0 \tag{VI-24}
\]

\[
\cos^\theta p_n^{m}(\cos^\theta) = \frac{(n-m+1)}{(2n+1)} p_n^{m+1}(\cos^\theta) + \frac{(n+m)}{(2n+1)} p_{n-1}^{m}(\cos^\theta) \tag{VI-25}
\]

and (VI-10) we find:

\[
(\cos^\theta \frac{\partial}{\partial \theta} + \frac{(m+1)}{\sin^\theta} ) p_p^{m+1}(\cos^\theta) =
\]

\[
-\frac{-p(p-m)(p-m+1)}{(2p+1)} p_p^{m}(\cos^\theta) + \frac{(p+1)(p+m)(p+m+1)}{(2p+1)} p_{p-1}^{m}(\cos^\theta) \tag{VI-26}
\]

Using (VI-23) we can write:
(cosθ \frac{d}{dθ} - \frac{(m-1)}{sinθ} ) P_{m-1}^p(\cosθ) = cosθP_m^p - (m-1)sinθP_{m-1}^p \quad (VI-27)

Using (VI-9) and (VI-25) this can be worked out further:

(cosθ \frac{d}{dθ} - \frac{(m-1)}{sinθ} ) P_{m-1}^p(\cosθ) = \frac{1}{(2p+1)} \left\{ pP_p^{m+1} + (p+1)P_{p-1}^m \right\} \quad (VI-28)

We can now integrate over the angle θ and obtain:

\frac{(2n+1)}{C_1 2\pi} \frac{(n-m)!}{(n+m)!} \int_0^\pi \sinθ P_n^m(\cosθ)dθ

\frac{2π}{C_1 2\pi} \int_0^\pi \cosθcosθ \frac{d}{dθ} - \frac{sinθ \frac{d}{dθ}}{sinθ} \sum_{p=0}^{∞} \sum_{q=0}^{∞} A_{pq} P_q^{m+1} \cosθdθ

= \sum_{p=0}^{∞} \sum_{q=0}^{∞} \left[ \frac{n+2}{k} \left( Ω^{1(1)} + Ω^{2(2)} \right) - \frac{n-1}{k} \left( Ω^{3(3)} + Ω^{4(4)} \right) \right] nmpq A_{pq} \quad (VI-29)

In a similar way we find:

\frac{(2n+1)}{C_1 2\pi} \frac{(n-m)!}{(n+m)!} \int_0^\pi \sinθ P_n^m(\cosθ)dθ

\frac{2π}{C_1 2\pi} \int_0^\pi \cosθcosθ \frac{d}{dθ} - \frac{sinθ \frac{d}{dθ}}{sinθ} \sum_{p=1}^{∞} \sum_{q=1}^{∞} B_{pq} P_q^{m+1} \sinθdθ

= \sum_{p=1}^{∞} \sum_{q=1}^{∞} \left[ \frac{n+2}{k} \left( Ω^{1(1)} + Ω^{2(2)} \right) - \frac{n-1}{k} \left( Ω^{3(3)} + Ω^{4(4)} \right) \right] nmpq B_{pq} \quad (VI-30)
\[
\frac{(2n+1) (n-m)!}{c_12\pi (n+m)!} \int_0^\pi \sin^m \theta \cos^n \theta d\theta
\]

\[
2\pi \int_0^\pi \cos^m \psi \sin^m \theta \frac{\partial}{\partial \theta} + \sin^m \psi \frac{\partial}{\partial \psi} \sum_{p=1}^\infty \sum_{q=1}^\infty B_{pq} \psi^q \sin^p \psi d\psi
\]

\[
= \sum_{p=1}^\infty \sum_{q=1}^\infty \left[ \frac{n+2}{k} (\Omega^{(1)} - \Omega^{(2)}) + \frac{n-1}{k} (\Omega^{(3)} - \Omega^{(4)}) \right]_{nm;pq} B_{pq}
\]

(VI-31)

\[
\frac{(2n+1) (n-m)!}{c_12\pi (n+m)!} \int_0^\pi \sin^m \theta \cos^n \theta d\theta
\]

\[
2\pi \int_0^\pi \sin^m \psi \cos^m \theta \frac{\partial}{\partial \theta} + \sin^m \psi \frac{\partial}{\partial \psi} \sum_{p=0}^\infty \sum_{q=0}^\infty A_{pq} \psi^q \cos^p \psi d\psi
\]

\[
= \sum_{p=0}^\infty \sum_{q=0}^\infty \left[ \frac{n+2}{k} (\Omega^{(1)} + \Omega^{(2)}) - \frac{n-1}{k} (\Omega^{(3)} + \Omega^{(4)}) \right]_{nm;pq} A_{pq}
\]

(VI-32)

We now calculate the coefficients of the expansion of the function \(g(k)\).

\[
g(\theta, \psi) = \sum_{n=0}^\infty \sum_{m=1}^\infty \left[ C_{nm} \cos^m \psi + D_{nm} \sin^m \psi \right] P_n^m (\cos \theta)
\]

(VI-33)

We follow the derivation of the components as was given in Chapter III paragraph 1. This time however we insert the expansion (VI-34) in (II-7).
\[ g(k) = \frac{V}{(2\pi)^3} \int_0^{\infty} k'^2 dk' \sum_{p=0}^{\infty} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} S_{p}(k,k')(A_{nm}I^{(1)} + B_{nm}I^{(2)}) \]

(VI-34)

where

\[ I^{(1)} = \int_0^{\pi} \int_0^{\pi} P_n^m(\cos\theta') \cos\psi' \, d\theta' \, d\psi' \]

\[ = \int_0^{\pi} \int_0^{\pi} P_n^m(\cos\theta') \cos\psi' \, d\theta' \, d\psi' \]

(VI-35)

\[ I^{(2)} = \int_0^{\pi} \int_0^{\pi} P_n^m(\cos\theta') \sin\psi' \, d\theta' \, d\psi' \]

(VI-36)

With:

\[ \cos(k'\theta - \theta') = \sin k' \sin \theta + \cos k' \cos \theta \]

the integrations over \( \theta' \) and \( \psi' \) will give:

\[ g(k) = \frac{V}{(2\pi)^3} \int_0^{\infty} k'^2 dk' \left[ 4\pi \sum_{n=0}^{\infty} S_{0}(k',k)A_{n0} P_n(\cos\theta) + \right. \]

\[ \left. \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} S_n(k',k) \frac{4\pi}{2n+1} \left[ A_{nm}(k') \cos m\psi + B_{nm}(k') \sin m\psi \right] P_n^m(\cos\theta) \right] \]

(VI-37)

Equation (VI-37) shows that the calculation of the coefficients of the expansion of \( g(k) \) remains very simple each coefficient is given by

\[ C_{nm}(k) = \frac{V}{(2\pi)^3} \frac{4\pi}{(2n+1)} \int_0^{\infty} k'^2 dk' S_n(k',k)A_{nm}(k') \]

(VI-38)
\[ D_{nm}(k) = \frac{V}{(2\pi)^3} \frac{4\pi}{(2n+1)} \int_0^{k'}^2 dk' S_{n}(k',k) B_{nm}(k') \] (VI-39)

We can now form the following sets of coupled equations:

\[ \frac{\partial}{\partial t} A_{nm} + \]
\[ + \sum_{p=0}^{p} \sum_{q=0}^{q} \left\{ \Omega^{(1)} + \Omega^{(2)} + \Omega^{(3)} + \Omega^{(4)} \right\}_{nm pq} \left[ \frac{e}{h} E_x \frac{\partial}{\partial k} + v(k) \frac{\partial}{\partial k} \right] A_{pq} \]
\[ + \sum_{p=1}^{p} \sum_{q=1}^{q} \left\{ \Omega^{(1)} - \Omega^{(2)} - \Omega^{(3)} + \Omega^{(4)} \right\}_{nm pq} \left[ \frac{e}{h} E_y \frac{\partial}{\partial k} + v(k) \frac{\partial}{\partial k} \right] B_{pq} \]
\[ + \sum_{p=0}^{p} \sum_{q=0}^{q} \left\{ \frac{n+2}{k} \left( \Omega^{(1)} + \Omega^{(2)} \right) - \frac{n-1}{k} \left( \Omega^{(3)} + \Omega^{(4)} \right) \right\} \frac{e}{h} E_x A_{pq} \]
\[ + \sum_{p=1}^{p} \sum_{q=1}^{q} \left\{ \frac{n+2}{k} \left( \Omega^{(1)} - \Omega^{(2)} \right) + \frac{n-1}{k} \left( \Omega^{(3)} - \Omega^{(4)} \right) \right\} \frac{e}{h} E_y B_{pq} = C_{nm} \] (VI-40)

\[ \frac{\partial}{\partial t} B_{nm} + \]
\[ + \sum_{p=1}^{p} \sum_{q=1}^{q} \left\{ \Omega^{(1)} + \Omega^{(2)} + \Omega^{(3)} + \Omega^{(4)} \right\}_{nm pq} \left[ \frac{e}{h} E_x \frac{\partial}{\partial k} + v(k) \frac{\partial}{\partial k} \right] B_{pq} \]
\[ + \sum_{p=0}^{p} \sum_{q=0}^{q} \left\{ -\Omega^{(1)} + \Omega^{(2)} + \Omega^{(3)} - \Omega^{(4)} \right\}_{nm pq} \left[ \frac{e}{h} E_y \frac{\partial}{\partial k} + v(k) \frac{\partial}{\partial k} \right] A_{pq} \]
\[ + \sum_{p=1}^{p} \sum_{q=1}^{q} \left\{ \frac{n+2}{k} \left( \Omega^{(1)} + \Omega^{(2)} \right) - \frac{n-1}{k} \left( \Omega^{(3)} + \Omega^{(4)} \right) \right\} \frac{e}{h} E_x A_{pq} \]
\[ + \sum_{p=0}^{p} \sum_{q=0}^{q} \left\{ \frac{n+2}{k} \left( -\Omega^{(1)} + \Omega^{(2)} \right) - \frac{n-1}{k} \left( \Omega^{(3)} - \Omega^{(4)} \right) \right\} \frac{e}{h} E_y A_{pq} = D_{nm} \] (VI-41)
The sets (VI-40) and (VI-41) contain two independent sets. One which couples all the coefficients $A_{nm}$ and $B_{nm}$ with $n+m$ even. The other set couples all the coefficients with $n+m$ odd. It can be shown that the coefficients of this last set will either be zero or approach zero under the supposed conditions ($E_z = 0$, spherical bandstructure etc.) The coupling between the coefficients of the first set is shown in the following figure.

For the macroscopic quantities we have:

\[
n(x,y,t) = 4\pi \int_0^\infty k^2 dk A_{00}(k) \quad (VI-42)
\]

\[
v_x(x,y,t) = -\frac{4\pi}{3n} \int_0^\infty v(k)k^2 dk A_{11} \quad (VI-43)
\]

\[
v_y(x,y,t) = -\frac{4\pi}{3n} \int_0^\infty v(k)k^2 dk B_{11} \quad (VI-44)
\]

\[
\varepsilon(x,y,t) = \frac{4\pi}{n} \int_0^\infty \varepsilon(k)k^2 dk A_{00} \quad (VI-45)
\]
An expansion of the radial part of the D.F. in Hermite polynomials can also be tried here.

\[ A_{nm}(k) = \xi^n \sum_{i=0}^{\infty} \frac{H_{2i}(\xi)}{\xi^n} \left( \frac{d}{d\xi} + \frac{m+2}{\xi} \right) \exp(-\xi^2) \]  

(VI-46)

\[ B_{nm}(k) = \xi^n \sum_{i=0}^{\infty} \frac{H_{2i}(\xi)}{\xi^n} \exp(-\xi^2) \]  

(VI-47)

with (see III-72):

\[ \xi = k/\kappa \]

We introduce the following matrices (see III-77):

\[ \phi(a)_{ip} = \frac{1}{\kappa} \int_0^\infty \frac{H_{2i}(\xi)}{\xi^n} \left( \frac{d}{d\xi} + \frac{m+2}{\xi} \right) \xi^n \exp(-\xi^2) \]  

(VI-48)

which has the following non-zero elements:

\[ \phi(a)_{ii} = 2(i - n - 1) \]  

(VI-49)

\[ \phi(a)_{i,j-1} = 2 \sqrt{i(i-\frac{1}{\kappa})} \]

and

\[ \phi(b)_{ip} = \frac{1}{\kappa} \int_0^\infty \frac{H_{2i}(\xi)}{\xi^n} \left( \frac{d}{d\xi} - \frac{n+1}{\xi} \right) \xi^n \exp(-\xi^2) \]  

(VI-50)

which has the following non-zero elements:
\[ \phi(b)_{i-s,i} = (-1)^s 2^{i+1} \frac{i! \sqrt{(2i-2s)!}}{(i-s)! \sqrt{2i!}} \]  

(VI-51)

We also introduce the matrices (see IV-19):

\[ v(a)_{i-s,i} = \sum_{0}^{\infty} H_{2i}(\xi) v(k) \xi H_{2s}(\xi) \exp(-\xi^2) \]  

(VI-52)

\[ v(b)_{i-s,i} = \sum_{0}^{\infty} H_{2i}(\xi) \frac{v(k)}{\xi} H_{2s}(\xi) \exp(-\xi^2) \]

Using these matrices we can construct the transport equations in two dimensions:

\[
\begin{align*}
\frac{\partial}{\partial t} F_{nm}^{i} + & \sum_{s} \left[ \frac{e}{h} E_{x} \phi_{nm}^{(a)is} + v(a)_{i-s,i} \frac{\partial}{\partial x} \right] F_{nm}^{s} \, \left( n+1, m+1 \right) \\
+ & \sum_{s} \left[ \frac{e}{h} E_{x} \phi_{nm}^{(b)is} + v(b)_{i-s,i} \frac{\partial}{\partial x} \right] F_{nm}^{s} \, \left( n-1, m-1 \right) \\
+ & \sum_{s} \left[ \frac{e}{h} E_{x} \phi_{nm}^{(a)is} + v(a)_{i-s,i} \frac{\partial}{\partial y} \right] F_{nm}^{s} \, \left( n+1, m-1 \right) \\
+ & \sum_{s} \left[ \frac{e}{h} E_{x} \phi_{nm}^{(b)is} + v(b)_{i-s,i} \frac{\partial}{\partial y} \right] F_{nm}^{s} \, \left( n-1, m+1 \right) \\
- & \sum_{s} \left[ \frac{e}{h} E_{y} \phi_{nm}^{(a)is} + v(a)_{i-s,i} \frac{\partial}{\partial y} \right] G_{nm}^{s} \, \left( n+1, m-1 \right) \\
- & \sum_{s} \left[ \frac{e}{h} E_{y} \phi_{nm}^{(b)is} + v(b)_{i-s,i} \frac{\partial}{\partial y} \right] G_{nm}^{s} \, \left( n-1, m+1 \right) \\
+ & \sum_{s} \left[ \frac{e}{h} E_{y} \phi_{nm}^{(a)is} + v(a)_{i-s,i} \frac{\partial}{\partial y} \right] G_{nm}^{s} \, \left( n+1, m+1 \right) \\
+ & \sum_{s} \left[ \frac{e}{h} E_{y} \phi_{nm}^{(b)is} + v(b)_{i-s,i} \frac{\partial}{\partial y} \right] G_{nm}^{s} \, \left( n-1, m-1 \right)
\end{align*}
\]
\[
\frac{\partial}{\partial t} G_{nm}^{1} + \Omega_{nm}^{(1)} \sum_{s} \left\{ \frac{e}{h} E_{x} \phi(a)_{is} + v(a)_{is} \frac{\partial}{\partial x} \right\} G_{n+1,m+1}^{s} \\
+ \Omega_{nm}^{(2)} \sum_{s} \left\{ \frac{e}{h} E_{x} \phi(b)_{is} + v(b)_{is} \frac{\partial}{\partial x} \right\} G_{n-1,m-1}^{s} \\
+ \Omega_{nm}^{(3)} \sum_{s} \left\{ \frac{e}{h} E_{x} \phi(a)_{is} + v(a)_{is} \frac{\partial}{\partial x} \right\} G_{n+1,m-1}^{s} \\
+ \Omega_{nm}^{(4)} \sum_{s} \left\{ \frac{e}{h} E_{x} \phi(b)_{is} + v(b)_{is} \frac{\partial}{\partial x} \right\} G_{n-1,m+1}^{s} \\
- \Omega_{nm}^{(1)} \sum_{s} \left\{ \frac{e}{h} E_{y} \phi(a)_{is} + v(b)_{is} \frac{\partial}{\partial y} \right\} F_{n+1,m+1}^{s} \\
+ \Omega_{nm}^{(2)} \sum_{s} \left\{ \frac{e}{h} E_{y} \phi(b)_{is} + v(b)_{is} \frac{\partial}{\partial y} \right\} F_{n-1,m-1}^{s} \\
+ \Omega_{nm}^{(3)} \sum_{s} \left\{ \frac{e}{h} E_{y} \phi(a)_{is} + v(a)_{is} \frac{\partial}{\partial y} \right\} F_{n+1,m-1}^{s} \\
- \Omega_{nm}^{(4)} \sum_{s} \left\{ \frac{e}{h} E_{y} \phi(b)_{is} + v(a)_{is} \frac{\partial}{\partial y} \right\} F_{n-1,m+1}^{s} = \sum_{n} S_{n}^{1p} G_{nm}^{P}
\]

(VI-53)

The scattering matrices S are exactly the same as those defined in Chapter III paragraph 6 (see III-78). Recovering the macroscopic quantities is very similar to (III-79,80,81).

\[
n = \kappa^{-3/2} n^{5/4} (F_{00}^{0} + \sqrt{2} F_{00}^{1})
\]

(VI-54)

\[
n_{x} = - \sum_{s} \alpha s F_{s}^{G}
\]

(VI-55)

\[
n_{y} = - \sum_{s} \alpha s F_{s}^{G}
\]

(VI-56)
\[ n\varepsilon = \sum_{s} \beta_{s} F_{s00} \]  

(VI-57)

where the coefficients \( \alpha_{s} \) and \( \beta_{s} \) are the same as in (III-80) and (III-81).

The number of parameters that needs to be stored in order to simulate a device of reasonable proportions is now enormous. This means that only very small devices may be candidates for such a simulation. Considering only \( F_{00}^{1}, F_{11}^{1} \) and \( G_{11}^{1} \) will reduce the number of parameters considerably. The results are then not very accurate but will give very good estimates.
References


VII. CONCLUSIONS.

In semiconductor devices of submicron dimensions it has been found necessary to use modeling methods that represent the physical processes in more detail than the usual drift-diffusion approach. In practice this means that the carrier distribution function (henceforth called D.F.) has to be calculated rather accurately. Especially for the III-V compounds like GaAs the Distribution Function has a wide variety of shapes at higher electric fields. In fig.III-4 a few of these shapes are shown. This is due to the existence of different minima (valleys) in the conduction bands of these compounds. When the applied electric field is zero nearly all the charge carriers are in the lowest energy minimum, the central valley. Under the influence of an applied electric field a great proportion of carriers are scattered to higher lying minima, the so called satellite valleys. The D.F.'s shown in fig.III-4 are those of the central valley. For a sufficiently accurate description of the macroscopic quantities a reasonably accurate determination of the D.F. in each valley is necessary.

Over the past 10 years a number of methods have come into use which accomplish this to different degrees of extent, e.g. Monte Carlo techniques, iterative methods, Displaced Maxwellian methods and energy relaxation methods. Of these the M.C. and iterative techniques are accurate but very costly, whereas the others are much faster but their accuracy is difficult to establish.

The main aim of this work was to develop a method which is less costly than the Monte Carlo or iterative ones but more accurate than the energy relaxation or Displaced Maxwellian approach.

From results we may conclude that a great reduction in computing effort is possible by sacrificing some detail of the D.F. while keeping accurate knowledge of the average velocity, energy and particle density in each valley.
Three different, but closely related methods were tried consecutively. In the first method the angular part of the D.F. was developed in Legendre polynomials. The radial part was represented by a number of points in k-space. In our examples 200 points were used, although less points would still give very good results. Only space independent cases were treated. This expansion leads to a set of equations which can be solved numerically. The method is described in Chapter III, paragraph 1, 2, 3 and 4. Using only two terms of the expansion the method is very efficient. A 100 iterations then take about 20 seconds of CPU time. However for the III-V compounds at least four terms are necessary. Using six terms one will get very accurate results. If the problem would require more than six terms this method would loose it attractiveness since the number of calculations needed for one iteration is at least proportional to the square of the number of terms.
Including space-dependence in this method is out of the question since this would require an enormous amount of memory and computer time.

In the second method the radial dependence was represented by a number of integrals over k-space. In this way a great reduction of the number of parameters representing the D.F. is possible. We have called these integrals Generalized Transport Quantities. The time-dependent problem of GaAs can successfully be handled by this method. In Chapter III, paragraph 5 it is shown how one can obtain detailed information of the particle density, average velocity and energy in each valley separately. To do so accurately one has to consider at least ten G.T.Q.'s per valley. The preparatory calculations and efforts are however expensive and difficult. To include space dependence may be possible but will be difficult. From our work no conclusions can be drawn regarding the question whether the space dependent problem of the III-V compounds can be handled in this manner. For other materials where the scattering is more dominant calculations have shown us that this method is
successful, accurate and fast.

In the third method, described in Chapter III, paragraph 6 we expanded the radial dependence in Hermite polynomials. Not only the time dependent but also the one dimensional space dependent problem can be handled successfully using this method. The number of coefficients describing the D.F. can be reduced to 32,12 and 8 in the $\Gamma$, L and X valleys. The method is however considerably slower than the energy relaxation method. For the space independent problem the method is still very fast. A 100 iterations take about 3 seconds of CPU time. The accuracy is dependent on the weightfactor introduced in the expansion (see III-71). A small weightfactor gives excellent accuracy at low fields but large errors at fields higher than a certain limit value. A larger weightfactor shifts this limit to higher values but decreases the accuracy at lower fields. A compromise value has been found which gives good accuracy from zero to 100 kV/cm, using 8 Hermite polynomials. To handle higher field strengths one has to choose a larger weightfactor and one has to increase the number of Hermite polynomials.

In dealing with the space dependent problem the question of numerical instabilities will arise. Having tried several integration schemes it was found that a straight-forward first-order scheme is the only stable one. To obtain stability some extra dissipation has to be added to some terms or some smoothing has to be applied. This does not involve those terms that describe the macroscopic quantities, therefore they do not suffer and can be obtained with high accuracy.

By adding the space dependence the interrelationship of the parameters requires expensive matrix multiplications. These matrix multiplications can only be reduced at the cost of accuracy. This means that this method can only compete with the M.C. method if the problem requires a small number of grid points in real space.

Using the three valley model for GaAs, a division of 1 $\mu$m in 100
grid points and 32 coefficients for the central valley, the calculation of the evolution of this 1 μm long piece of material during 1 psec. takes about 20 minutes of CPU time on a Gould SEL 32/77 computer. Using only 16 coefficients for the central valley the same calculation takes about 5 minutes, but then the results are far less accurate.

The great advantage of this method compared to M.C. are the accurate plots one can obtain for the particle density, average velocity and energy for each valley. It has been applied to a millimeter wave Gunn diode under applied d.c. and a.c. voltages as well as the same diode placed in an oscillator circuit with only a d.c. voltage applied. This has been described in chapter V. The advantage and importance of accurate plots is demonstrated there. They appear to be essential for the understanding of the operation of the device. To obtain such smooth plots using the M.C. method would require an enormous amount of simulated electrons. The LHE method then clearly has the advantage.

Extension of this method to more than one space dimension is possible and its principle is demonstrated in Chapter 6. The simulation of a two dimensional device then requires many coefficients. A computational facility which possesses a large memory and fast vector or matrix processing capabilities will make such an approach feasible.
VIII SUMMARY.

In this thesis modeling methods are developed that represent the physical processes in more detail than the usual drift-diffusion approach and at the same time are less costly than the Monte Carlo or iterative techniques. The short dimensions and time scales in which modern devices operate make a more detailed approach necessary. In practice this means that the distribution function (henceforth called the D.F.) has to be calculated rather accurately.

We have restricted ourselves to cases where the bandstructure has spherical symmetry and the electric field has only one component in real space. The methods that are developed can be applied to III-V semiconductor materials since they are the most difficult to describe. They can however be applied to other materials as well.

To give the methods a test GaAs is chosen as material.

Chapter II gives the basic transport equations and the scattering mechanisms.

Chapter III deals with the space independent problem. Under the assumed conditions the angular part of the D.F. can be expanded in Legendre polynomials. Transport equations for the expansion coefficients are derived from the Boltzmann transport equation. This leads to an infinite set of differential equations which, after truncation, can be solved iteratively. In order to avoid instabilities this truncated set is transformed into an integral form. An efficient way to solve the set of integral equations is given. A few results are shown and discussed.

In order to reduce the computation time two new methods are developed and tested. In paragraph 5 the radial dependence of the D.F. is represented by a number of integrals over k-space. These integrals are called Generalized Transport Coefficients. A coupled set of equations for these coefficients is derived. How to express the scattering processes in this method is explained and discussed in detail. A few results are shown.
The second method to reduce the computation time is given in paragraph 6. Here the radial dependence of the D.F. is expanded in Hermite polynomials. The D.F. is now represented by a number of expansion coefficients. The transport equations for these coefficients are derived. The scattering processes can be represented by a scattering matrix. The elements of this matrix can be obtained in a simple and straightforward manner. How to avoid some difficulties at high fields is discussed in detail.

Chapter IV deals with the space dependent problem. The feasibility of the different methods is discussed. Only the LHE method (Legendre-Hermite Expansion) is fully investigated. An extension of the transport equations which now contain the space derivatives are given in paragraph 2. Paragraph 3 shows how stable iteration schemes can be constructed which can solve the space dependent problem. Only first-order schemes appear to be stable. One of these stable first-order schemes is applied in Chapter V. The results of a millimeter wave Gunn diode under applied d.c. and a.c. voltages are given as well as the same diode placed in an oscillator circuit.

Chapter 6 shows how the LHE method can be extended to the two-dimensional space dependent problem.
APPENDIX

Physical constants.

Planck constant \( h = 1.0546 \times 10^{-34} \text{ J.s} \)
Electron rest mass \( m_0 = 9.1095 \times 10^{-31} \text{ kg} \)
Elementary charge \( q = 1.6022 \times 10^{-19} \text{ C} \)
Dielectric constant \( \varepsilon_0 = 8.8542 \times 10^{-12} \text{ F/m} \)
Boltzmann constant \( k_B = 1.3807 \times 10^{-23} \text{ J/K} \)

Parameters of the three-level model of GaAs according to Littlejohn.

<table>
<thead>
<tr>
<th>( \Gamma(0,0,0) )</th>
<th>( L(1,1,1) )</th>
<th>( X(0,0,0) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{m}{m_0} )</td>
<td>0.063</td>
<td>0.222</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>0.610 eV(^{-1})</td>
<td>0.461 eV(^{-1})</td>
</tr>
<tr>
<td>( \Delta_{j} )</td>
<td>1.439 eV</td>
<td>1.769 eV</td>
</tr>
<tr>
<td>( \varepsilon_{ac} )</td>
<td>7.00 eV</td>
<td>9.20 eV</td>
</tr>
<tr>
<td>( D_{ij} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \Gamma )</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>( L )</td>
<td>10(^9) eV/m</td>
<td>10(^9) eV/m</td>
</tr>
<tr>
<td>( X )</td>
<td>10(^9) eV/m</td>
<td>5 \times 10(^8) eV/m</td>
</tr>
<tr>
<td>( h\omega_{ij} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \Gamma )</td>
<td>-</td>
<td>0.0278 eV</td>
</tr>
<tr>
<td>( L )</td>
<td>0.0278 eV</td>
<td>0.0290 eV</td>
</tr>
<tr>
<td>( X )</td>
<td>0.0299 eV</td>
<td>0.0293 eV</td>
</tr>
<tr>
<td>( Z_j )</td>
<td>1</td>
<td>4</td>
</tr>
</tbody>
</table>
SAMENVATTING.

In dit proefschrift zijn verschillende modelleermethoden ontwikkeld die de fysische processen in meer detail weergeven dan de gebruikelijke drift-diffusie benadering en die tevens minder kostbaar zijn dan de Monte Carlo of iteratieve technieken. De kleine afmetingen en de korte tijdschalen waarin de moderne halfgeleider-componenten werken maken zo'n gedetailleerde benadering noodzakelijk. In de praktijk betekent dit dat de distributiefunctie (vanaf nu de D.F. genoemd) min of meer nauwkeurig berekend moet worden.

We hebben ons beperkt tot die gevallen waarbij de bandstructuur een sferische symmetrie heeft en het electrische veld slechts één component in de plaatsruimte. De methoden die ontwikkeld zijn kunnen toegepast worden op de III-V halfgeleider-materialen omdat deze het moeilijkst zijn. De methoden kunnen echter net zo goed op andere materialen toegepast worden. Om de methoden te testen werd als materiaal GaAs gekozen.

Hoofdstuk II geeft de basisvergelijkingen van het transport en de verstrooingsprocessen.


Om de rekentijd te verminderen zijn er twee nieuwe methoden ontwikkeld en beproefd. In paragraaf 5 wordt de radiale afhankelijkheid van de D.F. vertegenwoordigd door een aantal


Een van deze stabiele eerste-orde schema's is toegepast in hoofdstuk V. De resultaten van een millimetergolf Gunn diode onder een aangelegde wissel- en gelijkspanning worden gegeven evenals de resultaten voor het geval waarbij deze diode in een oscillator circuit wordt geplaatst.

Hoofdstuk VI laat zien hoe de LHE methode uitgebreid kan worden naar het tweedimensionale plaatsafhankelijke probleem.
LEVENSLoop

Stellingen behorende bij het proefschrift van

S.C. van Someren Gréve

De rechtvaardiging van een op energie relaxatie tijd gebaseerde analyse van III-V compounds door deze af te leiden van de verstrooilingsintegralen is niet juist.


II

Het verkrijgen van goede resultaten met behulp van de methode van de gegeneraliseerde verschoven Maxwell-verdeling door het aanpassen van de verstrooilings parameters aan deze methode kan deze niet rechtvaardigen.


III

Het voldoen aan de kconditie van von Neumann van een differentie-schema voor het oplossen van een hyperbolisch stelsel differentiaalvergelijkingen, waarbij de vergelijking van Poisson mede het transport bepaalt, is niet voldoende voor stabiliteit.

Dit proefschrift, hs IV.

IV

Het sommeren van de macroscopische grootheden van alle valleien bij de energie relaxatie tijd methode dient niet alleen om rekentijd te besparen maar ook om onnauwkeurigheden te verbergen.

V

Bij het postuleren van morphogenetische velden veronderstelt Sheldrake dat deze toevallig van aard zijn. Als men veronderstelt dat God de mens naar zijn beeld geschapen heeft en men vertaalt het woord beeld in morphogenetisch veld, dan is dit veld niet toevallig van aard en is de evolutie de poging van de materie om in morphogenetische resonantie te komen met dit veld.

De pogingen van Capra om de inzichten van de quantummechanica in verband te brengen met de ideeën van de oosterse mystiek zijn erop gericht deze ideeën een mentale vorm te geven. De weg van de oosterse mystiek gaat in de tegenovergestelde richting en tracht ieders mentale vorm juist los te laten.

F. Capra. *The Tao of Physics.*

Met de komst van het informatie-tijdperk wordt een tijd van verwarring ingeluid.

Als de maatschappij de vrijgekomen creatieve energie van werkeloze schoolverlaters en academici niet weet te kanaliseren in zinvol werk, dan zal deze creatieve energie omslaan in een destructieve kracht.