# MATHEMATICAL MODELLING OF SEMI CONDUCTOR DEVICES AND PROCESSES

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# THESIS SUMMARY

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Mathematical models of semiconductor devices are developed using the nearly isotropic approximation to the Boltzmann transport equation. The formalism treats the steady state inhomogeneous cases and an electric field is included in the analysis. As well as developing the equations to describe the charge transport appropriate boundary value problems are discussed.

A general equation can be developed which, by the inclusion or exclusion of certain parameters, is able to describe the twelve models that are being considered: the type of scatterers, whether non-polar optical, piezoelectric or acoustic phonons, the presence or absence of an electric field and the order of expansion of the collision integral in terms of the phonon energy. Restricted cases of this equation are considered and general solutions given.

One particular model, that of non-polar optical phonon scattering in the presence of an electric field with first order phonon energy expansion is discussed in detail. The electron distribution function and associated current due to an arbitrary injected energy distribution of electrons is determined by novel semi-analytical means.

The other possible models, and solutions, are discussed and methods of validating the analysis are mentioned.

ACKNOWLEDGMENTS

There are several people who have helped me to complete this work. I would particularly like to thank my supervisor Dr W. Cox whose enthusiasm and cheerfulness made my research, and the production of this thesis, an enjoyable experience.

The members of staff and my fellow research students in the department also provided a cordial environment in which to pursue this research.

Credit for the typing goes to Sheila Allen who has ensured that the production of this thesis was far less protracted than had been anticipated.

CONTENTS

## List of Illustrations

## DECLARATION

This thesis contains my own research work performed in the Department of Computer Science and Applied Mathematics between October 1984 and October 1987 under the supervision of Dr W Cox.

Parts of this work have been published in the scientific literature:

1 Semi-analytical treatment of electron transport in the presence of an electric field
W Cox and E J Bailey
Solid State Electronics 31, (7), pp 1169-1178, 1988

# CHAPTER ONE

## DEVICE MODELLING

### §1. Introduction

Pioneering semiconductor work was performed less than fifty years ago. The production of working devices then contained an element of luck. In the 1980's, it is possible to fabricate devices with geometrical features of dimensions less than one micron, and yields of eighty percent are not uncommon. This is mainly due to the rapid improvement in process and process control technology. However it is only useful to have very high yields of the devices if they behave as predicted: a one hundred percent yield of a transistor that only has a tenth of the gain expected is useless. Thus as well as having tight control over the process it is essential to be able to predict the electrical behaviour of the devices that are produced. Assuming that the production process could be perfectly controlled then geometries and doping profiles must be defined that give the required behaviour. This leads to the necessity of developing a semiconductor device modelling capability such that all required quantities can be predicted accurately, with acceptable precision. Obviously, there are two main ways to mathematically model the device, and to achieve this aim - computationally or analytically. The former has had a great deal of effort directed towards it as it is an extremely useful practical tool while the latter has been somewhat ignored. This is the opposite to what has happened in other

areas of mathematical modelling, such as fluid mechanics. For example, in fluid mechanics the basic equations have been well known for over a century and it is relatively recently, in the last couple of decades, that computational fluid mechanics has come to the fore. This is a more natural progression in that time has been spent investigating the mathematical aspects of the subject giving a firm base to computational approaches. As the advent of semiconductors and computing machines has occurred nearly simultaneously (the latter depending on the development of the former) there has been emphasis on numerical approaches without a particularly well developed analytical background. Although computational modelling has proved valuable in the analysis and design of device structures [1], analytic modelling has a place in this scheme and one that is complementary to computational simulations. The area to be developed in this thesis is that of analytical semiconductor modelling and analytic or semi- analytic mathematical methods.

Computational models offer several useful features; they can nearly remove the iterative approach to device design that was prevalent before the advent of such methods; using this approach a design was achieved by a combination of simple textbook formula [2] and experience. The design usually failed i.e. the observed electrical characteristics did not match the predicted ones. Then the iterative process would begin, and finish when, or if, a satisfactory design was achieved. This could take many steps, and prove to be very costly. For present day devices this approach is not feasible. Important device characteristics (such as gain, junction-breakdown voltage and thermal variation of characteristics) may be predicted and thus

controlled. This is a key element in device models. Another crucially important aspect of simulation is that it allows design modifications and also totally original device structures to be investigated without ever producing an actual device. Very flexible simulations exist that may be used in this manner. This again offers a capability that was impossible before such software was produced. Finally another aspect that needs to be mentioned is that simulations can provide information on physically unobservable quantities both in a practical or actual sense, such as the electron distribution function. Such quantities can prove invaluable in device design.

Thus computational modelling has a leading role to play in device design. However analytic models offer other features.

Firstly it must be ensured that the modelling problem is formulated correctly; if it is not then the only indication of this from simulations may be non-convergence, which is an extreme waste of resources. Analytical approaches can offer answers to such questions, although due to the inherent difficulty of semiconductor device modelling the topic is still in its infancy [3]. Secondly analytic models provide exact answers (modulo the background assumptions) and are hence capable of validating computer codes. This can be a valuable comparison technique as although codes may converge it is no guarantee that they have converged to the (unique) solution. Analytical results can also provide an initial input to simulations providing the first approximation to the solution [4]. All computational models rely on numerical iteration, and usually are based on Newton-Raphson iteration which only converges locally and

then quadratically. Thus an accurate initial solution can save vast amounts of computer time.

The two aspects of analytical models that will be of concern in this thesis are that analysis can provide general models, which can then be used to predict the variation of observables with respect to certain parameters. The methods and models developed mathematically also form a basis for further research and are thus useful in themselves.

## §2. Mathematical modelling

Essentially this involves the abstraction of the physics, and physical environment of the device into a mathematical form. It generally is a compromise between reality and tractability. The mathematical model will involve mainly partial differential equations (cf Chapter 2 and Chapter 4) which are then generally solved numerically although more esoteric formulations are necessary such as the Boltzmann transport equation (BTE), a non-linear integrodifferential equation (see Chapter 2). Whatever the model, it must include all the essential physics. This may be extremely difficult (see [5] for example) and has to be achieved by experience, intuition and iteration; comparing observed results with predicted results and modifying the equations as necessary.

The process may be viewed as two distinct steps: the first involves setting up the mathematical equations with appropriate conditions to describe the situation and the second involves the solution of such a model. The latter stage may be achieved in several ways (analytically/computationally/approximately ) and

is in some ways secondary. If the model is insoluble it can be useful to simplify the basic assumptions until the mathematics is tractable and then refine.

Modelling has, in some quarters, become synonymous with computational modelling or simulation, particularly finite element and finite difference methods. Although the latter approaches are providing detailed knowledge of previously unknown phenomena they are only part of the secondary procedure - namely a solution tool.

It is essential to firstly develop the correct equations: these are well known for medium small devices but for the high field regime or in the quantum domain or both, the analysis and interpretation of such formulations is controversial. In quantum transport theory there is little experimental evidence for comparison.

In this thesis mathematical modelling will mean analytic (or semi-analytic) treatment of the appropriate equations, involving formulation and, where possible, solution.

## §3. Semiconductor device models

The previous two sections have explained the necessity for semiconductor device models and given a brief introduction to the modelling idea. Here, the topic of discussion will be semiconductors and the essentials for modelling such materials will be discussed.

In the case of semiconductors the abstraction of the physical data is an extremely complex operation. Semiconductor device physics involves a large number of

charged electrons and uncharged phonons which are interacting. Surprisingly, simple approximations are quite often adequate: the effective electron mass may often be taken as constant and the electrons themselves may be treated semi-classically. As in most modelling situations it is generally impossible to quantitively predict the final effect of an earlier simplification and the justification of the ones used in this thesis is that they have a firm physical basis. Particular assumptions will be noted at the appropriate juncture.

There are a number of semiconducting materials each requiring a different description and there are also a large number of semiconducting devices (MOS and bipolar being the two main categories), each having different modes of operation and requiring different types of models. It is convenient to divide the device models into four different regimes and discuss each material/device within the particular regime.

i) Textbook models

These give simple and useful equations relating the various device parameters and characteristics. Typical of such results is (see [6])

$$BV_{CEO} = BV_{CBO} (1 + \beta)^{-1/m}$$

where (in the case of bipolar transistors)

$BV_{CEO}$ : collector emitter breakdown voltage (open base)

$BV_{CBO}$ : collector base breakdown voltage (open base)

$\beta$ : current gain

m : exponent, satisfying $4 \leq m \leq 10$.

These may be treated as rules to optimise the design. Generally, however, such rules have limited accuracy as they are often empirically based and also have limited ranged of validity. They do not offer a practical mathematical model for sophisticated devices and will not be considered further.

ii) Hydrodynamic models

The majority of computational effort (excluding Monte Carlo simulations) has been directed in solving the following set of hydrodynamical equations:

$$\nabla^2 \psi = q\,(n - p - c)\,/\varepsilon$$

$$-\,q\frac{\partial n}{\partial t} + \nabla \cdot \vec{J}_n = q\,R$$

$$q\frac{\partial p}{\partial t} + \nabla \cdot \vec{J}_p = -\,q\,R$$

$$\vec{J}_n = qn\,\mu_n \vec{E}_n + qD_n \nabla n + D_n \nabla T^{qn}$$

$$\vec{J}_p = qp\mu_p \vec{E}_p - qD_p \nabla p + D_p^T \nabla T \, qp$$

$$\nabla \cdot (k(T)\nabla T) = \rho c \frac{\partial T}{\partial t} - H$$

where:

| | |
|---|---|
| $\psi$ | electrostatic potential |
| $q$ | elementary charge |
| $\varepsilon$ | absolute permittivity |
| $n$ | electron concentration |
| $p$ | hole concentration |
| $C$ | net ionized impurity concentration |
| $J_n$ | electron current density |
| $R$ | net carrier recombination rate |
| $J_p$ | hole current density |
| $\mu_n$ | electron mobility |
| $\vec{E}_n$ | effective electron field |
| $D_n$ | effective electron diffusivity |
| $\mu_p$ | hole mobility |
| $\vec{E}_p$ | effective hole field |
| $D_p$ | effective hole diffusivity |
| $\rho$ | specific mass density |
| $c$ | specific heat |
| $T$ | lattice temperature |
| $t$ | time |
| $H$ | thermal generation |
| $k(T)$ | thermal conductivity |
| $D_{n,p}^T$ | effective thermal carrier diffusivity. |

These constitute a coupled non-linear system of partial differential equations, and represent a formidable mathematical problem. In most simulations the dimensionality of the problem is restricted (usually to two) and transient and thermal behaviour is ignored, although for certain applications these aspects [5] must be included. The simplified equations given above then become

$$\lambda^2 \nabla^2 \psi = n - p - C$$

$$\nabla \cdot (\nabla_n - n\nabla\psi) = R$$

$$\nabla \cdot (\nabla_p + p\nabla\psi) = R$$

plus associated boundary conditions, where the current relations have been substituted in the continuity equations and the Einstein relation has been assumed - namely $D/\mu = \frac{k_b T}{q}$, $k_b$ being the Boltzmann constant. Appropriate dimensional scales have been used to produce this simplified form. These form a coupled non-linear system of elliptic equations with $\lambda$ being a numerically small parameter. Note that as $\lambda$ is small singular perturbation techniques are available to study the system [7].

As they are non-linear equations the most common numerical technique of solution is to apply Newton-Raphson iteration to the set. This generates a set of matrix equations which then have to be solved, either coupled together or uncoupled (Gummel algorithm). The matrices have specific properties such as sparsity which can be taken advantage of [7] Once $\psi$, n, p are known, then other physical observables may be calculated, such as the electric field $E = -\nabla\psi$.

Accurate results can be produced providing that the limitations of the formulation and the numerical methods are remembered: for example it is assumed that medium small (or larger) devices are being treated. There are also assumptions pertaining to the simplification of the Maxwell equations to the Poisson equation. Problems can arise in the numerical analysis as convergence is a notoriously difficult problem. However, accuracy within a few percent may be achieved by simulation in calculations of say breakdown voltages.

MOS devices are simpler to simulate than bipolar structures as they are essentially unipolar and recombination can be ignored, reducing the complexity of the governing equations. Bipolar devices can be successfully simulated but require the full set of equations as contributions from both carriers must be considered.

Computational modelling is thus an essential design tool. However, it requires mainframe computational resources and accurate input of data that is difficult to determine. This then introduces more problems; to exemplify the latter point consider C, the net impurity profile which is the difference between the number of ionized donor and acceptor atoms. For a typical MOS structure, it would be difficult to measure (in two dimensions) the impurity profile, and this is essential input. The only sensible answer is to simulate the manufacturing process. The problem with this approach is that there can be many stages that affect the re-distribution of dopants and the physics and chemistry is not well understood.

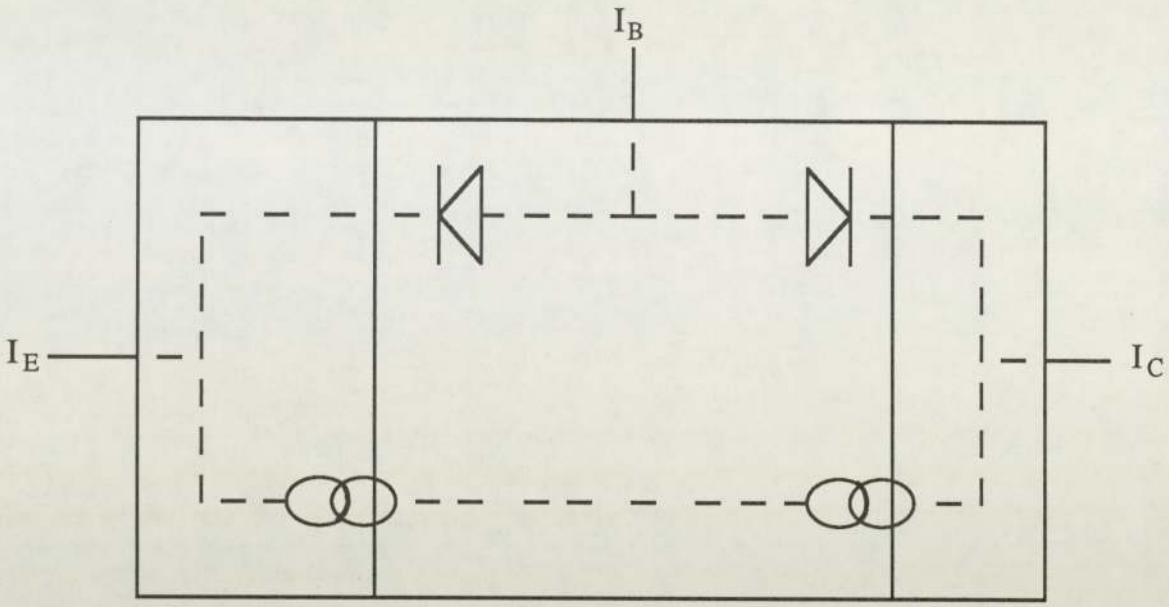
However some progress has been made in one and two dimensions [8], but there is a price to pay; computer run times for such simulations can be excessive.

Thus it seems possible to overcome the problem of impurity profile distribution, and thus provide accurate initial data.

It is also possible to reduce the time required to run simulations by generating an equivalent circuit model; here the device is divided into regions and each region is approximated by a combination of simple devices such as resistors and capacitors whose behaviour may be readily predicted. For example, by applying the one dimensional hydrodynamic equations to a bipolar transistor it is possible to generate expressions for the characteristics (such as the collector current) which depend on a small set of measurable parameters [9]. These parameters may be also determined by simulation or measurement. These analytic expressions for the device characteristics including the simulated/measured parameters may then be coded onto a computer. Due to the relative simplicity of such expressions run times may be greatly reduced although it can be difficult to model all regions of the device accurately due to the inherent simplifying assumptions.

It is possible to derive mathematical expressions for the behaviour of other components (resistors, capacitors, diodes) and hence simulate the complete circuit [10]. Figure (1.1) illustrates the basic ideas:

Figure 1.1




$$\begin{bmatrix} I_C \\ I_B \\ I_E \end{bmatrix} = \begin{bmatrix} \alpha_F & -1 \\ 1-\alpha_F & 1-\alpha_R \\ -1 & \alpha_R \end{bmatrix} \begin{bmatrix} I_F \\ I_R \end{bmatrix}$$

$$I_F = I_{ES}\,(e^{qV_{BE}/k_bT} - 1)$$

$$I_R = I_{CS}\,(e^{qV_{BC}/k_bT} - 1)$$

where:

$I_U$ = junction current (U = C, B, E)

$\alpha_{F,R}$ = forward/reverse current gains

$V\alpha\beta$ = $\alpha\beta$ junction voltage

$I_{VS}$ = saturation current of v-junction

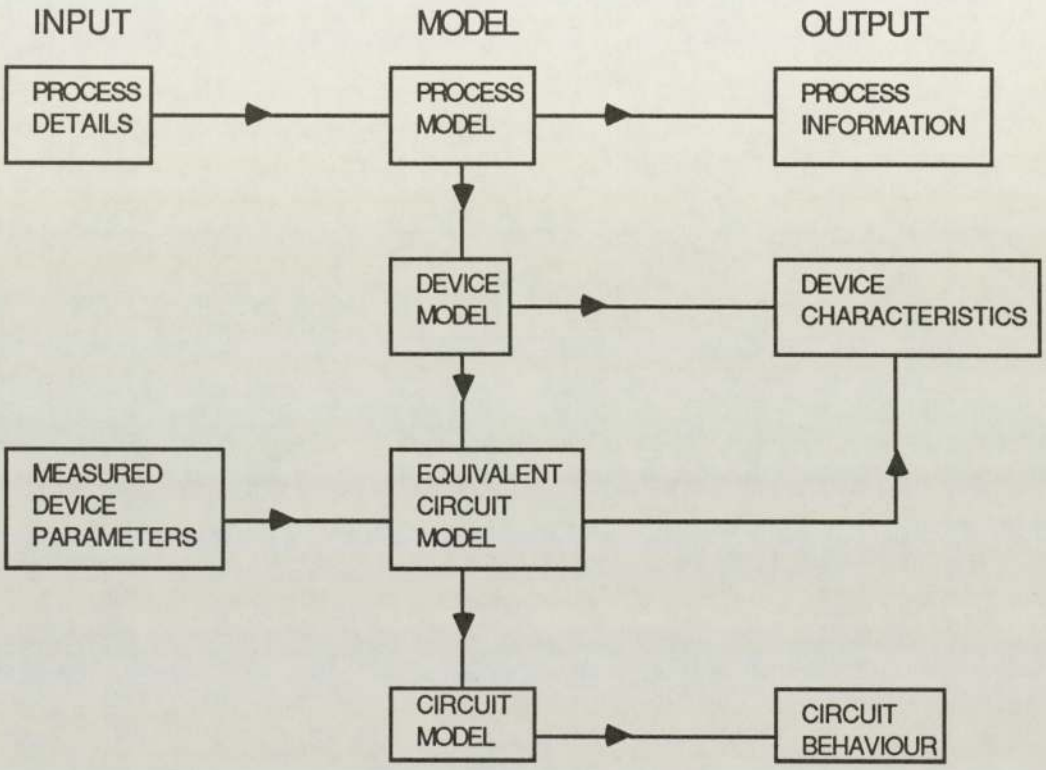
and the subscripts C, B and E refer to the collector, base and emitter of the transistor.

From easily measurable parameters, the simple model of the bipolar transistor given above may be derived and used to

predict the terminal currents. More complex and accurate models are available [9] .

Hence a typical simulation chain may be:

Figure 1.2




Hence it is possible purely from the process data to predict the device's behaviour in an arbitrary circuit without ever fabricating a device. This illustrates the flexibility of the computational approach.

Some analytical work has been undertaken on the hydrodynamic equations, mainly in one dimension. Other areas investigated include numerical analysis [11], singular perturbation theory [4], and mathematical analysis [12] of the equations.

iii) Boltzmann transport theory

The hydrodynamic equations are not universally valid and at small enough dimensions (for example) they are not appropriate. A more sophisticated model is then required and for medium small devices the BTE is necessary

$$D_t f(\underline{x}, \underline{v}, t) = C\left[f(\underline{x}, \underline{v}, t)\right]$$

$D_t$ denoting the convective derivative:

$$D_t \equiv \frac{\partial}{\partial t} + \underline{v}\cdot\frac{\partial}{\partial \underline{x}} + \underline{F}\cdot\frac{\partial}{\partial \underline{v}}$$

$\underline{F}$ being the external force per unit mass, $f(\underline{x}, \underline{v}, t)$ the carrier distribution function which depends on the position $\underline{x}$ and velocity $\underline{v}$ of the particle at time t. C denotes the scattering functional. The hydrodynamic equations may be derived from the BTE by the method of moments [13]. This statistical formulation in terms of the above transport equation is considerably richer in structure involving a 6n dimensional phase space (n being the number of particles). This deeper structure gives, and requires, more information and hence is more complex.

Computational approaches are generally based on the Monte Carlo method [14] . The carrier's motion within the lattice is simulated as a series of free flights and scattering events. The interval between collisions and the specific

scattering process are generated stochastically by the use of a random number sequence. For steady state homogeneous phenomena one carrier may be considered representative but under more complex conditions a large number of carriers must be dynamically modelled. Physical observables (such as the current) may be calculated in this way. As a solution method, the Monte Carlo technique may be viewed as "experimental" providing that accurate physical models are used. This is usually the case - the fact that electrons have differing effective masses in different valleys can be taken into account. The major drawback of this method is that excessive time and computational resources are required. However, in certain areas [15] the Monte Carlo method is providing extremely useful new information.

Analytically the BTE is intractable and simplifying assumptions are essential. This approach is the main topic of this thesis and discussion of such methods will be deferred to Chapter 2. It becomes more apparent that it is necessary to use simple analytical methods in this region as computational requirements are prohibitively large.

iv) Quantum transport models

Only a brief overview shall be given here.

Two main branches can be identified: quantum ballistic and quantum statistical transport.

Quantum ballistic transport deals with the electrons independently and treats their motion ballistically.[16]

Quantum statistical transport is a very sophisticated theory and is a superset of all the transport theories discussed previously; indeed one of the tests of a quantum statistical transport is to derive a Boltzmann-like equation from the quantum transport equation under suitable assumptions [17]. Quantum statistical transport is expected to be applicable to the next generation of sub-micron devices and as such should develop rapidly.

## §4 Motivation

Initially, the work detailed in this thesis began as a generalization of a model developed some time ago [18]. The model investigated the distribution of electrons and the current generated in the base region of a transistor when electrons are injected into it from the emitter. The scattering mechanism considered was that of non-polar optical phonon scattering and the distribution function was assumed to satisfy the nearly isotropic approximation (NIA). The treatment was extended to include an electric field. However as noted by [19] other aspects of the device physics need to be incorporated, namely higher (second) order phonon energy contributions than in [18]. Thus the model has been extended to include these contributions as well. This forms the basis of the models to be discussed in this thesis. The formulation was extended to other scattering mechanisms (namely acoustic and piezoelectric phonon scattering) rather than just non-polar optical phonon scattering.

An analytical approach to the solution has been adopted. The reasons for this are that the general models can be developed and also to illustrate the potential that analytic, and particularly semi-analytic, approaches have.

## §5 Summary of thesis

This thesis considers the problem of the formulation of analytic boundary problems in Boltzmann transport theory and their solution using analytical and semi-analytical means.

Chapter 2 discusses the simplification of the BTE from a non-linear integrodifferential equation into a second order linear partial differential equation using the nearly isotropic approximation. It is found that this equation with essentially two adjustable parameters may describe a wide range of physical phenomena. However, the equation is complicated (as the coefficients depend on the independent variables) and is not amenable to direct solution.

Chapter 3 discusses the mathematical boundary value problems that are appropriate for the different physical solutions described by the equation; the latter include the presence or absence of an electric field and the degree of truncation of the Taylor series expansion of the collision integral. An important point raised is that problems that seem physically well posed may not be mathematically well posed. Also a general case of the partial differential equation derived in Chapter 2 is solved providing a generalization of previously published work and indicating the economy of a general approach.

Chapter 4 is the culmination of the previous two chapters: it takes a specific model of a semiconductor device (namely that of a device governed by non-polar optical phonon scattering in an electric field) which is a generalization of the models considered in the previous chapter due to the inclusion of the electric field, and attempts to determine the electric current that would be observed in the sample, purely by analytical means. There are several stages: firstly a boundary value problem has to be solved, and although the solution can be determined by separation of variables [20] the boundary conditions are difficult to fit, and incidentally difficult to model. To satisfy the conditions it is necessary to invert a non standard singular Fredholm integral equation of the first kind. A model is then necessary for the injected current distribution. Once one is decided upon then the current may be obtained as an integral. No further progress is possible analytically so the current and electron distribution function are evaluated numerically.

Chapter 5 discusses methods of solution for the other cases of the partial differential equation derived in Chapter 2 that have not been discussed in Chapters 3 and 4. Several other cases are soluble and general solutions and details are given. The applicability of the method developed in Chapter 4 is also discussed.

Chapter 6 gives a summary of the work, the results obtained and the major conclusions reached.

# CHAPTER TWO

## THE TRANSPORT EQUATION

### §1. The Boltzmann equation

The most important object to be determined in transport theory is the distribution function $f(\underline{x},\underline{p},t)$ which gives the number of points in a volume element centred at $(\underline{x},\underline{p})$, $\underline{x}$ being the position vector and $\underline{p}$ the momentum vector of a particle. From the distribution function the ensemble average of any dynamical quantity may be calculated via

$$\langle A \rangle = \frac{\int A(\underline{x},\underline{p}) f(\underline{x},\underline{p},t) d\underline{p} d\underline{x}}{\int f(\underline{x},\underline{p},t) d\underline{p} d\underline{x}}$$

where $\langle\ \rangle$ denotes the operation of ensemble averaging, which (as shown in [21]) gives the physically observed value at time t.

The distribution function satisfies the classical Liouville equation

$$\frac{\partial f}{\partial t} - \{f, H\} = 0 \qquad (2.1.1)$$

where H is the Hamiltonian of the system (assumed explicitly time independent) and $\{f,H\}$ denotes the Poisson bracket of f and H defined by

$$\{f,H\}=\sum_{i=0}^{n}\left(\frac{\partial f}{\partial x_i}\frac{\partial H}{\partial p_i}-\frac{\partial f}{\partial p_i}\frac{\partial H}{\partial x_i}\right) \qquad (2.1.2)$$

n being the number of degrees of freedom of the physical system under question. For any realistic Hamiltonian (2.1.1) is impossible to solve in general and recourse to approximations is necessary. Further it is implicitly assumed in the above discussion that the system that is being described is classical in the sense that no quantum mechanical effects are included in the above formulation. However it is possible to extend the formalism to quantum systems [22] by replacing the distribution function by a density matrix [23] which is the sum over the quantum states of the system, appropriately weighted to take account of their relative probabilities and replacing the Poisson bracket with its quantum counterpart, the commutator (up to a multiplicative constant). The commutator is defined by

$$[A,B] = AB-BA$$

where A,B are now operators, as is usual in quantum theories; classical quantities (such as position, momentum) are replaced by corresponding operator forms, these being defined by the postulates of quantum mechanics. The corresponding quantum Liouville equation is

$$i\hbar\frac{\partial\Omega}{\partial t}=\left[\hat{H},\Omega\right]$$

$\Omega$ now being the density matrix of the system and $\hat{H}$ the Hamiltonian operator, $\hbar$ denotes Planck's constant. The

ramifications of this replacement are fundamental: concepts such as phase space and distribution functions have to be revised as simultaneous measurement of (say) position and momentum is no longer considered possible, a consequence of the Heisenberg Uncertainty Principle. It is possible to accommodate the change in structure of phase space and the generalization and extensions have proven to be particularly fruitful in high field quantum transport [17].

(2.1.1) may be viewed as the fundamental kinetic equation describing the phase space evolution of the distribution function from which other equations may be derived ( such as: BBGKY hierarchy; Pauli Master Equation; Boltzmann equation). The emphasis here shall be on the particular transport equation which is widely used in semiconductor device modelling although originally derived for gas like interactions, namely the Boltzmann equation. Several derivations are given in the literature [24], and we shall use the form most appropriate to our discussion

$$\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} + F_i \frac{\partial f}{\partial v_i} = C(f) \qquad (2.1.3)$$

(summation convention assumed) where $F_i$ are the components of the external force per unit mass and C(f) denotes the collision integral which is taken to have the form for binary collisions [25]

$$C(f) = \sum_{\underline{v}'} \left\{ f'(1-\mu f)P_{\underline{v}\,\underline{v}'} - f(1-\mu f')P_{\underline{v}'\underline{v}} \right\} \qquad (2.1.4)$$

where $f'=f(\underline{x},\underline{v}',t)$ and $P_{\underline{v}\,\underline{v}'}$ denotes the transition probability from the velocity state $\underline{v}$ to the velocity state $\underline{v}'$.

The BTE treats the collision integral quantum mechanically and the convective derivative classically although the wave nature of the electron is taken into account via the relationship $mv=\hbar k$. $\mu$ is a parameter which must be included to take account of degeneracy : $\mu=1$ is the degenerate case (when the Pauli exclusion principle applies, that is account has to be taken of the fact that electrons are fermions and cannot occupy the same quantum state) and $\mu=0$ is the non-degenerate case. That $\mu$ must be included is an indication of the inherent quantum nature of the electron, and that it cannot be treated purely classically. The ultimate justification comes from quantum transport theory [17], and the semiclassical form of (2.1.3) will be used :

$$\frac{\partial f}{\partial t}+\frac{\hbar \underline{k}}{m_e}\cdot\frac{\partial f}{\partial \underline{x}}+\frac{q\underline{\xi}}{\hbar}\cdot\frac{\partial f}{\partial \underline{k}}=\sum_{\underline{k}'}\left\{f'(1-\mu f)P(\underline{k},\underline{k}')-f(1-\mu f')P(\underline{k}',\underline{k})\right\} \quad (2.1.5)$$

where the electron wavevector $\underline{k}$ and the renormalised electron mass $m_e$ have been introduced. $\underline{\xi}$ is the electric field and q the electronic charge. Summation and integration will be interchanged in the collision term whenever necessary, depending on whether a discrete or continuous system is being considered. (2.1.5) is the basic transport equation used for the rest of this thesis, although in the following sections it will be recast in a form appropriate to high field transport.

As has been mentioned the Boltzmann transport equation has proven to be very useful in semiconductor device modelling but when device dimensions become small (of submicron order) and/or high electric fields are present the

implicit assumptions upon which (2.1.5) is based become invalid. Pertinent ones include:

1) Small interactions between particles
2) Weak electric fields
3) Low carrier densities
4) Point like collisions
5) Coarse graining in phase space

Various papers [17],[26] have discussed the range of validity of the BTE, and unusual effects ( such as the intra-collisional field effect -a prediction that the field may have some affect during a scattering event ) are possible for small devices and/or high fields. For our purposes we shall assume that the BTE equation is valid.

Mathematically, (2.1.5) constitutes a non-linear partial integrodifferential equation for the distribution function which should be solved self consistently with the Poisson equation

$$\varepsilon \nabla 2\varphi = -\rho$$

where $\varepsilon$ is the permitivity, $\varphi$ the electric potential and $\rho$ the space charge density and exact analytical solution for any realistic or interesting situation is impossible. Even if the distribution function could be evaluated exactly it is functionals of the distribution function that are required - the transport coefficients, such as the current. Computational approaches require expensive mainframe resources. There is thus a place for simple analytical approaches which can prove useful in themselves and also as initial input to computer codes.

Perturbative techniques have proven themselves in many areas of Mathematics and this is the basis of the method to be discussed.

§2. The collision integral.

From (2.1.4) we have the following form for the collision integral

$$C(f) = -{}^{V}/_{(2\pi)^3} \int_{\underline{k}'} \{ P(\underline{k},\underline{k}')f(\underline{k}) - P(\underline{k}',\underline{k})f(\underline{k}') \} dk' \qquad (2.2.6)$$

where the position and time dependence have been omitted. A factor of ${}^{V}/_{(2\pi)^3}$ has been included as the continuous form of the collision integral is being used, V denoting the volume of the system. Note that the multiplicative factor is included as we have changed from summation to integration. The non-degenerate case is being considered in which $f(\underline{k})<<1$ and $P(\underline{k},\underline{k}')$ has been written for the transition probability density from $\underline{k}$ to $\underline{k}'$ states. According to first order quantum perturbation theory [23] it has the form (Fermi Golden Rule)

$$P(\underline{k},\underline{k}') = \frac{2\pi}{\hbar} | M(\underline{k},\underline{k}') |^2 \delta(E(\underline{k}) - E(\underline{k}') \pm \hbar\omega_q) \qquad (2.2.7)$$

Here $M(\underline{k},\underline{k}')$ is the transition matrix which depends on the particular electron phonon interaction being considered [28] and the presence of the delta functional ensures conservation of energy, $\omega_q$ denoting the phonon frequency. The plus (minus) sign in (2.2.7) corresponds to the absorption (emission) of a phonon of frequency $\omega_q$. Any processes for which

$\underline{k}-\underline{k}'\pm\underline{q}\neq 0$ (Umklapp processes)

will not be considered.

Note that (2.2.7) is only a semiclassical approximation and is not universally legitimate [17] - for example, it requires infinite time between collisions. Generally in Boltzmann transport theory (2.2.7) is valid if the time between collisions is much greater than the duration of the collision event.Again for the purpose of this thesis the necessary approximations will be assumed valid.

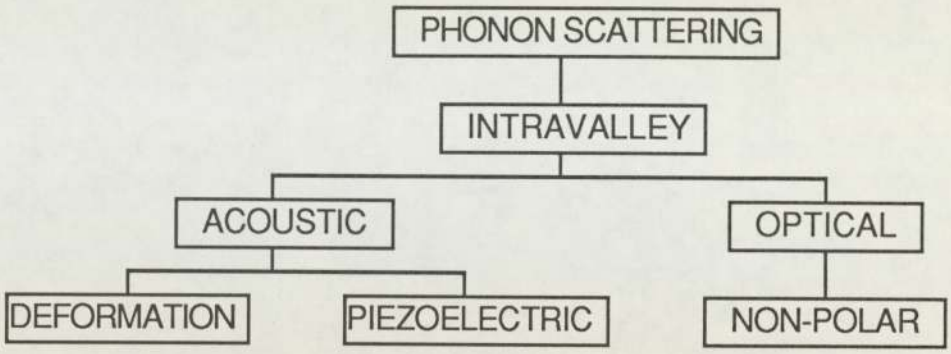
Below 300K, only single phonon processes are important [29] and we have

$$M(\underline{k},\underline{k}') = \sqrt{A(q)}\ \sqrt{n_q+\frac{1}{2}\pm\frac{1}{2}} \qquad (2.2.8)$$

The plus (minus) sign corresponding to the absorption (emission) of a phonon of frequency $\omega_q$. A(q) depends only on the particular scattering process and $n_q = k_bT/h\omega_q$ is the occupation number of the state q assuming an infinite equilibrium phonon bath. Assumptions pertaining to the use of (2.2.8) and its derivation are detailed in [28].

There are many types of scattering processes involving electrons - with impurities, phonons and other carriers (both electrons and holes). The scattering mechanisms of interest in this thesis are shown in Figure (2.1)

FIGURE 2.1




Mathematical models of these scattering processes will be developed later in this chapter.

The discussion shall now be restricted to the nearly isotropic approximation (NIA) to the collision integral; the full distribution is assumed to be well approximated by a perturbative expansion about its isotropic component

$$f(x,\underline{k}) = f_0(x,E)P_0(\cos\theta) + kf_1(x,E)P_1(\cos\theta) \qquad (2.2.9)$$

where E denotes the electron energy usually taken to satisfy $E=\frac{\hbar k^2}{2m_e}$ - the parabolic band approximation, $\theta$ the angle between wave vector and electric field. $P_i$ denotes the Legendre polynomial of degree i and $f_0$ , $f_1$ the symmetric and asymmetric components of the full distribution function f respectively. Physically, (2.2.9) corresponds to a distribution function that is nearly isotropic in momentum space; it is assumed that $| f_1 | << f_0$ .The validity of (2.2.9) is discussed in [30]. Note that some care is needed when comparing with other authors as some use an alternative expansion of f :

$$f(x,\underline{k}) = f_o(x,E)P_o(\cos\theta) + f_1(x,E)P_1(\cos\theta)$$

omitting the k factor multiplying $f_1$ [31]

Substituting (2.2.9) into (2.2.6) and using (2.2.7),(2.2.8) gives upon simplification

$$C(f) = \frac{V}{(2\pi)^3}\int_{\underline{k}'} d\underline{k}'\, A(q)\,\big[\delta(\Delta_+)\{(n_q+1)f_o(E_{\underline{k}'})-n_q\, f_o(E_{\underline{k}})\} + \delta(\Delta_-)$$
$$\{n_q f_o(E_{\underline{k}'})-(n_q+1)f_o(E_{\underline{k}})\} + \delta(\Delta_+)\{(n_q+1)\underline{k}'\cos\theta' f_1(E_{\underline{k}'}) -$$
$$n_q\underline{k}\cos\theta f_1(E_{\underline{k}})\} + \delta(\Delta_-)\{n_q\underline{k}'\cos\theta' f_1(E_{\underline{k}'}) - (n_q+1)\underline{k}\cos\theta f_1(E_{\underline{k}})\}\big] \qquad (2.2.10)$$

where

$$\Delta_\pm = E(\underline{k})-E(\underline{k}')\pm\hbar\omega_q$$

and the x-dependence of the functions in (2.2.10) has been suppressed. In low field transport $f_o$ may be taken to be the equilibrium Maxwellian distribution function, and contributions to the collision integral from terms involving $f_o$ vanish [10]. In high field situations it cannot be assumed that $f_o$ is the equilibrium distribution and the terms involving it constitute the symmetric part of the collision integral $C_o$ where

$$C_o(f_o) = \frac{V}{(2\pi)^3}\int_{\underline{k}'} d\underline{k}' A(q)\,\big[\delta(\Delta_+)\{(n_q+1)f_o(E_{\underline{k}'})-n_q\, f_o(E_{\underline{k}})\} +$$
$$\delta(\Delta_-)\{n_q f_o(E_{\underline{k}'})-(n_q+1)f_o(E_{\underline{k}})\}\big] \qquad (2.2.11)$$

Similarly, terms involving $f_1$ constitute the asymmetric part of the collision integral

$$C_1(f_1) = \frac{V}{(2\pi)^3}\int_{\underline{k}'} d\underline{k}'\, A(q)\big[\delta(\Delta_+)\{(n_q+1)\underline{k}'\cos\theta' f_1(E_{\underline{k}'})-$$

$(n_q \underline{k}\cos\theta) f_o(E_{\underline{k}})\} + \delta(\Delta_-)\{n_q \underline{k}'\cos\theta' f_o(E_{\underline{k}'}) - (n_q+1)\underline{k}\cos\theta f_o(E_{\underline{k}})\}\Big]$

(2.2.12)

Further simplifications to (2.2.11) and (2.2.12) will now be discussed.

## §3 Relaxation time approximations

Further simplification of (2.2.11) and (2.2.12) is essential so that the equations derived using the NIA are soluble.A relaxation time approximation to the collision integrals will be developed [28].

Firstly, only scattering processes for which the asymmetric part of the collision integral can be written in the form

$$C(f_1) = -k\cos\theta \frac{f_1(E)}{\tau_1(E)} \qquad (2.3.13)$$

will be considered, where $\tau_1(E)$ is the energy dependent momentum relaxation time [32]. (2.3.13) is valid only for randomizing collisions (for example, non-polar optical phonon scattering) and elastic collisions (acoustic phonon, piezoelectric phonon and impurity scattering being in this latter category), although relaxation time approximations have been used to gain qualitative information about scattering mechanisms which are neither randomizing nor elastic (carrier-carrier and polar optical phonon scattering being cases in hand). When (2.3.13) is applicable explicit expressions may be derived for the relaxation time: from (2.2.6) and (2.2.9)

$$C(f) = -\frac{V}{(2\pi)^3}\int_{\underline{k}'}\{P(\underline{k},\underline{k}')f(\underline{k})-P(\underline{k}',\underline{k})f(\underline{k}')\}\,d\underline{k}'$$

$$f = f_o + kf_1\cos\theta$$

Thus

$$C(f) = C(f_o + kf_1\cos\theta)$$

$$= C(f_o) - \frac{V}{(2\pi)^3}\int_{\underline{k}'}\{P(\underline{k},\underline{k}')kf_1(\underline{k})\cos\theta-P(\underline{k}',\underline{k})k'f_1(\underline{k}')\cos\theta'\}d\underline{k}' \qquad (2.3.14)$$

Consider randomizing collisions; the probability of transition from the state $\underline{k}$ to the state $\underline{k}'$ is independent of $\underline{k}$. Hence

$$\int_{\underline{k}'} P(\underline{k},\underline{k}')k'f_1\cos\theta'd\underline{k}' = 0$$

as the integral of cos $\theta'$ over $\theta'$ (which runs from 0 to $2\pi$) vanishes. (2.3.14) then simplifies to

$$C(f) = C(f_o) - \frac{V}{(2\pi)^3}\,kf_1\cos\theta\int_{\underline{k}'}P(\underline{k},\underline{k}')dk'$$

$$= C_o(f_o)\,P_o + kC_1(f_1)\,P_1(\cos\theta) \qquad (2.3.15)$$

making the obvious identifications.

For elastic scattering :

$$C(f_o + kf_1\cos\theta) = C(f_o) - \frac{V}{(2\pi)^3}\int_{\underline{k}'}P(\underline{k},\underline{k}')\{kf_1(\underline{k})\cos\theta-k'f_1(\underline{k}')\cos\theta'\}d\underline{k}'$$

(as, for elastic scattering, $P(\underline{k},\underline{k}') = P(\underline{k}',\underline{k})$ )

$$= C(f_o) - \frac{V}{(2\pi)^3}k\cos\theta f_1\int_{\underline{k}'}d\underline{k}'P(\underline{k},\underline{k}')\left(1 - \frac{\underline{k}'\cos\theta'}{\underline{k}\cos\theta}\right)$$

$$= C_o(f_o)\,P_o + kC_1(f_1)\,P_1(\cos\theta) \qquad (2.3.16)$$

again making the obvious identifications. Hence for the above scattering mechanisms the stated form for the asymmetric part of the collision has been derived. Note that its functional form (2.2.13) arises from the assumptions made about the scattering mechanisms and the use of the NIA to the distribution function (2.2.9) assumed ; it is not a Legendre expansion of the collision integral (see [33]).Comparing (2.2.13) and (2.2.15), (2.2.16) gives expressions for the relaxation time :

$$\text{Randomizing:}\quad \tau_1(E) = \frac{(2\pi)^3}{V}\left( \int_{\underline{k}'} P(\underline{k},\underline{k}')d\underline{k}' \right)^{-1} \qquad (2.3.17)$$

$$\text{Elastic:}\quad \tau_1(E) = \frac{(2\pi)^3}{V}\left( \int_{\underline{k}'} P(\underline{k},\underline{k}')\left(1 - \frac{k'\cos\theta'}{k\cos\theta}\right) d\underline{k}' \right)^{-1} \qquad (2.3.18)$$

Generally, $\tau_1(E)$ may be expressed in the form:

$$\tau_1(E) = \tau_{sm}\, E^{\pm 1/2} \qquad (2.3.19)$$

(for the models to be considered here) where $\tau_{sm}$ and the sign chosen depend on the particular scattering mechanism under consideration (see Table 2.1).

TABLE 2.1

| | $\tau_0$ | $\tau_1$ | K |
|---|---|---|---|
| NPOP | 1/2 | −1/2 | 1 |
| AP | −1/2 | 1/2 | 2 |
| PP | 1/2 | 1/2 | 1 |

$\tau_o(E)$ being the energy relaxation rate.
(the values given in columns one and two of table represent the values of the exponent n in the formula

$$\tau_i(E) = (\tau_i)_{sm} E^n \qquad (i=0,1)$$

$(\tau_i)_{sm}$ being a constant, and K is introduced in (2.3.21).

Secondly, as it is high field transport that will be considered it may be assumed that $E >> \hbar\omega_q$ : i.e. that the carrier energy is much greater than the phonon energy (a major assumption that restricts the analysis to 'hot' electron theory). Using this assumption the symmetric part of the distribution may be expanded by Taylors theorem :

$$f_o(E \pm \hbar\omega_q) = \sum_{n=0}^{\infty} f_o^{(n)}(E) \frac{(\pm\hbar\omega_q)^n}{n!} \qquad (2.3.20)$$

enabling (2.2.11) to be considerably simplified by substituting (2.3.20) in (2.2.11) and truncating at either first (as in [18]) or second order (as in [20]). Both options will be retained here. The expression obtained for $C_o$ is

$$C_o(f_o) = \frac{1}{(\tau_o(E))_{sm}} \left( K f_o + W\frac{\partial f_o}{\partial W} + \beta_{sm}\left( K\frac{\partial f_o}{\partial W} + W\frac{\partial^2 f_o}{\partial^2 W}\right)\right) \qquad (2.3.21)$$

with W being the scaled energy. The particular scale factor will be introduced shortly. K, $\beta_{sm}$ are constants ( all scatterer dependent); $\beta_{sm}$ representing a second order phonon energy contribution to the symmetric collision integral while K is a

parameter introduced for convenience. The form of the collision integral relevant to this thesis has now been discussed and the specific form for the differential equations will now be derived.

## §4. Hot electron transport

### i) Drifted Maxwellian

Although the sole concern of this thesis shall be the use of the nearly isotropic approximation to the BTE, a simpler method which has found favour in hot electron modelling - the displaced Maxwellian approach [35] - is of interest. This amounts to assuming a specific functional form for the distribution function, with three adjustable parameters

$$f(E) = A \exp\left\{ - \frac{(E - \underline{v}_d . \underline{p})}{k_b T_e} \right\} \qquad (2.4.22)$$

where A is a constant, $\underline{v}_d$ the electron drift velocity, $\underline{p}$ its momentum and $T_e$ the electron gas temperature. Frohlich has shown [36] that if the carrier concentration can be considered large and the anisotropic component small, then (2.4.22) is valid.

To determine the three parameters take moments of the original BTE (2.1.5), recasting it in momentum space (using natural units)

$$\partial_t < \varphi > + \partial_r < \varphi v > + < eF \partial_p \varphi > = < \int dp' [\varphi(p') - \varphi(p')] P(p,p') > \qquad (2.4.23)$$

with $<\ >$ denoting the process of ensemble averaging, (noting that f is assumed to be normalized) $\varphi$ being some arbitrary function. Taking

$$\varphi = p^r \quad (r= 0,1,2)$$

gives

$$\begin{aligned} &\langle 1\rangle = n \\ &\langle p\rangle = mv_d \\ &\langle p^2\rangle = 3mk_bT_e \end{aligned} \tag{2.4.24}$$

The three equations (2.4.24) are coupled equations which may be solved by numerical methods self consistently to give the parameters A, $\underline{v}_d$ and $T_e$.

This method has given useful insight into device operation but has one serious flaw ; to obtain consistent results from such truncation schemes then the analysis is limited to at most two moments of the original equation [22] .

ii) Legendre expansion

If the assumptions necessary to ensure the validity of the displaced Maxwellian approximation [36] cannot be made then the full BTE (2.1.5) must be solved. This is not feasible analytically due to its mathematical complexity. If however it is assumed that the distribution function is nearly isotropic in momentum space, the BTE may be simplified by applying the NIA giving two coupled partial differential equations

$$\frac{2E}{3\hbar}\partial_x f_1 + \frac{2e\xi E^{-1/2}}{3\hbar}\partial_E(E^{+3/2}f_1) = C_o(f_o) \tag{2.4.25}$$

$$\frac{\hbar}{m_e}\partial_x f_o + \frac{e\hbar\xi}{m_e}\partial_E(f_o) = C_1(f_1) \tag{2.4.26}$$

(where the fact that Legendre functions are orthogonal to each other over [-1,1] has been used).

(2.4.25) and (2.4.26) constitute two coupled non-linear partial integrodifferential equations when explicit forms for the collision integrals are inserted. Use of the approximations detailed in this chapter, namely the NIA, the assumption that $E >> \hbar\omega q$ and the relaxation time form of the collision terms enables them to be reduced to one second order elliptic partial differential equation. Making the substitutions gives

$$\frac{2E_c}{3m_e x_c}\ \tau_1 \frac{\partial}{\partial X}\left(\frac{1}{x_c}\frac{\partial f_o}{\partial X} - \frac{\lambda}{E_c}\frac{\partial f_o}{\partial W}\right)$$

$$+\ \frac{2\lambda}{3m_e} W^{-1/2}\frac{\partial}{\partial W}\left(W^{3/2}\,\tau_1\left(\frac{1}{x_c}\frac{\partial f_o}{\partial X} - \frac{\lambda}{E_c}\frac{\partial f_o}{\partial W}\right)\right) = C_o \qquad (2.4.27)$$

where $\lambda = -e\xi$ and dimensionless variables X,W have been introduced by the relations

$$x = x_c X$$
$$E = E_c W \qquad (2.4.28)$$

$x_c$, $E_c$ are characteristic length and energy scales (respectively), which will be introduced at the appropriate juncture. (2.4.27) applies to all the scattering mechanisms to be discussed - the specific form of $C_o$ will change depending on which is considered. However it is possible to generalize (2.4.27) to a single partial differential equation that depends on five parameters to cover all cases to be considered :

$$(\alpha^2+\beta s m W^n)\frac{\partial^2 f_o}{\partial W^2} - 2\alpha\gamma\frac{\partial^2 f_o}{\partial W\,\partial X} + \gamma^2\frac{\partial^2 f_o}{\partial X^2} -$$
$$m\frac{\alpha\gamma}{W}\frac{\partial f_o}{\partial X} + \left(\frac{m\alpha^2}{W} + W^n + (m+n)\beta s m W^{n-1}\right)\frac{\partial f_o}{\partial W} +$$
$$(m+n)W^{n-1} f_o = 0 \qquad (2.4.29)$$

where

$$\alpha^2 = \frac{\lambda^2}{\mu E_c^2} \qquad \gamma^2 = \frac{1}{\mu x_c^2} \qquad \mu = \frac{3m_e}{2E_c\tau_1\tau_o} \tag{2.4.30}$$

with the doublet of integers (m,n) given in Table 2.2 below. It is to be expected that an equation of the form (2.4.29) would result, as $C_o$ has a similar functional form for all the scattering mechanisms considered here (see (2.3.27)) and the energy and momentum relaxation times $\tau_o(E)$, $\tau_1(E)$ have similar energy dependence (see table 2.1).

TABLE 2.2

| | n | m |
|---|---|---|
| NPOP | 0 | 1 |
| AP | 1 | 1 |
| PP | - 1 | 2 |

The identification of (m,n) in (2.4.29) has been by inspection rather than by derivation; the functional form of the collision term for the scattered mechanisms stated was examined and a mathematical description, in terms of the two parameters (m,n) obtained. The general formalism developed, namely a Legendre expansion of the BTE and relaxation time approximation to the collision integral will now be used to model devices in various environments.

## §5. Summary

In this chapter the partial differential equations that will form the basis of the study of boundary value problems to be discussed in the next chapter have been derived and particular assumptions stated. The following specific approximations have been made :

1) that the device may be modelled by the Boltzmann transport equation
2) the distribution function is nearly isotropic in velocity space
3) the scattering mechanisms are either elastic or randomizing

These approximations allow the Boltzmann transport equation to be reduced to a single linear second order partial differential equation for the symmetric part of the distribution function. Mathematically the NIA may be viewed as a perturbative expansion of the distribution function about its isotropic component, enabling it to be reduced to a tractable partial differential equation, when suitable assumptions are made about the scattering mechanisms.

# CHAPTER THREE

## BOUNDARY VALUE PROBLEMS IN SEMICONDUCTOR DEVICE MODELLING

### §1. Introduction.

Mathematical modelling of transport processes will, in general, generate non-linear integrodifferential equations. In particular, for semiconductor structures, the actual equation (which is assumed to incorporate the essential physics) is only one aspect of the modelling process: the device geometry and appropriate auxiliary conditions must be included.

The particular kinetic equation used (quantum, semiclassical or hydrodynamic) depends on such factors as the device geometry, environment and the accuracy required, although the effect that the choice of equation has on the latter factor can only be judged qualitatively. At the most fundamental level when device size is of submicron order and we are considering the high field regime perhaps 100 kV $cm^{-1}$, quantum transport equations are essential, either statistical or ballistic depending on the prevailing physics. At larger geometries, and lower fields, Boltzmann transport theory is applicable which is a semiclassical approximation to the full quantum transport equations [17], [22]. In many situations the BTE may be reduced to hydrodynamic equations, which form the basis of the majority of numerical device models. Rate equations have also proved useful in device modelling [37]. Note that care is needed to ensure that the correct equation is used as there is

not universal agreement on the ranges of validity of the various approaches. [38].

As well as the equation the device geometry, which will be fixed, has to be included. Only for simple geometries, usually one dimensional geometries, will analytic approaches be feasible, whereas the scope for numerical simulations is unlimited although even these are usually restricted to two dimensions, with the hydrodynamic equations forming the mathematical basis [39]. Considerations such as symmetry may help, and approximations such as semi-infinite domain can alleviate some problems in analytic approaches. The geometry may in fact intimate a method of solution as in the case of spherical symmetry which suggests a transformation of the coordinate system or a particular perturbative expansion, in terms of the spherically symmetric functions. It may even dictate an approximation if it is required to continue analytically; equations on infinite domains are much more amenable to treatment by integral transforms or separation or variables than those posed on finite domains.

Another crucial aspect is the question of auxiliary conditions (initial/final values and boundary conditions). They will be mathematical abstractions of the physical situation, such as Neumann conditions at contacts representing the fact that the field is normal to the contact and apart from general considerations to ensure that a realistic compromise between mathematical tractability and physical actuality is achieved it must also be ensured that the problem is well posed; that is a solution exists which is unique and also depends continuously on the data. The last condition is very significant physically as the

accuracy of all data is limited, both practically and theoretically. It would not be expected that any bifurcations in the solution for infinitesimal changes in the data would exist. However this is not the case as shown in [34] ; models which seem well-posed physically may in fact be ill-posed mathematically and non-uniqueness of solution may result (however ill-posed problems do have a place in mathematics - see [40]). Before leaving the discussion there is a point worthwhile of mention: although it shall be ensured that the boundary value problems discussed in this thesis are well-posed, this does not necessarily infer that the BTE is well posed as only linear approximations to the BTE are being used. Appropriate auxiliary conditions for non-linear partial integrodifferential equations have not been mentioned and will not be discussed; it is difficult to ensure that such problems are mathematically well posed. Physical intuition may act as a guide but the mathematical implications are important; thyristors exhibit bistable states and this may be a manifestation of an improperly posed non-linear boundary value problem [41].

The discussion has been of the essential ingredients to a device model: mathematical equation, device geometry and boundary value problems. The first two factors have been implicit in the formulation of the problem(s) (see Chapter 2). The latter factor shall now be discussed, in the context of particular examples.

## §2. Boundary value problems

Appropriate boundary value problems for the equation

$$(\alpha^2+\beta_{sm}W^n)\frac{\partial^2 f_o}{\partial W^2} - 2\alpha\gamma\frac{\partial^2 f_o}{\partial W\partial X}+\gamma^2\frac{\partial^2 f_o}{\partial X^2} -$$

$$m\frac{\alpha\gamma}{W}\frac{\partial f_o}{\partial X}+\left(\frac{m\alpha^2}{W}+W^n+(m+n)\beta_{sm}W^{n-1}\right)\frac{\partial f_o}{\partial W} + (m+n)W^{n-1}f_o = 0 \qquad (3.2.1.)$$

(introduced in Chapter 2, equation (2.4.29)) shall be discussed. For convenience the notation discussed below shall be used to avoid repetition.

i) Notation

There are twelve cases of (3.2.1) to be considered; they correspond to the particular scattering mechanism (characterized by m,n), the presence or absence of an electric field (represented by $\alpha$) and the order of Taylor expansion of $f_o$ (whether truncated at first or second order in the phonon energy). The choice $\alpha=0$ corresponds to no electric field, while $\beta_{sm}=0$ corresponds to truncating the Taylor expansion at first order ($\beta_{sm}>0$ for second order expansion). Write

$$L_{sm}^{\{u\ v\}} = (\alpha^2+\beta_{sm}W^n)\frac{\partial^2}{\partial W^2} - 2\alpha\gamma\frac{\partial^2}{\partial W\partial X}+\gamma^2\frac{\partial^2}{\partial X^2} -$$

$$m\frac{\alpha\gamma}{W}\frac{\partial}{\partial X}+\left(\frac{m\alpha^2}{W}+W^n+(m+n)\beta_{sm}W^{n-1}\right)\frac{\partial}{\partial W} + (m+n)W^{n-1} \qquad (3.2.2)$$

where

$$u = \begin{cases} 0 & \text{No electric field} \\ 1 & \text{Non-zero constant electric field} \end{cases} \qquad v = \begin{cases} 0 & \text{first order truncation} \\ 1 & \text{second order truncation} \end{cases}$$

and the subscript $sm$ ($\in$ {NPOP, AP, PP}) refers to the scatterer; NPOP referring to non-polar optical phonons, AP to acoustic phonons and PP to piezoelectric phonons.

For example the boundary value problem posed in [18] corresponds to

$$L^{\{0\ 1\}}_{NPOP}\ f_o = 0 \quad \text{(and associated auxiliary conditions).}$$

This classification (in terms of the mathematical structure of the operator (3.2.2)) is complementary to that given in [34], where the problems were characterized physically in terms of the scatterer.

The four categories of boundary value problems

$$\left( L^{\{0\ 0\}}_{sm},\ L^{\{1\ 0\}}_{sm},\ L^{\{0\ 1\}}_{sm},\ L^{\{1\ 1\}}_{sm} \right)$$

will now be discussed.

(ii) No electric field, first order scattering

These relatively simple cases, without an electric field and first order Taylor series truncation, will be discussed first and in detail as they illustrate the salient points and can be treated fully. Now, from (3.2.2)

$$L^{\{0\ 0\}}_{sm} = \frac{\partial^2}{\partial X^2} + W^n \frac{\partial}{\partial W} + (m+n)W^{n-1} \qquad (3.2.3)$$

(X has been rescaled to $X/\gamma$). This is a linear second order adjoint parabolic differential operator in canonical form. To transform it to a more familiar form, write

$$L^{\{0\ 0\}}_{s\ m}\ f_o = 0$$

and define

$$j(X,W) = \frac{\partial}{\partial X}(W^m f_o) \tag{3.2.4}$$

Physically (3.2.4) corresponds to the current density per unit energy interval in the field free case. Operating on $f_o$ with (3.2.3) and then differentiating with respect to X and substituting (3.2.4) gives

$$\frac{\partial^2 j}{\partial X^2} + \frac{\partial}{\partial W}(W^n j) = 0 \tag{3.2.5}$$

Define a new coordinate U by

$$U = \int^W \frac{ds}{s^n}\ ;\quad U = f(W) \Leftrightarrow W = f^{-1}(U) \tag{3.2.6}$$

and a function Q(X,W) by

$$Q(X,W) = W^n j(X,W) \tag{3.2.7}$$

Substitution of (3.2.6) and (3.2.7) in (3.2.5) gives

$$\frac{\partial^2 Q}{\partial X^2} + \frac{\partial Q}{\partial U} = 0 \tag{3.2.8}$$

The above transformations (on both the dependent and independent variables) have thus reduced (3.2.3) to the adjoint diffusion operator. Note that an important feature of (3.2.8) is that it does not admit the same boundary value problems as the (one-dimensional) diffusion equation

$$\frac{\partial^2 Q}{\partial X^2} - \frac{\partial Q}{\partial U} = 0 \qquad (3.2.9)$$

To ensure that the problem is well posed mathematically (3.2.9) requires an initial boundary value problem of the form:

$$\begin{aligned} & Q(X=0, U) = h(U) \\ \lim_{U\to 0} \; & Q(X,U) = g(X) \end{aligned} \qquad (3.2.10)$$

whereas an appropriate boundary value problem for (3.2.8) is a final boundary value problem of the form [42]

$$\begin{aligned} & Q(X=0,\ U) = h(U) \\ \lim_{U\to U_o} \; & Q(X,U) = 0 \qquad (U_o>0) \end{aligned} \qquad (3.2.11)$$

Imposition of (3.2.10) on (3.2.8) will give an improperly posed boundary value problem and unexpected results will occur, Here, (3.2.8) shall be considered subject to conditions imposed on a physical observable - namely the current density per unit energy interval j(X,W). Various models are considered in the literature (see [43]) and for illustrative purposes a simple model (with direct physical interpretation) for j(X,W) has been chosen to satisfy

$$j(O,W) = J_o\,\delta(W-W_o) \qquad (J_o \text{ constant})$$

$$\lim_{W\to W_o} j(X,W) = 0 \qquad (W \leqq W_o) \tag{3.2.12}$$

where $\delta(z)$ denotes the delta functional of argument z. (3.2.12) represents a monoenergetic injected stream of electrons (of energy $W_o$). Use of the relationships (3.2.6) and (3.2.7) enables the boundary value problem to be recast in the form:

$$\frac{\partial^2 Q}{\partial X^2} + \frac{\partial Q}{\partial U} = 0$$

$$Q(O,U) = J_o[f^{-1}(U)]^n\,\delta(f^{-1}(U) - f^{-1}(U_o)) := h(U) \tag{3.2.13}$$

$$\lim_{f'(U)\to f^{-1}(U_o)} [f^{-1}(U)]^n\, Q(X,U) = 0$$

where $U_o = f(W_o)$. The solution to (3.2.13) may be obtained by the use of the appropriate Green's function; the required function being [44]

$$G(x,u;\xi,u_o) = \begin{cases} \dfrac{(x-\xi)}{\sqrt{4\pi(u_o-u)^3}} \exp\left(\dfrac{-(x-\xi)2}{4(u_o-u)}\right) & u<u_o \\ 0 & u\geq u_o \end{cases} \tag{3.2.14}$$

and the solution to (3.2.13) is given by:

$$Q(X,U) = \int_o^\infty G(X,U;0,\tau)h(\tau)d\tau$$

with the function h as defined as in (3.2.13). Thus

$$Q(X,U) = \int_{o}^{W_o} \frac{J_o X}{\sqrt{4\pi(\tau-U)^3}} \exp\left\{\frac{-X^2}{4(\tau-U)}\right\} [f^{-1}(\tau)]^n \, \delta\left(f^{-1}(\tau)-f^{-1}(U_o)\right) d\tau$$

which gives upon integration

$$Q(X,U) = \frac{J_o X}{\sqrt{4\pi(f(W_o)-U)^3)}} \exp\left\{\frac{-X^2}{4(f(W_o)-U)}\right\} \quad W_o^n f'(W_o)$$

(3.2.15)

Finally we have for the current density per unit energy interval (noting that $W_o^n f'(W_o)=1$ for the functions defined by (3.2.6)) using (3.2.7)

$$j(X,W) = \frac{J_o X}{W^n \sqrt{4\pi(f(W_o)-f(W))^3}} \exp\left\{\frac{-X^2}{4(f(W_o)-f(W))}\right\} \qquad (3.2.16)$$

and from (3.2.4)

$$f_o(X,W) = J_o W^{-(n+m)} \sqrt{\frac{f(W_o)-f(W)}{\pi}} \exp\left\{-\frac{X^2}{4(f(W_o)-f(W))}\right\}$$

(3.2.17)

(up to a multiplicative constant).

Figure 3.1 gives a representation of $f_o(X,W)$ in the case of piezoelectric phonon scattering, taking various values of X. (3.2.16), (3.2.17) may be used, as in [18], to calculate such quantities as the current transfer ratio $\alpha$ in a transistor where a particular scattering mechanism (non-polar optical, piezoelectric or acoustic phonon) operates.

$$J_o(X) = \int_o^{W_o} j(X,W)\,dW = \frac{J_o' X}{2\sqrt{\pi}} \int_o^{W_o} \frac{\exp\left(-\frac{X^2}{4(f(W_o) - f(W))}\right)}{\sqrt{(f(W_o) - f(W))^3}}\, dW$$

$J_o'$ being a constant (see (3.2.16))

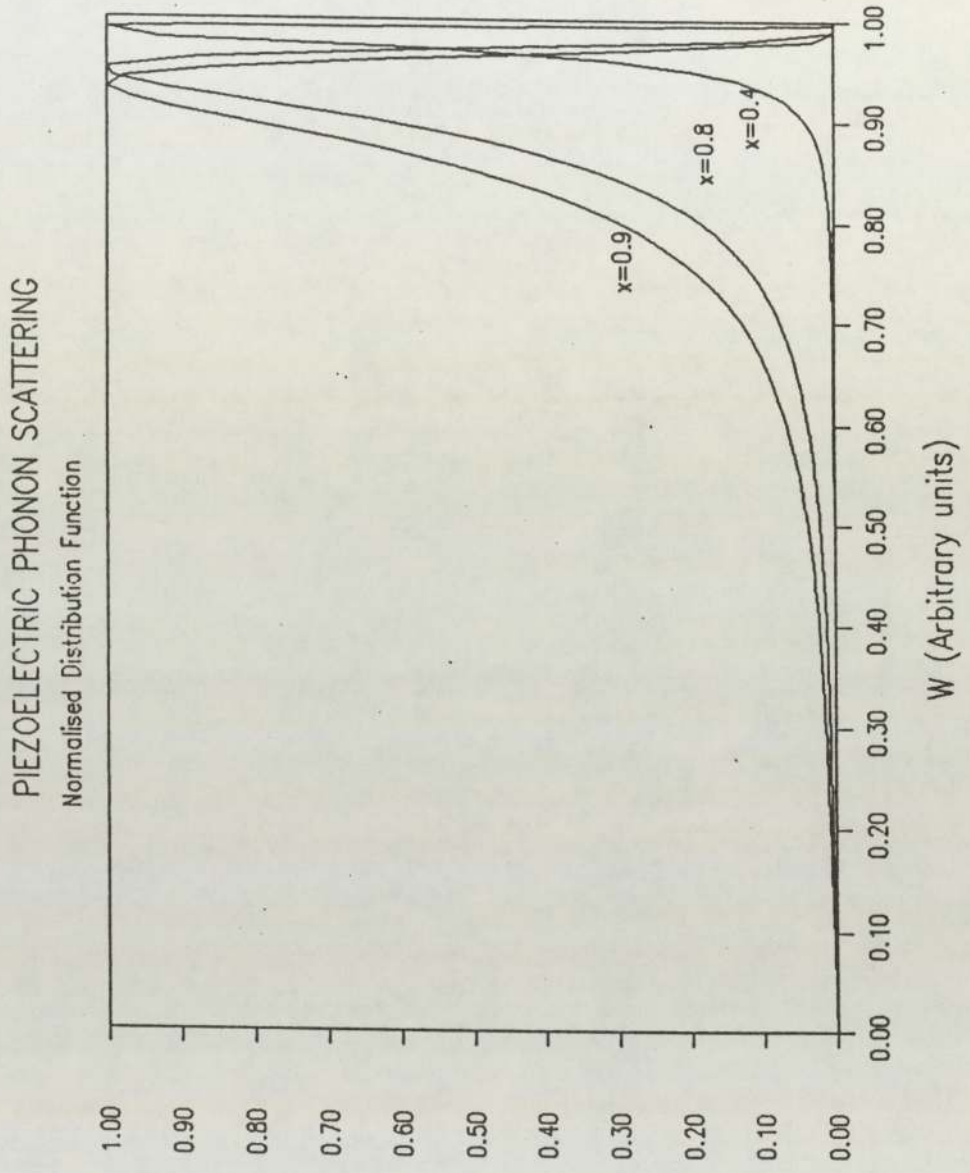
Using a change of variable

$$\sigma = \frac{X}{2\sqrt{f(W_o) - f(W)}}$$

enables the integral to be transformed to

$$J_o(X) = J_o' \frac{2}{\sqrt{\pi}} \int_{\sigma_o}^{\infty} e^{-\sigma^2}\, d\sigma \; := \; J_o' \operatorname{erfc}\left\{\frac{X}{2\sqrt{f(W_o) - f(O)}}\right\}$$

Figure 3.1


PIEZOELECTRIC PHONON SCATTERING
Normalised Distribution Function
x=0.9
x=0.8
x=0.4
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
W (Arbitrary units)

$\sigma_o$ denoting the value of $\sigma$ corresponding to W=O.

Inserting the specific functional forms for f (see (3.1.16) and Table 3.1)

TABLE 3.1

| Scattering Mechanism | n | f(x) |
|---|---|---|
| NPOP | 0 | x |
| PP | -1 | $\frac{1}{2}x^2$ |
| AP | +1 | ln(x) |

gives the following results for the current: in the case of non-polar optical phonon scattering

$$J_o(X) = J_o' \text{ erfc } \left(\frac{X}{2\sqrt{W_o}}\right)$$

whilst in the case of piezoelectric phonon scattering

$$J_o(X) = J_o' \text{ erfc } \left(\frac{X}{\sqrt{2}W_o}\right)$$

The most interesting result occurs in the case of acoustic phonon scattering when the mathematical model predicts that

$$J_o(X) = J_o'$$

-a constant.

The current transfer ratio $\alpha$ then evaluates as

$$\alpha = \text{erfc}\left\{\frac{X}{2}(f(W_o) - f(O))^{-1/2}\right\}$$

suggesting that, for acoustic phonon scattering, the current transfer ratio $\alpha$ is constant.

iii) Electric field, first order scattering

In these cases an arbitrary electric field is included. The operator is still of an adjoint parabolic form and thus admits boundary value problems of the type discussed in the previous section

$$L_{s\,m}^{\{1\ 0\}} := \alpha^2 \frac{\partial^2}{\partial W^2} - 2\alpha\gamma \frac{\partial^2}{\partial X \partial W} + \gamma^2 \frac{\partial^2}{\partial X^2}$$

$$- \frac{m\alpha\gamma}{W}\frac{\partial}{\partial X} + \left(\frac{m\alpha^2}{W} + W^n\right)\frac{\partial}{\partial W} + (m+n)W^{n-1} \qquad (3.2.18)$$

Particular solutions to the equation $L_{s\,m}^{\{1\ 0\}} f_o = 0$ will be discussed in detail in Chapter 4 (for non-polar optical phonon scattering) and Chapter 5 (for piezoelectric and acoustic phonons). However there are some points relevant to this chapter; the canonical form of (3.2.18) is (after suitable scaling)

$$L_{s\,m}^{\{1\ 0\}} = \frac{\partial^2}{\partial \eta^2} + \left(\frac{m}{\eta} + \eta^n\right)\frac{\partial}{\partial \eta} + \eta^n \frac{\partial}{\partial \xi} + (m+n)\eta^{n-1} \qquad (3.2.19)$$

using canonical coordinates $\xi = X+W \quad \eta = W$. (3.2.19) is still an adjoint parabolic equation and a final boundary value problem is thus appropriate (cf (3.2.11),(3.2.19)).

Note that although physically we would expect that when the electric field is removed (ie, $\alpha \to 0$) the unique solution to (3.2.19) tends to that of (3.2.8), care must be exercised as the boundary value problems associated with the problems are not necessarily the same. Mathematically stated

$$\text{As } L_{s\,m}^{\{1\ 0\}} \underset{\alpha\to 0}{\to} L_{s\,m}^{\{0\ 0\}} \quad \text{then} \quad (f_o)_{s\,m}^{\{1\ 0\}} \underset{\alpha\to 0}{\to} (f_o)_{s\,m}^{\{0\ 0\}}$$

if, and only if,

$$(BVP)_{s\,m}^{\{1\ 0\}} \underset{\alpha\to 0}{\to} (BVP)_{s\,m}^{(0\ 0)}$$

i.e. the distribution functions will only correspond if the boundary value problems are equivalent as $\alpha$ tends to zero.

An example of the fact that the above behaviour does occur may be seen by comparing the solutions of [18] and [34] the solutions do not correspond as they use different boundary value problems.

iv) No field, second order scattering

In this case:

$$L_{s\,m}^{\{0\ 1\}} := \beta_{sm} W^n \frac{\partial^2}{\partial W^2} + \gamma^2 \frac{\partial^2}{\partial X^2} + (W^n + \beta_{sm}(m+n)W^{n-1}) \frac{\partial}{\partial W} +$$

$$(m+n)W^{n-1} \qquad (3.2.20)$$

Physically, higher order contributions from the phonon energy (represented by the positive constant $\beta_{sm}$) are included. This changes the nature of the operator from parabolic to elliptic. If contributions higher than second order were included then the operator would correspondingly increase in order, and complexity. As the electron energy is considerably higher than the phonon energy these higher order contributions would have little physical significance and hence the latter possibility will not be considered. Due to the change in the nature of the operator the type of boundary value problems admitted is fundamentally changed; generally, second order elliptic partial differential equations admit Robbins conditions

$$a(X,W)\, f_{o\hat{n}} + b(X,W) f_o = c(X,W) \qquad (3.2.21)$$

where a(X,W), b(X,W) and c(X,W) are functions of the independent variables. The subscript $\hat{n}$ denotes the normal derivative of $f_o$ and the values of it are prescribed on the boundary of the domain. Dirichlet and Neumann conditions are special cases, corresponding to the choices a(X,W) = 0 and b(X,W) = 0 respectively. Again, particular cases of (3.2.20) will be considered in later chapters and the discussion here will be restricted to overall properties of the operator (3.2.20). Firstly (3.2.20) will be considered on a finite domain, usually a rectangle [a,b]x[c,d]. This makes the analysis more difficult as it usually disqualifies separation of variables and recourse to numerical computation may be necessary (for which efficient software is available see [45]) (3.2.20) may be rewritten in terms of the

current density per unit energy interval J(X,W) (which is defined as in (3.2.4)) as

$$\frac{\partial}{\partial W}(\beta_{sm} W^{m-n} \frac{\partial}{\partial W}(W^m J) + W^n J) + \gamma^2 \frac{\partial^2 J}{\partial X^2} = 0 \qquad (3.2.22)$$

(cf (3.2.5) with $\beta sm = 0$) which is unfortunately of little analytical use. Again due to the increased complexity of the operator (3.2.20), particular examples will be discussed in Chapter 5. Similar comments also apply to the correspondence of solutions of (3.2.20) and (3.2.3) if we notice that

$$\lim_{\beta sm \to o} L_{s\,m}^{\{0\,1\}} = L_{s\,m}^{\{0\,0\}};$$

the solutions to these operators may not behave in a similar manner as they are subject to totally different boundary value problems : compare for example Laplace's equation $\nabla^2 f = 0$ with the heat equation $\nabla^2 f = \alpha \frac{\partial f}{\partial t}$ ; the former is elliptic and the latter parabolic. As $\alpha \to 0$ then they tend to the same equation but it is possible to construct solutions that are independent of $\alpha$ which will not correspond as completely different BVP have been imposed on the equations.

v) Electric field, second order scattering

This is the most general case and is a formidable operator (it includes field and second order phonon energy and is analytically intractable)

$$L^{\{1\ 1\}}_{s\ m} f_o := (\alpha^2+\beta s m W^n)\frac{\partial^2 f_o}{\partial W^2} - 2\alpha\gamma\frac{\partial^2 f_o}{\partial W \partial X}+\gamma^2\frac{\partial^2 f_o}{\partial X^2} -$$

$$m\frac{\alpha\gamma}{W}\frac{\partial f_o}{\partial X} +\left(\frac{m\alpha^2}{W} + W^n+(m+n)\beta s m W^{n-1}\right)\frac{\partial f_o}{\partial W} + (m+n)W^{n-1}f_o = 0$$

(3.2.23)

(3.2.23) is an elliptic equation and the appropriate BVP's are those mentioned in (2.3.(iii)).

## §3. Summary

A general description of the boundary value problems associated with the mathematical modelling of electron transport in semiconductors (subject to the assumptions given in Chapter 2) has been given. Two important points are the dramatic increase in complexity when an electric field is included and the change in nature of the boundary value problems (from parabolic to elliptic) when higher order contributions from the phonon energy are included.

Explicit solutions to particular problems are the topic of the next chapter.

# CHAPTER FOUR

## ELECTRON TRANSPORT IN AN ELECTRIC FIELD

### §1. Solution of the governing equation

The previous chapter discussed the type of mathematical problems that the nearly isotropic approximation to the BTE poses. As an example we now discuss in detail the case of non-polar optical phonon scattering in the presence of an electric field, with a first order truncation of the Taylor series (2.3.20).

The treatment is an extension of that given in [18] where non-polar optical scattering was treated in the absence of an electric field (i.e. assuming a purely diffusive phenomena) by the use of the NIA to the Boltzmann equation. The resulting partial differential equation was solved by a Green's function technique (cf. section 2, Chapter 3). The inclusion of the field considerably complicates the analysis, due to the fact that the equation satisfied by the distribution function changes from an adjoint diffusion equation with constant coefficients to one whose coefficients depend on the independent variables, and it becomes necessary to use numerical methods and analytic approximations.

The partial differential equation describing this particular model is:

$$\alpha^2 \frac{\partial^2 f_o}{\partial W^2} - 2\alpha\gamma \frac{\partial^2 f_o}{\partial W \partial X} + \gamma^2 \frac{\partial^2 f_o}{\partial X^2}$$

$$-\frac{m\alpha\gamma}{W}\frac{\partial f_o}{\partial X}+\left(\frac{m\alpha^2}{W}+W^n\right)\frac{\partial f_o}{\partial W}+(m+n)W^{n-1}f_o=0 \qquad (4.1.1)$$

(see (2.4.29)). The solution to (4.1.1) is discussed in [20] where the problem was formulated in velocity-position variables, rather than in energy position variables as used solely in this thesis, and the relevant points shall be reviewed here. Inserting the values of (m,n) appropriate to this case and choosing characteristic length and energy parameters to make $\alpha$ and $\gamma$ unity:

$$x_c=\frac{\lambda}{\mu} \qquad E_c=\frac{\lambda^2}{\mu} \qquad (4.1.2)$$

(with $\lambda$ and $\mu$ as defined in (2.4.30)) enables (4.1.1) to be written in dimensionless form:

$$\frac{\partial^2 f_o}{\partial W^2}-2\frac{\partial^2 f_o}{\partial X\partial W}+\frac{\partial^2 f_o}{\partial X^2}-\frac{1}{W}\frac{\partial f_o}{\partial X}+\left(\frac{1}{W}+1\right)\frac{\partial f_o}{\partial W}+\frac{1}{W}f_o=0 \qquad (4.1.3)$$

(4.1.3) is an adjoint parabolic equation and using canonical coordinates

$$\xi=X+W \qquad \eta=W$$

reduces it to the normal form:

$$\eta\frac{\partial^2 f_o}{\partial\eta^2}+\eta\frac{\partial f_o}{\partial\xi}+(1+\eta)\frac{\partial f_o}{d\eta}+f_o=0 \qquad (4.1.4)$$

As shown in [20], solutions to (4.1.4) exist for a final BVP of the form.

$$f_o(O,W) = h(W) \qquad (4.1.5)$$
$$\lim_{W\to\infty} f(X,W) = 0$$

and in terms of the original variables the solution is

$$f_o(X,W) = \int_o^\infty dt\, B(t)\ \exp(-(t+1)^2W)\ \exp(-(t^2+t)X)$$
$$x\quad {}_1F_1\left(\frac{t}{2t+1}\,;\,1\,;\,(2t+1)W\right) \qquad (4.1.6)$$

where B(t) is to be determined from the condition (see (4.1.5))

$$h(W) = \int_o^\infty dt\, B(t)\ \exp(-(t+1)^2W)\ {}_1F_1\left(\frac{t}{2t+1}\,;\,1\,;\,(2t+1)W\right) \qquad (4.1.7)$$

${}_1F_1$ denotes the confluent hypergeometric function [46] defined by

$${}_1F_1\,(a;\,b;\,x) = \sum_{n=o}^{\infty} \frac{(a)_n}{(b)_n} \cdot \frac{x^n}{n!} \qquad (4.1.8)$$

$(a)_n$ denoting the Pochammer symbol

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)} = a(a+1)....\ (a+n-1)$$

$\Gamma(z)$ being the gamma function of argument z

The main problem is to invert the singular Fredholm integral equation of the first kind (4.1.7). This is termed singular due to

the semi-infinite range of integration rather than any singularities in the kernel. The general form of Fredholm integral equations (of the first kind) is

$$h(W) = \int_a^b K(W,t)\ B(t)\ dt$$

Many integral transforms are particular examples of Fredholm integral equations of the first kind; one particularly relevant to this thesis is the Laplace transform defined by

$$h(W) = \int_0^\infty \exp(-Wt)\ B(t)\ dt = L_W\ (B(t))$$

Unfortunately however the kernel of the integral equation (4.1.7) viz

$$K(t,W) = e^{-(t+1)^2 W}\ {}_1F_1\ (\frac{t}{2t+1}\ ;\ 1;\ (2t+1)W)$$

cannot be converted to any standard form. Approximate (and computational) methods exist but would be difficult due to the nature of the confluent hypergeometric function. The approach developed here will entail deriving a simple analytic approximation to the kernel.

## §2. The boundary condition

An initial (or boundary) condition on the full distribution function satisfying (2.1.5) must be imposed to ensure a unique solution. In the NIA

$$f = f_o + k f_1 \cos\theta$$

and the single condition on f is in fact sufficient to determine conditions on both $f_o$ and $f_1$. The boundary value problem on $f_o$ (see section 3.3) is also sufficient to enable $f_o$ and $f_1$ to be uniquely determined. If a boundary value problem had been prescribed on $f_1$ then this would be equivalent to a Neumann problem for $f_o$ due to the relationship between $f_o$ and $f_1$

$$f_1(E) = -\tau_1(E) \left\{ \frac{\hbar}{m_e} \partial_x f_o + \frac{e\xi}{m_e} \partial_E f_o \right\}$$

- see (2.4.26) and (2.3.13).

The boundary value problem appropriate to this model shall be reformulated in terms of physical observables; either j(X,W) the current density per unit energy interval (when the boundary value problem is prescribed on $f_1$) or n(X,E) the particle number density per unit energy interval (when the boundary value problem is imposed on $f_o$). It is quite common in mathematical modelling to impose conditions on integrals of functions as certain observables, such as energy, are usually defined as such. Now

$$n(X)\, dX = dX\, N \int f(X,\underline{k})\, d\underline{k}$$

$$n(X,E) \propto \sqrt{E}\, f_o(X,E) \qquad (4.2.9)$$

N denoting the total number of particles and the symmetry (in k space) of $f_o$ has been used.

Similarly

$$j(X) \propto \int k_x f(\chi, \underline{k})\, d\underline{k}$$

$$j(X,E) \propto E^{3/2} f_1(X,E) \qquad (4.2.10)$$

As boundary value problems for $f_o$ are of interest here, then (4.2.9) will be used to translate between the models.

Some compromise between the realistic distribution (i.e. that based on experiment) and the form used for the following analysis is necessary, so that the calculations may be effected analytically. The functional form chosen for n(X,E) does not affect the inversion of (4.1.7), which depends only on the kernel and range of integration (providing it satisfies certain reasonable mathematical criteria such as continuity) but determines whether simple explicit formula can be derived for B(t). Various models are plausible to represent the injected current - a mono energetic beam of $n_o$ electrons at X=0 for example, which would be mathematically represented by a delta functional. For illustrative purposes and also to provide a useful toy model the form chosen is

$$n(0,W) = \frac{n_o e^{-W}}{\sqrt{\pi E_c W^{1/2}}} \qquad (4.2.11)$$

giving a total number of particles at the origin of

$$\int_0^\infty n(O,W)dW = n_o$$

and, from (4.2.9)

$$f_O(O,W) = \frac{Ce^{-W}}{W} = h(W) \qquad (4.2.12)$$

with C being a normalization constant. Other models for n(O,W) will be discussed in section (4.5). B(t) shall now be evaluated with h(W) as defined in (4.2.12).

§3. Solution of the integral equation

The singular Fredholm integral equation of the first kind (4.1.7) possesses a daunting kernel namely

$$K(t,W) = e^{-(t+1)^2W} \; {}_1F_1\left(\frac{t}{2t+1}\,;\; 1\;;\; (2t+1)W\right) \qquad (4.2.13)$$

It is highly unlikely that it will be possible to invert an integral equation with a kernel of the form (4.3.13) analytically, a major difficulty being that the integration variable t appears in two parameters of the confluent hypergeometric function. Numerical methods are available [47] but are not unconditionally stable and so in keeping with the general approach of this work, a simple semi-analytic solution will be determined. It is intended to develop an approximation to the kernel (4.3.13) that will enable the integral equation to be inverted.

Firstly using the relation [3]

$$ {}_1F_1\,(a\,;\,b\,;\,x) \xrightarrow[x\ \text{large}]{} \frac{\Gamma(b)}{\Gamma(a)}\, e^{x}\, x^{a-c} \quad (x \in R^{+}) $$

it can be seen that for large t and/or W the exponential factor $e^{-(t+1)^2 W}$ dominates the kernel. W represents the scaled energy viz

$$ W = \frac{E}{E_c}\,; \quad E_c = \frac{\lambda^2}{\mu} $$

Now $\mu \alpha D_o^4$ where $D_o$ is the deformation potential constant [18] and has an experimentally determined value in the range $10^9$ - $10^{11}$ $eVm^{-1}$. If the applied field is in the range $10^5$ - $10^7$ $Vm^{-1}$ then $E_c$ varies over twelve orders of magnitude. As $E_c$ represents the energy scale against which E is measured, $W = {}^{E}/_{E_c}$ will show a similar variation. Taking the field to be 100 kV $cm^{-1}$ and $D_o = 10^{10}$ $eVm^{-1}$ gives $W \sim 10^{-3}$ for appropriate carrier energies. W will thus be considered to be of small magnitude in the following analysis, although this is not strictly necessary.

If W is considered small then the following approximation will be shown to be valid

$$ e^{-(t+1)^2 W}\ {}_1F_1\left(\frac{t}{2t+1}\,;\,1\,;\,(2t+1)W\right) \sim e^{-(t+1)^2 W}\ (1+tW) \qquad (4.3.14) $$

Analytically:

$$\left| e^{-(t+1)^2W} {}_1F_1\left(\frac{t}{2t+1}\,;\ 1\ ;\ (2t+1)W\right) - (1+tW)\, e^{-(t+1)^2W} \right|$$

$$= e^{-(t+1)^2W} \left| \frac{t(3t+1)W^2}{(2!)^2} + \frac{t(3t+1)(5t+2)}{(3!)^2} W^3 + t(3t+1)(5t+2)(7t+3) \right.$$
$$\left. \times \frac{W^4}{(4!)^2} + \ldots \right|$$

{ Using the expansion

$${}_1F_1\left(\frac{t}{2t+1}\,;\ 1\ ;\ (2t+1)W\right) = 1 + \sum_{j=1}^{\infty} \frac{W^j}{(j!)^2} \left\{ \prod_{n=o}^{j-1} [\,(2n+1)t+n] \right\} \}$$

$$\leq e^{-(t+1)^2W} \left| \frac{3!\ t(t+1)}{2(2!)^2} W^2 + \frac{5!t(t+1)^2W^3}{2(2!)(3!)^2} + \frac{7!t(t+1)^3}{2(3!)(4!)^2} W^4 \ldots \right|$$

$$\leq e^{-(t+1)^2W} \left| t(t+1)W^2 + t(t+1)^2W^3 + t(t+1)^3W^4 + \ldots \right|$$

$$\left[ \text{as } \frac{(2n-1)!}{(n-1)!(n!)^2}\ ,\ \leq\ 1 \text{ by induction} \right]$$

$$= e^{-(t+1)^2W} \left| \frac{tW^2.(1+t)}{1-(t+1)W} \right|$$

assuming $(1+t)W < 1$

Hence for $t < \left(\frac{1}{W} - 1\right) \approx \frac{1}{W}$ (for W small) the above approximation is valid. As $W \sim 10^{-3}$ this is valid for $t<1000$. This error term is obviously small over the range of interest. This linear truncation is valid as for large t the exponential term dominates, and has small magnitude, while for small t, terms of $O(W^2)$ again are negligible. The difference in magnitude between (4.3.14) and (4.3.13) has also been studied numerically, and the above

reasoning verified. Using the approximation defined in (4.3.14) an explicit solution to the resulting integral equation

$$\int_0^\infty B(t)e^{-(t+1)^2W}\,(1+tW)\,dt \;=\; h(W) \qquad (4.2.15)$$

will now be constructed [48].

Integrating (4.3.15) by parts gives

$$\lim_{t\to o}\left[\frac{t.B(t)}{2(t+1)}\right]+\int_o^\infty\left\{B(t)+\frac{d}{dt}\left[\frac{tB(t)}{2(t+1)}\right]\right\}e^{-(t+1)^2W}\,dt=h(W) \qquad (4.3.16)$$

providing that B(t) is exponentially bounded as $t\to\infty$.

Assuming the result

$$\lim_{t\to o}\left[\frac{tB(t)}{(t+1)}\right] \;=\; 0 \qquad (4.3.17)$$

(4.3.16) becomes

$$\int_0^\infty \varphi(t)e^{-(t+1)^2W}\,dt \;=\; h(W) \qquad (4.3.18)$$

with

$$\varphi(t) \;=\; \frac{d}{dt}\left\{\frac{tB(t)}{2(t+1)}\right\} \;+\; B(t) \qquad (4.3.19)$$

Consider (4.3.18):

$$e^{-W}\int_0^\infty \varphi(t)e^{-(t+1)^2W}\,dt = e^{-W}\int_0^\infty \frac{\varphi(\sqrt{u+1}-1)}{2\sqrt{u+1}}e^{-uW}\,du = h(W) \tag{4.3.20}$$

after using the substitution $u = t^2 + t$. (4.3.20) is in the form of a Laplace transform with variable W :

$$L_w\{\varphi(u)\} = e^W h(W)$$

($L_w$ denoting the operation of Laplace transforming) which upon inversion gives

$$\varphi(t) = 2(t+1)\,p(t^2+t) \tag{4.3.21}$$

$$p(t) = L_w^{-1}\{e^W h(W)\} \tag{4.3.22}$$

Thus, formally, an expression for $\varphi(t)$ has been derived. B(t) may be evaluated from the first order linear ordinary differential equation (4.3.19). The solution is

$$B(t) = \frac{(t+1)}{t^3}e^{-2t}\left[\delta + 2\int_0^t p^2 e^{2p}\varphi(p)\,dp\right] \tag{4.3.23}$$

The constant of integration $\delta$ must be chosen so that (4.3.23) satisfies (4.3.17). Putting

$$a(t) = \int^{t} p^2 \, e^{2p} \, \varphi(p) \quad dp$$

the limit required is:

$$\lim_{t \to 0} \; e^{-2t} \left[ \frac{\delta + 2a(t)}{t^2} \right]$$

Using a Taylor expansion of a(t), noting that $a'(t)\big|_{t=o} = a''(t)\big|_{t=o}$ gives

$$\delta = -\, 2a(t)\big|_{t=0}$$

Hence:

$$B(t) = \frac{(t+1)}{t^3} \, e^{-2t} \int_{p=0}^{p=t} p^2 \, e^{2p} \, \varphi(p) \; dp \qquad (4.3.24)$$

with $\varphi(p)$ defined in (4.3.21), (4.3.22). Hence, for arbitrary h(W), the integral equation (4.3.15) has been inverted, and an exact solution to the boundary value problems (4.1.5), (4.1.6) has been derived, subject to the approximations detailed in this section.

## §4. Evaluation of the current

Although the distribution function is of primary importance; physical observables, such as the current are of interest experimentally.

From (4.2.10) and (2.4.26), (2.3.13)

$$j(x) = k \int_0^\infty E^{3/2} f_1 (x,E) \; dE \tag{4.4.25}$$

$$= k_1 \int_0^\infty E \left( \frac{\partial f_o}{\partial x} + e\xi \frac{\partial f_o}{\partial E} \right) dE \tag{4.4.26}$$

$k, k_1$ being constants. Note that dimensionless variables are not being used in (4.4.26). Integrating (4.4.26) by parts gives

$$j(x) = k_1 \left\{ \frac{d}{dx} \int_0^\infty E f_o \; dE - e\xi \int_0^\infty f_o \; dE \right\} \tag{4.4.27}$$

the boundary terms vanishing due to the limits of integration.

Strictly, the limits on the integrals are not (o, ∞); it has been assumed that $E > \hbar\omega$ (see section 2.3), and this dictates the lower bound. However low energy carriers furnish little current and the lower bound shall be taken to be zero. There have been attempts to overcome this problem (see [49]), by using solutions appropriate to each energy interval. This is not feasible in this analysis.

In low field transport (see [28]) $f_o$ is now assumed to be a Maxwell-Boltzmann distribution, and (4.4.27) may be evaluated exactly. Generalizations of this procedure have included that in [50] which assumed a temperature dependent $f_o$, and extended the simple drift-diffusion expression

$$j = - en\mu_e\xi + e D_e \frac{dn}{dx} \qquad (4.4.28)$$

(n being the electron number density, $\mu_e$ the electron mobility and $D_e$ its diffusion coefficient) to the temperature dependent form

$$j = -e\xi n(x)\mu_e(T) + e \frac{d}{dx} \left[n(x)\, D_e(T)\right] \qquad (4.4.29)$$

the temperature being spatially dependent. Neither of these treatments are appropriate to this analysis as hot electron transport is being treated and a Maxwellian distribution is not applicable. However the precise functional form for $f_o$ is known, for an arbitrary injected stream of electrons from Chapter 4, although a specific model has been used. This shall be used in (4.4.27) to evaluate j(x). Note that (4.4.27) can be expressed in drift-diffusion format as (using dimensionless variables)

$$j(X) = \frac{d}{dX} \left(D(X,\xi)\, n(X,\xi)\right) - \mu(X,\xi)\, n(X,\xi) \qquad (4.4.30)$$

with n given as in (4.2.9), and the explicit dependence of the functions involved has been advanced. $D(X,\xi)$ and $\mu(X,\xi)$ have now become functions of field and position, being generic diffusion and mobility coefficients respectively, given by

$$D(X,\xi) = \frac{I_1}{I_{1/2}} \qquad \mu(X,\xi) = \frac{I_o}{I_{1/2}}$$

with

$$I_n = \int_0^\infty W^n f_o(X,W)\ dW \qquad (4.4.31)$$

Dimensionless variables have been used in (4.4.31) and multiplicative constants have been omitted.

The current j(X) can be expressed in the form

$$j(X) = \frac{d}{dX} I_1 - I_o \qquad (4.4.32)$$

where E has been replaced by W via $E = WE_c$ and the definition of $I_n$ given by (4.4.32) has been used. A specific functional form for h(W) must be used to determine B(t). For simplicity and to generate a toy model, taking

$$n(W) = \frac{Ce^{-W}}{W^{1/2}} \qquad (4.4.33)$$

(see (4.2.11), (4.2.12)) C being a constant, gives

$$h(W) = \frac{Ce^{-W}}{W} \qquad (4.4.34)$$

and from (4.3.21), (4.3.22)

$$\varphi(t) = 2C(t+1) \qquad (4.4.35)$$

Evaluating the integral (4.3.24), with $\varphi(t)$ given as above gives,

$$B(t) = 2C \cdot \frac{(t+1)}{t^3} \left\{ e^{-2t} + 4t^3 - 2t^2 + 2t - 1 \right\} \qquad (4.4.36)$$

This satisfies the condition (4.2.17) (by construction).
By substitution (4.4.36) satisfies (4.2.15), with the choice of boundary condition used ((4.4.34)). From (4.1.6)

$$f_o(X,W) = 2C \int_o^\infty \frac{(t+1)}{t^3} \left[ e^{-2t} + 4t^3 - 2t^2 + 2t - 1 \right] e^{-(t+1)^2 W}$$

$$e^{-(t^2+t)X} \cdot {}_1F_1 \left( \frac{t}{2t+1} ; 1 ; (2t+1)W \right) dt \qquad (4.4.37)$$

$$\approx 2C \int_o^\infty \frac{(t+1)}{t^3} \left[ e^{-2t} + 4t^3 - 2t^2 + 2t - 1 \right] e^{-(t+1)^2 W} e^{-(t^2+t)X}$$

$$(1 + tW)\, dt \qquad (4.4.38)$$

(using the approximation (4.3.14)).

For the solution (4.4.38) reversing the order of integration and performing the W-integration gives (using (4.4.32) and (4.4.31))

$$j(X) = \int_o^\infty B(t)\, e^{-(t^2+t)X} \left\{ \frac{(t^3 + 5t^2 + 4t + 1)}{(t+1)^5} \right\} dt \qquad (4.4.39)$$

(38) converges, but is not readily evaluated. (4.4.39) will be evaluated numerically; taking the device to be of size 10μm and $\xi$ = 100kV $cm^{-1}$ gives Figures (4.1) and (4.2) for $f_o(X,W)$ and $j(X)$ respectively.

## §5. High field solution

Sections two and three of this chapter detail the evaluation of the generalized Fourier coefficient B(t) via the assumption that W is small. This is not necessarily true as W varies over several orders of magnitude, depending on the values of the field $\xi$ and the deformation potential constant $D_o$. W is inversely proportional to the characteristic energy scale Ec which itself is a function of the applied field and deformation potential constant. The magnitude of W will be determined by the range of Ec via the relationship $W=E.E_c^{-1}$. If their values are such that W is large (in the sense that (4.5.40) is a valid approximation) another solution to the boundary value problem (4.1.5), (4.1.6) may be determined. This approach is somewhat artificial in that it dictates a value of Ec, and hence applied field for its validity. However the appropriate range of electric field is realistic and the solution to the boundary value problem does represent the exact distribution function rather than assuming a specific form with variable parameters, as in a drifted Maxwellian approach.

For large $z$, the confluent hypergeometric function has the following asymptotic form

$$ {}_1F_1(a\,;1\,;z) \underset{z\to\infty}{\longrightarrow} \frac{e^z z^{a-1}}{\Gamma(a)} \qquad (4.5.40) $$

Thus, the following approximation is valid for large W

$$ {}_1F_1\left(\frac{t}{2t+1}\,;\,1\,;\,(2t+1)W\right) \underset{(2t+1)W\to\infty}{\longrightarrow} \frac{e^{(2t+1)W}[(2t+1)W]^{-(t+1)/(2t+1)}}{\Gamma\left(\frac{t}{2t+1}\right)} \qquad (4.5.41) $$

(Note that for $t \geq 0$ $(2t+1)W \geq W$). Using (4.5.41) in (4.1.7) gives

$$ \int_0^\infty B(t)\,\frac{[(2t+1)W]^{-\left(\frac{t+1}{2t+1}\right)}}{\Gamma\left(\frac{t}{2t+1}\right)}\, e^{-t^2W}\, dt = h(W) \qquad (4.5.42) $$

If a derivative problem was imposed on fo (i.e. a boundary value problem involving the current) then use of the relationship

$$ \frac{d}{dx}\,{}_1F_1\,(a\,;\,b\,;\,x) = \frac{a}{b}\,{}_1F_1\,(a+1\,;\,b+1\,;\,x) $$

would enable (4.5.40) to be applied to the resulting Fredholm integral equation of the first kind. Other problems (see Chapter 5 and [34]) may admit a similar asymptotic approach. The same argument applies to the analysis of section (4.3)

As it stands, (4.5.42) is intractable. However as W is large, and the argument of an exponential function, progress may be made: only in the vicinity of t=0 will the exponential function have appreciable magnitude; it is highly localized at the origin for large W. Hence to a good approximation, the function $W^{-\left(\frac{t+1}{2t+1}\right)}$ can be replaced by its functional form at t=0, namely $W^{-1}$. (4.5.41) then becomes

$$\int_0^\infty C(t)e^{-t^2W}\,dt = Wh(W) \qquad (4.5.43)$$

with

$$C(t) = \frac{B(t)\,(2t+1)}{\Gamma\left(\frac{t}{2t+1}\right)^{-\left(\frac{t+1}{2t+1}\right)}} \qquad (4.5.44)$$

(4.5.43) may be readily converted to a Laplace transform by the substitution $s=t^2$ giving

$$L_w\{\,C(\sqrt{s})\,\} = Wh(W) \Leftrightarrow C(t) = L_w^{-1}\,(Wh(W))\,\Big|_{s=t^2} \qquad (4.5.45)$$

and, from (4.5.44), B(t) is then known. As in the low W case, h(W) must be modelled. Again, a simple form will be used for n(0,W) and the ramifications of this choice investigated. A more realistic n(0,W) could be used and numerical techniques applied but the object of this analysis is illustrative.

Taking

$$n(0,W) = \alpha \cdot \frac{W^{1/2}}{(W+W_o)^2} \qquad (4.5.46)$$

($\alpha$ being a normalization constant, and $W_o$ an arbitrary positive dimensionless energy) gives (via (4.2.9))

$$f_o(O,W) = h(W) = \frac{\alpha}{(W+W_o)^2} \qquad (4.5.47)$$

(4.5.47) was chosen mainly to facilitate inversion of the Laplace transform. Using (4.5.47) in (4.5.45) gives, using (4.5.44)

$$B(t) = 2\alpha t\,\Gamma\left(\frac{t}{2t+1}\right)\,(1-W_o t^2)\,e^{-t^2 W_o\,(2t+1)}\left(\frac{t+1}{2t+1}\right) \qquad (4.5.48)$$

Substituting the value obtained for B(t) above gives fo(X,W) as

$$f_o(X,W) = 2\alpha \int_o^\infty \left[ t\Gamma\left(\frac{t}{2t+1}\right)\,(1-W_o t^2)\,e^{-t^2 W_o\,(2t+1)}\left(\frac{t+1}{2t+1}\right)\right.$$

$$\left. e^{-(t+1)^2 W}\; e^{-(t^2+t)X}\; {}_1F_1\left(\frac{t}{2t+1};\,1\,;\,(2t+1)W\right)\right] dt \qquad (4.5.49)$$

$$h(W) = f_o(O,W) = 2\alpha \int_o^\infty t\,\Gamma\left(\frac{t}{2t+1}\right)\,(1-W_o t^2)\,e^{-t^2 W_o\,(2t+1)}\left(\frac{t+1}{2t+1}\right)$$

$$\text{x}\quad e^{-(t+1)^2 W}\; {}_1F_1\left(\frac{t}{2t+1};\,1\,;\,(2t+1)W\right)\,dt$$

Thus this is the exact distribution function. The alternative viewpoint - that (4.5.49) represents an exact solution if the injected stream of electrons has the distribution defined in (4.5.49) - is valid: if such a distribution could be generated experimentally then the resultant current could be compared with the analytic results, providing a useful test of the model.

Using (4.4.32) the current corresponding to the above distribution may be evaluated: use of the result [46]

$$\int_0^\infty e^{-pt}\, t^{b-1}\, {}_1F_1\,(a\,;\,c\,;\,kt)dt = \Gamma(b)\; p^{-b}\; {}_2F_1\left(a\,,\,b;\,c;\,\frac{k}{p}\right)$$

(the necessary convergence criteria are satisfied) where ${}_2F_1\,(a, b; c; x)$ denotes Gauss' function, defined by

$${}_2F_1\,(a, b; c; x) = \sum_{n=o}^{\infty} \frac{(a)_n (b)_n}{(c)_n}\,\frac{x^n}{n!}$$

enables the W-integration to be performed analytically giving

$$I_1 = \int_0^\infty \frac{B(t)\; e^{-(t^2+t)X}}{(t+1)^2}\; {}_2F_1\left(\frac{t}{2t+1};\,1;\,1;\,\frac{2t+1}{(t+1)^2}\right)\,dt \qquad (4.5.50)$$

$$I_2 = \int_0^\infty \frac{B(t)\; e^{-(t^2+t)X}}{(t+1)^2}\; {}_2F_1\left(\frac{t}{2t+1};\,2;\,1;\,\frac{(2t+1)}{(t+1)^2}\right)\,dt \qquad (4.5.51)$$

Use of the identities

$${}_2F_1\,(a, 1; 1; x) \;=\; (1-x)^{-a}$$

$${}_2F_1\,(a, 2; 1; x) \;=\; \frac{1-(a+1)x}{(1-x)^{a+1}}$$

enables j(X) to be written as (see (4.4.32))

$$j(X) = \int_{o}^{\infty} \frac{(t^4+t^3+1)}{(t+1)^4} B(t) e^{-(t^2+t)X} dt \qquad (4.5.52)$$

with B(t) given by (4.5.48).

Figure (4.1) gives the $f_o(X,W)$ surface for a device of the order of $10\mu m$ subject to a field of the order of 100 $kVcm^{-1}$ with the boundary condition (4.4.34).

Figure (4.2) gives the electron current corresponding to the distribution function given in Figure (4.1).

**Figure (4.1) : Electron Distribution function $f_o(X,W)$**

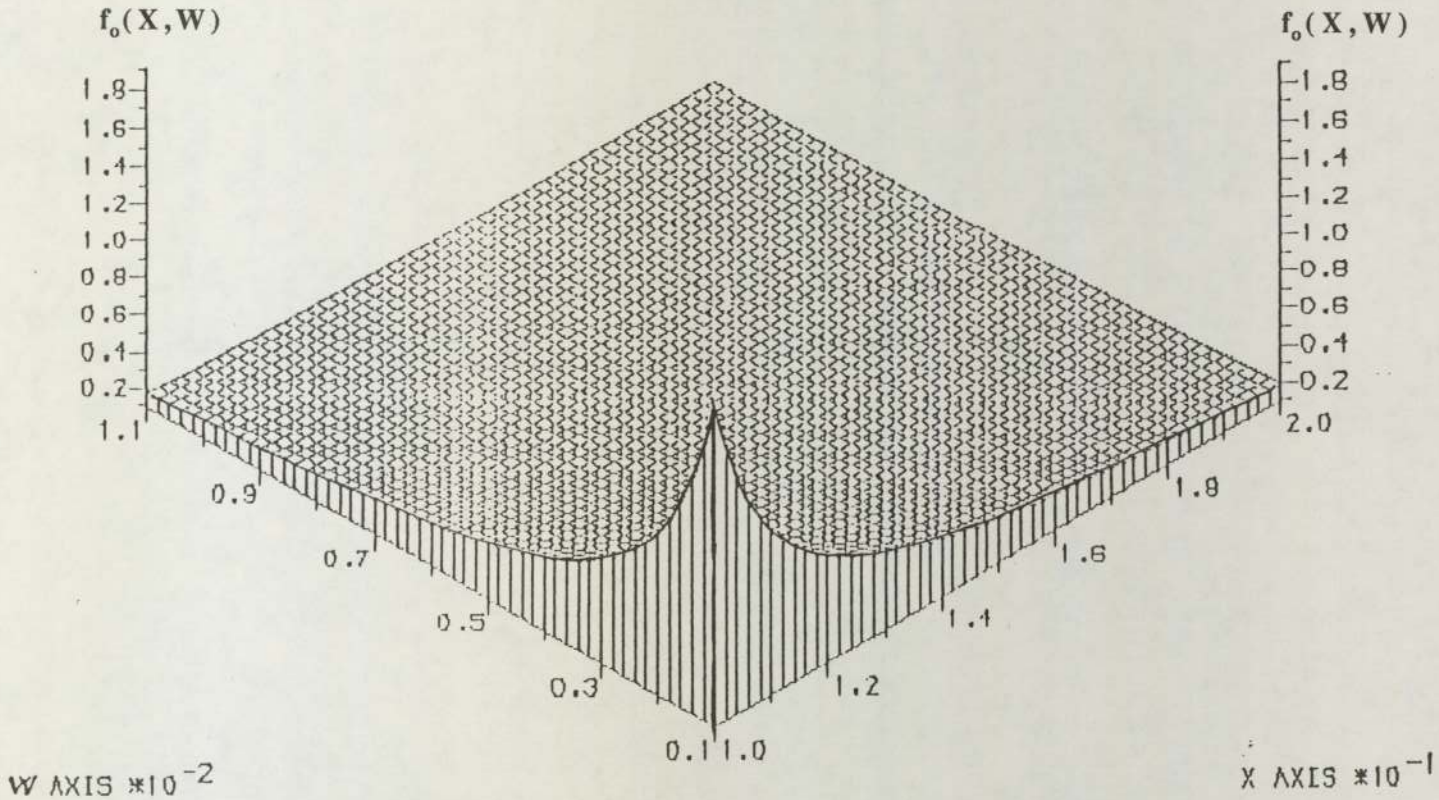
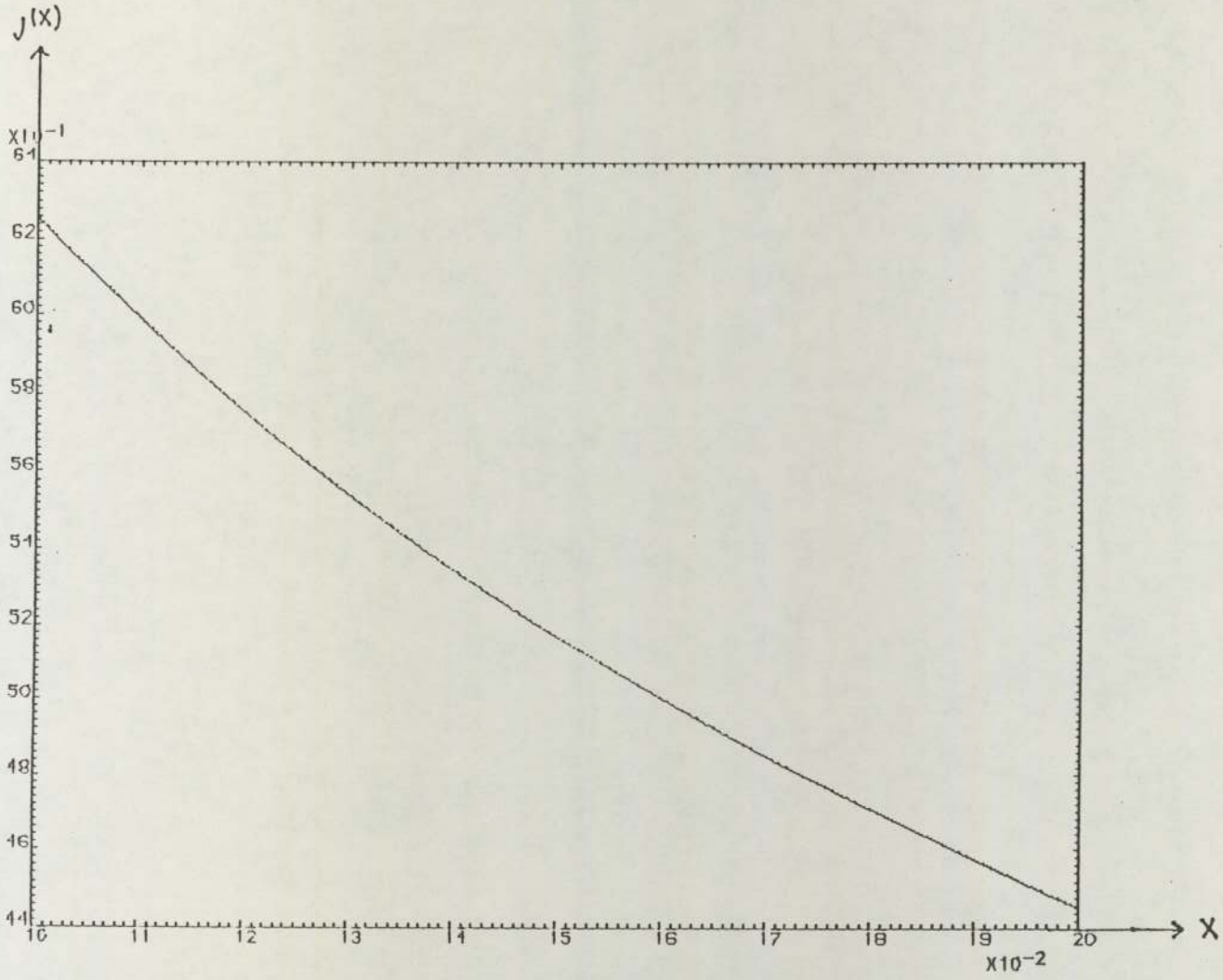


**Figure (4.2) : Current corresponding to distribution function given in Figure (4.1)**



# CHAPTER FIVE

## MODEL SOLUTIONS

### §1. Introduction

Chapter 3 discussed the general classes of problem to be discussed whereas Chapter 4 solved a particular example in detail. Here an intermediate viewpoint shall be used in that the method of solution shall be developed although not fully as in the previous chapter.

There are still a number of problems to be discussed, and apart from the $L_{s\,m}^{\{0\ 0\}}$ cases (those without an electric field and first order phonon energy expansion), the remaining boundary value problems require a large amount of work; the general approach expounded in Chapter 3 cannot be extended to these cases.

However some progress can be made analytically and once again the mathematical classification of the problems (see Chapter 3) provides useful insight.

### §2. Model solutions

#### i) Electric field, first order scatterers

These cases include an electric field but only consider the first order phonon energy contributions to the collision integral.
This is a parabolic operator, the corresponding partial differential equation being:

$$\frac{\partial^2 f_o}{\partial \eta^2} + \left( \frac{m}{\eta} + \eta^n \right) \frac{\partial f_o}{\partial \eta} + \eta^n \frac{\partial f_o}{\partial \xi} + (m + n)\eta^{n-1} f_o = 0. \quad (5.2.1)$$

with n having a value appropriate to the scattering mechanism as given in Table 3 of Chapter 3.

The canonical coordinates:

$$\eta = W \qquad \xi = X + W \quad (5.2.2)$$

have been utilized (cf. 3.2.19). Separating the variables in (5.1.1) gives:

$$f_o(\xi,\eta) = N(\eta)Z(\xi) \quad (5.2.3)$$

$$\frac{dZ}{d\xi} + \lambda Z = 0 \quad \text{(i)} \quad (5.2.4)$$

$$\frac{d}{d\eta}\left( \eta^m \frac{dN}{d\eta} \right) + \frac{d}{d\eta}(\eta^{m+n}N) - \lambda\eta^{m+n}N = 0 \quad \text{(ii)}$$

$\lambda$ being the separation constant. Note that the boundary conditions must also separate. (5.2.4(i)) is readily soluble but the second equation causes more difficulty. Instead of repeating the analysis of Chapter 4, and studying the second order ordinary differential equations (5.2.4.(ii)) in depth, a different approach will be used. Multiplying (5.2.1) by $\eta^m$ and simplifying gives:

$$\frac{\partial}{\partial \eta}\left( \eta^m \frac{\partial F}{\partial \eta} + \eta^{m+n} F \right) + \frac{\partial}{\partial \xi}(\eta^{m+n} F) = 0 \quad (5.2.5)$$

where $F \equiv f_o$.

Writing

$$F(\xi,\eta) = \exp\left\{ - \int^{\eta} v^{n} \, dv \right\} \Psi(\xi,\eta) \equiv p(\eta)\, \Psi(\xi,\eta) \qquad (5.2.6)$$

recasts (5.2.5) in the form

$$\frac{\partial \psi}{\partial \xi} + \frac{1}{\eta^{m+n} p(\eta)} \frac{\partial}{\partial \eta} \left( \eta^{m} \, p(\eta) \frac{\partial \psi}{\partial \eta} \right) = 0 \qquad (5.2.7)$$

(5.2.7) is still separable but this is of little practical value. Continuing in the spirit of the approach developed in Chapter 3, define a coordinate transformation

$$u = \chi(\eta) \qquad (5.2.8)$$

such that (5.2.7) becomes

$$\frac{\partial \psi}{\partial \xi} + \frac{\partial}{\partial u} \left( h(u) \frac{\partial \psi}{\partial u} \right) = 0 \qquad (5.2.9)$$

where the functional form of $\chi$ (and hence h) may be determined by comparison of (5.2.9) and (5.2.7). This approach illustrates the similarity between the models generated by the $L^{\{0\ 0\}}_{s\ m}$ and $L^{\{1\ 0\}}_{s\ m}$ operators, as one would expect as they only differ by the inclusion of the electric field in the latter. (5.2.9) cannot be solved in a general manner; each case shall be treated separately.

Non polar optical phonon scattering

This particular case was treated at length in chapter 4. It illustrates the increase in difficulty when the electric field is introduced; a purely analytic approach applicable in the case of zero field has to be replaced by semi-analytic methods.

Piezoelectric phonon scattering

In this case (5.1.7) reduces to (see Table 2)

$$\frac{\partial \psi}{\partial \xi} + \frac{\partial}{\partial \eta}\left(\eta \frac{\partial \psi}{\partial \eta}\right) = 0 \qquad (5.2.10)$$

(5.2.10) is in fact equivalent to the corresponding partial differential equation. given in [34]:

$$\eta^2 \frac{\partial^2 f_o}{\partial \eta^2} + 3\eta \frac{\partial f_o}{\partial \eta} + \eta \frac{\partial f_o}{\partial \xi} + f_o = 0$$

(see [34])

which may be reduced to

$$\frac{\partial}{\partial \eta}\left(\eta \frac{\partial}{\partial \eta}(\eta f_o)\right) + \frac{\partial}{\partial \xi}(\eta f_o) = 0$$

by elementary manipulation.

The substitution

$$\psi = \eta f_o$$

gives the required result.

The generalized adjoint diffusion equation (with a non-constant diffusion coefficient) may be approached using several

different techniques; for example, separation of variables is applicable. However by comparison with the adjoint equation

$$\frac{\partial \psi}{\partial \xi} - \frac{\partial}{\partial \eta}\left(\eta \frac{\partial \psi}{\partial \eta}\right) = 0 \qquad (5.2.11)$$

the Green's function technique offers scope as the Greens function for (5.2.11) is tabulated [44]. As the form of the separated solution is known, (see [34]) this suggests that a Hankel transform may also be helpful: putting

$$\eta = \frac{1}{4} r^2 \qquad (5.2.12)$$

transforms (5.2.10) into

$$\frac{\partial \phi}{\partial \xi} + \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial \phi}{\partial r}\right) = 0 \qquad (5.2.13)$$

whence the term involving derivates with respect to r is in fact a Bessel operator. Care must be exercised as the equation (5.2.13) is in fact adjoint to the more usual form of the equation, namely (5.2.11). Another consideration is although the boundary value problem appropriate to (5.2.1) is

$$\begin{aligned} & f_o\,(O,W) = h(W) \\ & \lim_{W \to \infty} f_o\,(X,W) = 0 \end{aligned} \qquad (5.2.14)$$

that appropriate to (5.2.10) as

$$\lim_{\xi \to \eta} \frac{1}{\eta} \psi(\xi,\eta) = h(\eta)$$

$$\lim_{\eta \to \infty} \frac{1}{\eta} \psi(\xi,\eta) = 0$$

whilst that for (5.2.13) is

$$\lim_{\xi \to \frac{r^2}{4}} \frac{4}{r^2} \phi(\xi,r) = H(r)$$

$$\lim_{r \to \infty} \frac{4}{r^2} \phi(\xi,r) = 0$$

This illustrates the care necessary when dealing with such problems: transformations may alleviate problems due to the form of the equation but aggravate the situation due to the boundary conditions. This particular case is an interesting boundary value problem which it may be possible to solve completely by analytical methods. It would offer a chance of comparing the approximate techniques developed in Chapter 4 with an exact analysis.

Finally the comments and treatment given here may be compared with that given in [34]: by using the method of separation of variables Cox derives a solution of the form

$$f_o(X,W) = \int_o^\infty A(w) e^{-wX} e^{-wW} I_o(2\sqrt{wW}) \, dw \quad (5.2.15)$$

which satisfies the final boundary value problems (5.2.14) where w is the separation constant, $I_o$ denotes the modified Bessel function of zeroth order and A(w) must be chosen to satisfy the singular Fredholm integral equation of the first kind

$$h(W) = \int_o^\infty A(w)\, e^{-wW}\, I_o\,(2\sqrt{wW})\, dw \qquad (5.2.16)$$

(i.e. the boundary condition).

The techniques developed in Chapter Four, of either using a "small W" approximation, or an asymptotic approximation, to the kernel of the integration equation, namely $e^{-wW} I_o(2\sqrt{wW})$ may be applicable. However (5.2.16) is in fact (formally) soluble, and is a special case of a more general Fredholm integral equation of the first kind:

$$\int_o^\infty f(x)\, K\,(xt)\, dx = g(t) \quad (t>0) \qquad (5.2.17)$$

(making the obvious identification $K(xt) = e^{-xt} I_o(2\sqrt{xt})$).

The method of solution given in [51]; if use is made of the Mellin transform defined by

$$M\{f(x)\,;\,s\} = \int_o^\infty x^{s-1} f(x)\, dx = f^*(s) \qquad (5.2.18)$$

(for suitable f(x)) and also the result

$$M\left[ x^{\lambda} \int_0^{\infty} u^{\mu} f(xu)g(u)du \; ; \; s \right] = f^*(s+\lambda)g^*(1-\lambda+\mu-s) \qquad (5.2.19)$$

then Mellin transforming (5.2.17) gives:

$$f^*(1-s) = K^*(s)g^*(s)$$

with solution

$$f(x) = M^{-1}\left\{ \frac{g^*(s)}{K^*(1-s)} \right\} \qquad (5.2.20)$$

($M^{-1}$ denoting the inverse Mellin transform)

In the case in hand:

$$g^*(s) = M\{h(W) \; ; \; s\} \qquad (5.2.21)$$

which is of course model dependent while

$$K^*(s) = M\{ e^{-W} I_0(2\sqrt{W}) \; ; \; s \}$$

$$= \int_0^{\infty} W^{s-1} e^{-W} I_0\left(2\sqrt{W}\right) dW$$

$$= \Gamma\left(s+\frac{1}{2}\right) {}_1F_1\left(\frac{1}{2} - s \; ; \; 1 \; ; \; -1\right) \qquad (5.2.22)$$

using the notation of Chapter 4. Hence (5.2.20) gives us the function A(w) in (5.2.16) and thus via (5.2.15) the exact form of the symmetric part of the distribution function. A similar procedure to that followed in chapter 4 may be used to evaluate the current due to the injected distribution. Suitable models are

necessary for h(W), and even then semi-analytic means may be required.

Acoustic phonon scattering

This case is analytically insoluble and separation of variables is inapplicable as it generates a second order ordinary differential equation of non-standard form namely: (see 5.2.4)

$$\frac{d}{d\eta}\left(\eta \frac{dN}{d\eta}\right) + \frac{d}{d\eta}(\eta^2 N) - \lambda\eta^2 N = 0 \qquad (5.2.23)$$

for which solutions are not immediately available.

Thus the only method of solution seems to be numerical and further analysis of this case shall be omitted.

ii) No electric field, second order scattering

These form a new class of problems in that the operators $L_{s\,m}^{\{0\ 1\}}$ are elliptic. They require different boundary value problems (see Chapter 3) and are more difficult to solve than the preceding cases.

The general equation to be considered is:

$$W^n \frac{\partial^2 f_o}{\partial W^2} + \frac{\partial^2 f_o}{\partial X^2} + (W^n + (m+n)W^{n-1}) \frac{\partial f_o}{\partial W} + W^{n-1} f_o = 0 \qquad (5.2.24)$$

(or alternatively in terms of the current density per unit energy interval:

$$\frac{\partial}{\partial W}\left(W^{m-n}\frac{\partial}{\partial W}(W^{m}J) + W^{n}J\right) + \frac{\partial^2 J}{\partial X^2} = 0$$

with J(X,W) defined as in (3.2.4)).

Again, (5.2.24) is separable; substituting $fo(X,W) = H(W)T(X)$ gives:

$$\frac{d^2T}{dX^2} + \lambda T = 0 \qquad (5.2.25)$$

$$W^{n}\frac{d^2H}{dW^2} + (W^{n} + (m+n)W^{n-1})\frac{dH}{dW} + ((m+n)\,W^{n-1} - \lambda)\,H = 0 \qquad (5.2.26)$$

(5.2.25) is readily soluble but (5.2.26) generally is not; in the cases of acoustic phonon scattering and non-polar optical phonon scattering (5.2.26) may be solved in terms of hypergeometric functions [34] whereas in the case of piezoelectric phonon scattering (5.2.26) is of non-standard form.

However the boundary value problems for elliptic partial differential equations accentuate the problems: the actual set of admissible boundary value problems for elliptic operators is a complex subject and the discussion shall be restricted to those posed on a finite domain [52]. The most general boundary value problem (see (3.3.21)) is of the Robbins type:

$$a(x,y)\,\phi_{\hat{n}} + b(x,y)\,\phi = c(x,y) \qquad (5.2.27)$$

with $\phi_{\hat{n}}$ denoting the normal derivative of the function $\phi$. The fitting of this type of boundary condition on a finite domain by the inversion of a generalized Fourier-Bessel series (generated by the solutions of (5.2.25),(5.2.26)) can require considerable ingenuity. For example, in the case of acoustic phonon scattering Cox has shown that a solution of the form [34]

$$f_o(X,W) = \sum_{\omega} \exp\left(-\sqrt{\omega X}\right) e^{-W}\, {}_1F_1(\omega; 2; W)\; C(\omega) \qquad (5.2.28)$$

exists, $C(\omega)$ being determined by the boundary value problem, $\omega$ being a separation constant and ${}_1F_1$ the confluent hypergeometric function. (5.2.28) is then subject to a condition of the form (5.2.27) on the rectangle [a,b] x [c,d] and inversion of such a problem on a finite domain is impractical analytically.

Thus no simple analytic solutions are possible. This is unfortunate as efficient software exists for elliptic problems and comparison of the solutions would have been interesting.

iii) Electric field, second order scatterers

This is included for completeness; there is little chance of solving the relevant equations as this case is a generalization of all other cases, including the effects of the electric field and also higher order contributions from the phonon energy.

Numerical methods provide the only feasible approach [45] and these shall not be considered in this thesis.

# CHAPTER SIX

## SUMMARY OF THESIS

### §1. Conclusions

The overall aim of this thesis has been to develop the theme of analytic and semi-analytic modelling and to show that it is a useful modelling tool, being in many ways complementary to computational modelling.

Chapter 1 introduced the overall scope of modelling and gave a brief review of the various approaches to device modelling, concentrating mainly on the comparison between analytic and hydrodynamic computational modelling. The main conclusion drawn was that computational modelling is an extremely useful, practical simulation tool whereas analytic modelling has extensive general predictive capabilities and is complimentary to the computational method.

Chapter 2 provides the backbone of the formulation: it introduces the BTE, the transport equation used to derive the models. The steady state spatially inhomogeneous case is considered rather than the more usual space-independent formulation. Also the presence of an electric field is included which extends previous treatments and provides a more appropriate model, in certain circumstances. The collision integral is also treated in such a manner that higher order phonon energy contributions to the scattering integral are included, up to second order. The model includes extensions to previous models such as

an arbitrary injected electron energy distribution is considered. Due to this formulation there is a need to use a combination of mathematical methods and physical approximations (as detailed in Chapter 4).

The mathematical equations used throughout the thesis are then developed from the BTE using several approximations and assumptions. Firstly it is assumed that the electrons are 'hot' - that the mean electron energy is much greater than the mean phonon energy, and that the distribution function of the electrons is nearly isotropic in momentum space (the NIA). This allows considerable simplification of the BTE, reducing it to a pair of coupled equations. A relaxation time approximation is then developed for the collision integral (on the assumption that the collisions are either elastic or randomizing) and allows the two partial integrodifferential equations to be reduced to one second order linear partial differential equation. This partial differential equation depends on five parameters and covers all cases of scatterers non-polar optical phonons, piezoelectric phonons or acoustic phonons. The presence or absence of an electric field and order of expansion in phonon energy (first or second) is also included. The investigation of solutions to this partial differential equation forms the major part of the work.

Chapter 3 introduced the more abstract details that need to be considered when performing mathematical modelling: as well as deriving appropriate equations the device environment must be included. This means practically that various types of boundary value problems must be considered for different types

of partial differential equations and subtle problems are encountered, such as the difference between initial and final boundary value problems. It was noted that the different equations which are limiting forms of each other, for example when the electric field is turned off, do not necessarily have solutions related in a similar way. This was ascribed in some cases to the fact that the nature of the boundary value problems was different. A particular subset of cases covered by the general partial differential equation was solved in general, illustrating the power of the approach and also the similarity between the models. It became apparent that the inclusion of an electric field and/or higher order phonon energy contributions considerably complicates the analysis.

Chapter 4 is the culmination of Chapters 2 and 3: it details the solution of a particular case of an equation derived in Chapter 2 - that for non-polar optical phonon scattering in an electric field with first order expansion of the phonon energy contribution, subject to a final boundary value problem. The derivation of a solution to the partial differential equation without incorporating the boundary condition has been achieved [20]. There are problems incorporating the boundary conditions : it is obviously necessary to model the physical distribution of electrons. There are several plausible options, and for the purpose of this thesis some compromise between the actual distribution and the mathematical model has been made. If it is desired to continue analytically then this is essential. The purpose of the chapter is the inversion of a singular Fredholm integral equation of the first kind. The method of solution is suggested by the physics of the

situation, and amounts to a functional approximation to the kernel of the integral equation, considerably simplifying it. The approximation is shown to be valid analytically and this fact has been verified numerically.

Thus a solution has been derived for the distribution of electrons within the emitter base region of a transistor in the presence of an electric field subject to non-polar optical phonon scattering with arbitrary injected distribution. No approximation (modulo calculational difficulties) to the form of the distribution function has been made. The distribution thus calculated has been evaluated numerically.

From the distribution function transport coefficients may be calculated. However due to the complicated nature of the distribution function this cannot be completed analytically. A semi-analytic approach is used and the necessary integrals evaluated numerically. This is seen to be a generalization of previous treatments.

It is worthwhile mentioning that this approach could have been used on the other two cases in this model category, and the technique may have general mathematical applications. There is no experimental work available for direct comparison. The purpose of this chapter is twofold: to extend a previously proposed model and also to illustrate the scope of semi-analytic modelling. Other cases could be treated in a very similar manner and this is where the power of this particular approach lies.

Chapter 5 discusses, in a more general way, other models, appropriate boundary value problems and their solution. An aspect of the approach developed in Chapter 5 becomes apparent: concise formulations may suggest methods of solution; in the case of piezoelectric phonon scattering in an electric field it is seen that the problem can be reduced to that of a generalized adjoint diffusion equation with concentration dependent diffusivity and standard techniques applied. A formal solution to this particular problem is derived.

The other cases are discussed but no simple solutions seem to exist, mainly due to the difficulty of incorporating the initial condition. Numerical methods are applicable and if necessary could be used.

## §2. Future Research

The work in this thesis introduces the ideas of semi-analytical Boltzmann modelling and indicates some of the advantages of such an approach.

However, there are many important areas to be developed from the work detailed, which has provided an introduction to the topic of semi-analytic modelling.

On the practical side there is the solution of the various models that have not been attempted here. The inclusion of an electric field has caused mathematical problems and it would be most interesting to completely solve the the case of piezoelectric

phonon scattering in an electric field with first order phonon collision term $\{ L^{(1\,0)}_{p\,p} f_0 = 0 \}$ analytically and to compare it with the solution derived in the absence of an electric field. This is presently being undertaken. Once the piezoelectric phonon case is solved analytically it would also provide a starting point to analytically investigate the implications of the 'small w' or asymptotic approximation made in other chapters. The methods developed, and applied, in Chapter 4 could also be applied to the other cases. The elliptic problems generally do not seem amenable to analytic (or semi-analytic) approaches and numerical methods seem to be appropriate for this category of model. This is feasible as efficient software exists for such problems. If this was undertaken it would provide a useful test of the semi-analytic approximations and also measure the effect of including the second order phonon energy connection.

One aspect of the models that has not been carefully considered is the relative importance of the various scattering mechanisms although the non-polar optical phonon scattering is usually taken to be the dominant mechanism. It would be possible to derive equations to include all, or combinations of, the scattering mechanisms considered singly here. Again solution to all possible cases would be difficult but certain cases would be expected to succumb to analytic methods. There is also the relationship between the various boundary value problems to be determined; as was noted previously, although the operators correspond when the field tends to zero, the solutions do not. This was ascribed to the differing boundary value problems. It would

be interesting to impose boundary value problems on the problems such that the boundary value problems became identical when the field was zero, and then to check that the solutions were identical.

One area that could be developed in detail is that of perturbative expansions: the nearly isotropic approximation represents only one such expansion and others have been applied to the BTE, although not in the context of semiconductor device modelling. These could be tailored to suit the specialized needs of device modelling and knowledge already gained here about objects such as the distribution function could be incorporated; it is often of Gaussian nature for example and this could be used in a similar manner to that in the drifted Maxwellian.

Ideally, an expansion method that could be applied in more general circumstances is required; schemes could be developed that amalgamate the nearly isotropic approximation and the maximum anisotropy approximation [31] to give one general scheme. This could then be used to derive information on the distribution function when neither of these approximations was appropriate.

Included within the above would be to extend the treatment to take account of two dimensional effects. For example, numerical simulations of vertical bipolar transistors suggest that the majority of the current flow is one dimensional (and equivalent circuit models take account of this fact); this would

suggest that analytic treatments can treat the lateral current flow perturbatively and an expansion of the form:

$$f(x,y) = g(y) \ ( f_0 (x) + kf_1(x) )$$

may be appropriate. Again appropriate expansions for various situations could be developed but this would be expected to be a difficult exercise, as it could involve a large number of coupled equations.

A topic that was mentioned briefly but demands the majority of effort is that of quantum transport theory. Although quantum transport equations have been developed there has been little application of them to actual devices. A perturbative treatment (in some situations) at least would be appropriate as there may only be small deviation from the classical solution. Thus the development of a NIA to a quantum distribution could be of particular interest.

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