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Discontinuous Galerkin Methods for Boltzmann - Poisson Models of Electron Transport in Semiconductors

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Discontinuous Galerkin Methods for Boltzmann - Poisson Models of Electron Transport in Semiconductors

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Dedicated to my parents, María del Carmen Patricia Escalante López and Aureliano Morales Vargas.

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Discontinuous Galerkin Methods for Boltzmann - Poisson Models of Electron Transport in Semiconductors

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The work presented in this dissertation is related to several lines of research in the area of Discontinuous Galerkin (DG) Methods for computational electronic transport in semiconductor devices using Boltzmann - Poisson (BP) models.

The first line of research is the use of EPM related energy bands in a DG solver for BP where we consider a $n^+ - n - n^+$ diode problem, in order to increase the accuracy of the physical modeling of the energy band structure and its derivatives, via a spherical average of the EPM band structure and the spline interpolation of its derivatives, as these functions are involved in the collision mechanism, such as electron - phonon scattering in silicon, and transport via the electron group velocity. The balance of these two mechanisms

is the core of the modeling of electron transport in semiconductors by means of Boltzmann - Poisson. The more physically accurate values of the spherical average EPM energy band and its derivatives interpolated by splines give a quantitative difference in kinetic moments related to the energy band model, such as average velocity, energy, and particularly the current given by our numerical solver. This highlights the importance of band models and features such as anisotropy and derivative interpolation in the BP numerical modeling of electron transport via DG schemes.

The second line of research is related to the mathematical and numerical modeling of Reflective Boundary Conditions (BC) in 2D devices and their implementation in DG-BP schemes. We have studied the specular, diffusive and mixed reflection BC on the boundaries of the position domain of the device. We developed a numerical equivalent of the pointwise zero flux condition at the position domain insulating boundaries for the case of a more general mixed reflection with a momentum dependant specularity parameter $p(\vec{k})$. We obtain this numerical zero flux condition by formulating the general mixed reflection BC as the solution of the problem of finding a function and parameter that balance the incident and reflected microscopic probability flow at each point of the insulating boundary. We compared the influence of the different reflection BC cases in the computational prediction of moments after implementing numerical BC equivalent to the respective reflective BC. There are expected effects due to the inclusion of diffusive reflection boundary conditions over the moments of the probability density function and over the electric field

and potential, whose influence is not only restricted to the boundaries but actually to the whole domain. We observe in our simulations effects in kinetic moments of the inclusion of diffusion in the BC, such as the increase of the density close to the reflecting boundary, the decrease of the mean energy over the domain and the increase of the momentum x-component over the domain.

The third line of research is related to the development of positivity preserving DG schemes for BP semiconductor models. We pose the Boltzmann Equation for electron transport in curvilinear coordinates for the momentum. We consider the 1D diode problem with azimuthal symmetry, which is a 3D plus time problem. We choose for this problem the spherical coordinate system $\vec{p}(|\vec{p}|, \mu = cos\theta, \varphi)$, slightly different to the choice in previous DG solvers for BP, because its DG formulation gives simpler integrals involving just piecewise polynomial functions for both transport and collision terms. Applying the strategy of Zhang & Shu, [63], [64], Cheng, Gamba, Proft, [36], and Endeve et al. [65], we treat the collision operator as a source term, and find convex combinations of the transport and collision terms which guarantee the positivity of the cell average of our numerical probability density function at the next time step. The positivity of the numerical solution to the pdf in the whole domain is guaranteed by applying the limiters in [63], [64] that preserve the cell average but modify the slope of the piecewise linear solutions in order to make the function non - negative. In addition of the proofs of positivity preservation in the DG scheme, we prove the stability of the semi-discrete DG scheme under an entropy norm, using the dissipative properties of our colli-

sional operator given by its entropy inequalities. The entropy inequality we use depends on an exponential of the Hamiltonian rather than the Maxwellian associated just to the kinetic energy.

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Chapter 1

Introduction

1.1 Motivation

Boltzmann - Poisson (BP) is a system coupling a partial differential integral equation such as the Boltzmann Equation with the Poisson Equation. The Boltzmann equation models the transport and collisions of electronic particles in semiconductors by following the time evolution of the probability density function representing the electronic charges in the respective phase space. The Poisson Equation is necessary in the model to obtain the electric field which is not only external, since the charges create a self consistent electric field, therefore the latter is dependent on the charge density and a fixed doping background as well. The BP system is nonlinear due to the dependance of the electric field on the charge density. It is also nonlocal due to the collision scatterings in momentum space, which can be related to different physical phenomena, but which scatter a momentum vector into another one that can differ significantly.

The BP system has been traditionally used in the electrical engineering community to model electronic transport in semiconductor devices of different dimensionality in position space, such as diodes (1D), MOSFETs (2D), and

FinFETs (3D). The lowest possible phase space dimensionality for the 1D problem in position space is, under certain symmetry assumptions, 2D plus time. For 2D problems and higher, the dimensionality of the momentum space is 3D plus time. Therefore, the total dimensionality of the problems treated by BP spans from 3D plus time (the lowest dimensionality in total) to 6D plus time, for a full 3D device.

These dimensionalities explain why BP was traditionally treated numerically by Monte Carlo solvers (DSMC) in the electrical engineering community. However, Monte Carlo methods have by its own nature an unavoidable statistical noise, dependant on the number of particles used in the simulation, and have some issues related to the treatment of boundary conditions [34]. Deterministic methods to solve the BP system do not have this kind of statistical error, give a much finer resolution of the time evolution of the probability density function and its moments from its transient state to its steady state, and can incorporate boundary conditions in an easier fashion, for example, using DG methods [34]. The downside of deterministic numerical methods is, in principle, the computational cost associated to the full dimensionality of the phase space problem plus time. The overall objective of deterministic numerical methods for Boltzmann - Poisson, such as Discontinuous Galerkin (DG) Finite Element Methods (FEM), is to provide accurate results of the pdf and its moments, that agree with Monte Carlo solvers but which provide a much higher resolution of the physical quantities, and that provide them at a fractional computational time compared to Monte Carlo.

DG, our particular deterministic numerical method of choice for BP, is a finite element method that was originally motivated for the modeling of hyperbolic transport problems such as neutron transport [1]. DG captures in its numerics the essence of the physics of transport, by propagating the information in the numerical domain according to the direction in which this information is traveling, via the numerical fluxes, such as the upwind rule, for example. It conserves mass locally, and because the transport part considers the local interaction of next neighboring cells, it gives sparse systems that are generally block diagonal that are easily invertible. The trade off is the higher number of degrees of freedom when compared to continous finite element methods, since DG allows discontinuous basis functions for the representation of hyperbolic problems. DG is a method designed to represent the physics of transport in its numerics. Therefore, the phase space advection part of the Boltzmann Equation is perfectly captured by DG when solving our BP system. The other main component of the Boltzmann Equation, namely the collision term, can be incorporated as a right hand side source term in the DG method. This collision term is also the one that is more computationally expensive when solving BP with DG methods. Finally, the Poisson Equation can be solved given the charge density by a method such as Local DG, which is an adaptation of DG to solve elliptic problems, which will be described later in this document, but which has been studied in detail in references [1], [50].

1.2 Literature Review

The semi-classical Boltzmann description of electron transport in 3D semiconductor devices is an equation in six dimensions plus time when the system is not in steady state. For a 1-D device model, under azimuthal symmetry assumptions, the phase space dimensionality can be reduced to 3D plus time, this being the BP problem modeling transport in semiconductors with the lowest dimensionality. The heavy computational cost is the main reason why the Boltzmann - Poisson (BP) system had been traditionally solved numerically by means of Direct Simulation Monte Carlo (DSMC) methods [19]. However, after the pioneer work [20], in recent years, deterministic solvers to the BP system were proposed in [21], [22], [23], [24], [25], [26], [27]. These methods provide accurate results which, in general, agree well with those obtained from Monte Carlo (DSMC) simulations, often at a fractional computational time. Moreover, these type of solvers can resolve transient details for the electron probability density function f, which are difficult to compute with DSMC simulators. The initial methods proposed in [23], [24], [25], [26] using weighted essentially non-oscillatory (WENO) finite difference schemes to solve the Boltzmann-Poisson system, had the advantage that the scheme is relatively simple to code and very stable even on coarse meshes for solutions containing sharp gradient regions. However, a disadvantage of the WENO methods is that it requires smooth meshes to achieve high order accuracy, hence it is not very flexible for adaptive meshes.

Motivated by the easy *hp*-adaptivity and the simple communication

pattern of the discontinuous Galerkin (DG) methods for macroscopic (fluid level) models [28], [29], [30],[31], it was proposed in [32], [33] to implement a DG solver to the full Boltzmann equation, that is capable of capturing transients of the probability density function.

In the previous work [32], [33], the first DG solver for (2.8)-(4.17) was proposed, and some numerical calculations were shown for one and two-dimensional devices. In [34], the DG-LDG scheme for the Boltzmann-Poisson system was carefully formulated, and extensive numerical studies were performed to validate the calculations. Such scheme models electron transport along the conduction band for 1D diodes and 2D double gate MOSFET devices with the energy band $\varepsilon(\mathbf{k}) = \varepsilon(|\mathbf{k}|)$ given by the Kane band model (valid close to a local minimum) in which the relation between the energy ε and the wavevector norm $|\mathbf{k}|$ is given by the analytic formula, referred as the Kane Band Model,

$$\varepsilon\,(1 + \alpha\varepsilon) = \frac{\hbar^2|\mathbf{k}|^2}{2m^*}, \tag{1.1}$$

where m^* is the effective mass for the considered material, Silicon for the case of this work, and α is a non-parabolicity constant. This band model can be understood as a first order variation from the parabolic band model, given by the particular case $\alpha = 0$.

A DG scheme for full band BP models was proposed in [35], following the lines of the schemes in [32], [33], [34], generalizing the solver that uses the Kane non-parabolic band and formulating it to treat a possible full band case. A preliminary benchmark of numerical results, using isotropic band models

with a dependence just on the momentum norm, shows that the direct evaluation of the Dirac delta function can be avoided, and so an accurate high-order simulation with comparable computational cost to the analytic band cases is possible. It would be more difficult or even unpractical to produce the full band computation with other transport scheme. It is worth to notice that a high-order positivity-preserving DG scheme for linear Vlasov-Boltzmann transport equations, under the action of quadratically confined electrostatic potentials, independent of the electron distribution, has been developed in [36]. The authors there show that these DG schemes conserve mass and preserve the positivity of the solution without sacrificing accuracy. In addition, the standard semi-discrete schemes were studied showing stability and error estimates.

In all of the aforementioned deterministic solvers previous to [35], the energy-band function $\varepsilon(\mathbf{k})$ is given analytically, either by the parabolic band approximation or by the Kane non-parabolic band model. The analytical band makes use of the explicit dependence of the carrier energy on the quasimomentum, which significantly simplifies all expressions as well as implementation of these techniques in the collision operator. However, some physical details of the band structure are partly or totally ignored when using an analytic approximation, which hinders its application to transport of hot carriers in high-field phenomena (the so called hot electron transport) where the high anisotropy of the real band structure far from the conduction band minimum becomes important. Full band models, on the other hand, are able to provide an accurate physical description of the energy-band function, portraying this anisotropic

band structure far from a conduction band minimum.

One of the most commonly used methods to compute full bands is the empirical pseudopotential method (EPM). Such method gives a full band structure truncating the Fourier series in the k-space [37] for a crystal lattice potential model given as the sum of potentials due to individual atoms and associated electrons, with few parameters fitting empirical data such as optical gaps, absorption rates, etc, to finally compute the energy eigenvalues of the Schrödinger equation in Fourier space. A more detailed discussion of this method can be found in [37], [38]. While full band models, as the ones given by EPM, have been widely used in DSMC simulators [19], their inclusion in deterministic solvers for the transport Boltzmann Equation is more recent; on [40], [41], full band models have also been combined with spherical harmonic expansion methods used to solve the Boltzmann equation numerically. However, high order accuracy is not always achieved by spherical harmonic expansion methods when energies vary strongly and only a few terms of the expansion are usually employed [42]. In contrast, the simulations for the BP system developed in our line of work, as in [32], [34], do not involve any asymptotics and so are very accurate for hot electron transport regimes.

The type of DG methods to be discussed in this work, as was done in [34], belongs to a class of finite element methods originally devised to solve hyperbolic conservation laws containing only first order spatial derivatives, e.g. [43–47]. Using a piecewise polynomial space for both the test and trial functions in the spatial variables, and coupled with explicit and nonlinearly stable

high order Runge-Kutta time discretization, the DG method is a conservative scheme that has the advantage of flexibility for arbitrarily unstructured meshes, with a compact stencil, and with the ability to easily accommodate arbitrary *hp*-adaptivity. For more details about DG scheme for convection dominated problems, we refer to the review paper [48], later generalized to the Local DG (LDG) method to solve the convection diffusion equations [49] and elliptic equations [50].

1.3 Main Contributions

The main contributions of this dissertation lie in the fields of computational electronic transport and Discontinuous Galerkin Methods for Boltzmann - Poisson models. These contributions are:

- The incorporation of conduction energy band structures such as EPM (Empirical Pseudopotential Method) in Discontinuous Galerkin Methods for BP, via spherical averages of the EPM band structure, and spline interpolations of its derivatives, in order to provide these methods of a more physically accurate modeling of the electron group velocity and collision mechanisms such as electron - phonon scattering in the case of silicon semiconductors.

- The formulation of numerical boundary conditions modeling diffusive and general mixed reflection with a momentum dependant specularity probability $p(\vec{k})$ for Discontinuous Galerkin Methods in BP, which sat-

isfy the numerical equivalent of a mathematical zero flux condition at an insulating boundary, conserving the mass by balancing the incident and reflected probability flow in momentum space pointwise at this boundary. The computational implementation of these boundary conditions for our numerical method to model devices with a 2D geometry (with a respective 3D momentum space) such as a 2D bulk silicon diode and a double gated MOSFET.

- The development of positivity preserving Discontinuous Galerkin schemes for BP models of electron transport in curvilinear momentum coordinates, treating in the scheme the time dependant electric field given by the Poisson equation and the collision term related to electron - phonon scattering. In the case of the symmetric diode problem in semiconductors, with dimensionality of 3D plus time, the coordinate system chosen in momentum space is such that all the integrals related to the DG formulation depend only on simple polynomial functions, which gives a simpler description than the one related to spherical coordinate systems for the momentum used in previous DG solvers for BP. In addition of the proofs of preservation of positivity of the numerical solution after each time step, we present as well a proof of the stability of the semi-discrete DG scheme with respect to an entropy norm depending on the Hamiltonian.

1.4 Dissertation Outline

Chapter 2 provides an introduction to kinetic models for semiconductors such as the Boltzmann - Poisson system, and its formulation as a mathematical problem. We also give an overview of the mathematical properties of the electron-phonon collision operator for silicon semiconductors, as well as a description of the family of entropy inequalities that can be derived from the structure of this collision operator. We include in this chapter too a brief introduction to the physics associated to electrons in semiconductors. We finalize with a brief introduction to the Discontinuous Galerkin Finite Element Method, giving as an example the case of a transport equation in one dimension.

Chapter 3 formulates the Boltzmann equation using spherical coordinates for the electron momentum vector. It shows then the Runge-Kutta Discontinuous Galerkin (RK-DG) formulation of the Boltzmann - Poisson problem in momentum spherical coordinates. It then presents the use of EPM related energy band models, its spherical average and the spline interpolation used to approximate its partial derivatives to obtain the respective electron group velocity, and its computational implementation in the DG solver for BP. The respective numerical results of the incorporation of the EPM spherical average energy band in our DG-BP solver are presented.

Chapter 4 concerns the formulation of numerical boundary conditions to model in a Discontinous Galerkin setting the mixing of specular and diffusive reflection with a momentum dependant specularity probability $p(\vec{k})$. It

presents the mathematical formulation of the specular, diffusive, and general mixed reflection boundary conditions, where we emphasize the role of the zero flux condition in all of these cases by formulating these BC as the solutions to the problem of finding functions and parameters such that a pointwise zero flux condition is satisfied balancing the incident and reflected microscopic flow in momentum space. We present the formulation of the numerical equivalents of these reflection BC and the numerical equivalent of the pointwise zero flux condition as well. In particular, we introduce the numerical formulation of the general mixed reflection BC with momentum dependant specularity probability $p(\vec{k})$, and posing it as the problem of finding a function and parameter such that the respective reflection BC satisfies a pointwise numerical equivalent of the zero flux condition, we find the numerical version of the general mixed reflection BC with $p(\vec{k})$ under the assumption of a finite element space made of tensor products of position and momentum functions. We present at the end the results of numerical simulations implementing specular, diffusive, and general mixed reflection BC for a 2D bulk diode and a double gate MOSFET.

Chapter 5 is concerned with the development of DG schemes that preserve the positivity of the probability density function (which mathematically is non negative by definition) for the Boltzmann - Poisson model of semiconductor transport. We formulate the Boltzmann - Poisson system with the momentum in curvilinear coordinates, motivated by the physics and math of our model. We use the work of Zhang & Shu [63], [64], and Cheng, Gamba, Proft [36] for our problem, incorporating our electron - phonon collision term

as a source in the scheme, and considering the time and charge dependence of the electric field. We choose a particular spherical coordinate system for the momentum which is slightly different from the choice of previous DG deterministic solvers. It is more convenient since, when applied to the symmetric diode problem, it renders integrals related to the DG formulation which just involve polynomial or piecewise polynomial functions, which are simpler than for other coordinate choices for $\vec{k}$ in previous DG-BP schemes. We mainly study and present our results for the symmetric diode problem, 1D in position, 3D plus time in total. We present at the end a proof of stability of the semi-discrete DG scheme formulated under an entropy norm dependant on the Hamiltonian. As a corollary, for the particular case of a time independent potential, the decay of this entropy norm follows directly.

Finally, the conclusions of this work are summarized in the last chapter. We discuss as well our goals for future work.

Chapter 2

Preliminaries

The presented research concerns the mathematical and computational modelling of the physical phenomena of charge transport in semiconductor devices, by means of the numerical method known as Discontinuous Galerkin applied to the Boltzmann - Poisson system. Its possible applications are related to problems of computational design for the performances of nano-scale transistors, or the modelling of electronic devices such as diodes or MOSFETS.

We present an introduction to the basics needed to understand the physics, mathematics, and numerics related to our proposed work. We first present to the reader a brief review of kinetic theory and the Boltzmann Equation. Then, the Boltzmann - Poisson (BP) mathematical model for transport in semiconductors is introduced and explained, explaining in detail the mathematical properties of the collision operator. We present then the fundamentals of semiconductor physics related to electronic transport. After that, an introduction to the Discontinuous Galerkin (DG) method is presented, explaining its formulation for the basic case of a transport equation in one dimension.

2.1 The Boltzmann-Poisson Model for Semiconductors

2.1.1 Kinetic Theory and the Boltzmann Equation

The Boltzmann Equation is a mathematical model for systems of a large number of particles, often having an underlying Hamiltonian structure, related to the interaction through a long range, mean force field, but also being under the influence of short range forces, which are called collisional mechanisms. The description of a system with such a large number of particles is described in a more practical way by means of a particle density approach rather than following the individual positions and velocities of each one of all the particles of the system. We go over the concepts necessary for a description of the physical system in terms of a density in its phase space.

Definition 2.1.1. Probability Density Function *Let* $(\mathbf{x}, \mathbf{p}) \in \mathbf{R}^d \times \mathbf{R}^d$, $d = 1, 2, 3$, *be a point in the phase space for one of the particles of the system. We define as the* Probability Density Function (pdf) *the function* $f : \mathbf{R} \times \mathbf{R}^d \times \mathbf{R}^d \to \mathbf{R}^+$ *such that* $f(\mathrm{t}, \mathbf{x}, \mathbf{p})\, d\mathbf{x}\, d\mathbf{p}$ *is the probability of finding a particle at time* t *on the infinitesimal phase space element of volume* $d\mathbf{x}\, d\mathbf{p}$ *centered at the point* $(\mathbf{x}, \mathbf{p})$*, related to position* $\mathbf{x}$ *and momentum* $\mathbf{p}$*. That is, if* $P|_{\mathrm{t}} \{(\mathbf{x}, \mathbf{p}) \in B\}$ *is the probability at time* t *of a particle being in the phase-space region* B*,* $f(\mathrm{t}, \mathbf{x}_0, \mathbf{p}_0)$ *is defined as*

$$f(\mathrm{t}, \mathbf{x}_0, \mathbf{p}_0) = \lim_{(\Delta\mathbf{x}, \Delta\mathbf{p}) \to \vec{0}} \frac{P|_{\mathrm{t}} \{(\mathbf{x}, \mathbf{p}) \in B\}}{\int_B d\mathbf{x}\, d\mathbf{p}} \quad , \tag{2.1}$$

$$B = \{(\mathbf{x}, \mathbf{p}) : |\mathbf{x} - \mathbf{x}_0| < \Delta\mathbf{x}\,,\ |\mathbf{p} - \mathbf{p}_0| < \Delta\mathbf{p}\}\ , \tag{2.2}$$

$$P|_{\mathrm{t}} \{(\mathbf{x}, \mathbf{p}) \in B\} = \int_B f(\mathrm{t}, \mathbf{x}, \mathbf{p}) d\mathbf{x}\, d\mathbf{p}\,. \tag{2.3}$$

A Vlasov model for a system of particles provides a macroscopic description of its motion assuming their interaction is driven just by long range forces, considered in the Hamiltonian of the system, disregarding scattering of particles generated by short range forces,

$$\frac{df}{d\mathrm{t}} = \frac{\partial f}{\partial \mathrm{t}} + \frac{\partial f}{\partial \mathbf{x}} \cdot \dot{\mathbf{x}} + \frac{\partial f}{\partial \mathbf{p}} \cdot \dot{\mathbf{p}} = 0\,, \quad \dot{\mathbf{x}} = \mathbf{v}(\mathbf{p}), \quad \dot{\mathbf{p}} = \mathbf{F}(\mathbf{x}, \mathrm{t})\,. \tag{2.4}$$

It can be interpreted as an equation for the conservation of probability. As stated in [17], it only represents a useful model for a collision-less system, or for a time scale much shorter than the mean time between two consecutive scattering events.

A Boltzmann model for a system of particles, on the other hand, considers that the total rate of change of the probability density function (its total derivative) is due to collisional mechanisms

$$Q(f) = \frac{df}{d\mathrm{t}} = \frac{\partial f}{\partial \mathrm{t}} + \dot{\mathbf{x}} \cdot \frac{\partial f}{\partial \mathbf{x}} + \dot{\mathbf{p}} \cdot \frac{\partial f}{\partial \mathbf{p}}\,, \tag{2.5}$$

where the short range forces are represented in the collisional operator $Q(f)$. This collisional operator models instantaneous scatterings of particles from one state to another, in such a way that their momentum vector changes extremely fast, while the change of the position vector takes place slowly [17].

For a classical system of particles, under the Laws of Newtonian Mechanics, we have

$$\dot{\mathbf{x}} = \mathbf{v}(\mathbf{p}), \quad \dot{\mathbf{p}} = \mathbf{F}(\mathbf{x}, \mathrm{t}), \tag{2.6}$$

where the function $\mathbf{v}(\mathbf{p})$ models the velocity of the particle in terms of the momentum, and $\mathbf{F}(\mathbf{x}, \mathrm{t})$ gives the force over the particle on the position $\mathbf{x}$ at time t. For electron transport problems, under the quasi-electrostatic approximation, the force is due just to the electric field, that is, $\mathbf{F} = -q\mathbf{E}(\mathbf{x}, \mathrm{t})$.

We obtain then the **Boltzmann Equation** model for the pdf $f(\mathrm{t}, \mathbf{x}, \mathbf{p})$ representing our system of particles .

Definition 2.1.2. Boltzmann Equation

$$\frac{\partial f}{\partial \mathrm{t}} + \frac{\partial f}{\partial \mathbf{x}} \cdot \mathbf{v}(\mathbf{p}) + \frac{\partial f}{\partial \mathbf{p}} \cdot \mathbf{F}(\mathbf{x}, \mathrm{t}) = Q(f). \tag{2.7}$$

2.1.2 Introduction to the Boltzmann - Poisson system

The Boltzmann-Poisson (BP) system is a semi-classical model for electric charge transport in semiconductors. The BP system can be used to describe the hot electron transport in modern semiconductor devices at nanoscales. As stated in [17], this model describes the long range interactions over charge carriers and the statistical evolution of its states that includes an account of the quantum scattering events. The BP system treats charge carriers partly as classical particles by describing them by means of a time-dependent probability density function $f(\mathrm{t}, \mathbf{x}, \mathbf{k})$ over the phase space $(\mathbf{x}, \mathbf{k})$, and using a Boltzmann equation to model the time evolution of the associated probability density function in the phase space. The quantum nature of the carriers is considered in several terms of the Boltzmann equation. The quantum crystal wave-vector $\mathbf{k}$ is used as the momentum phase space vari-

able in the model. The model for the local velocity of the charge carriers is the group velocity $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})$ of its quantum mechanical wave function, related to the electronic energy band function $\varepsilon(\mathbf{k})$ of the considered semiconductor material. As usual, $\hbar$ is the Planck constant divided by 2π. The collision integral operator models the quantum scattering mechanisms acting over the charge carriers. The flow of charge carriers is induced by the force over the electron charge $-q$, which is assumed to be given by a mean electric field, $\mathbf{F}(\mathrm{t}, \mathbf{x}) = -q\,\mathbf{E}(\mathrm{t}, \mathbf{x})$. This effective electric field, modeled by the Poisson Equation, takes into account long range interactions made of both internal carrier self-consistent and external contributions, such as an applied potential (bias). Hence, time-dependent solutions of the the BP system contain all the information on the transient of the carrier distribution and the time evolution of the total electric field. A phenomenological derivation of the BP model can be found in [17].

Consequently, the semi-classical **Boltzmann - Poisson (BP) system** for electron transport along an energy band is given by the system

$$\frac{\partial f}{\partial \mathrm{t}} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\,\varepsilon(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar}\mathbf{E}(\mathrm{t}, \mathbf{x}) \cdot \nabla_{\mathbf{k}} f = Q(f)\,, \tag{2.8}$$

and

$$\nabla_{\mathbf{x}} \cdot [\epsilon_r(\mathbf{x})\,\nabla_{\mathbf{x}} V(\mathrm{t}, \mathbf{x})] = \frac{q}{\epsilon_0}\,[\rho(\mathrm{t}, \mathbf{x}) - N_D(\mathbf{x})]\,, \quad \mathbf{E}(\mathrm{t}, \mathbf{x}) = -\nabla_{\mathbf{x}} V(\mathrm{t}, \mathbf{x})\,, \tag{2.9}$$

where $f(\mathrm{t}, \mathbf{x}, \mathbf{k})$ represents the probability density function (*pdf*) of finding an electron being at the physical location $\mathbf{x}$ with momentum wave-vector $\mathbf{k}$ at

time t, $V(\mathbf{x})$ is the electric potential for the total charge, the associated mean electric field is the negative potential gradient, denoted by $\mathbf{E}(\mathbf{x}, \mathrm{t})$, and $\varepsilon(\mathbf{k})$ is the energy band function.

The collision integral operator $Q(f)$ describes the scattering over the electrons, where several quantum mechanisms can be taken into account. In the low density approximation, the collisional integral operator becomes linear in f, having the form

$$Q(f) = \int_{\Omega_{\mathbf{k}}} \left[S(\mathbf{k}', \mathbf{k}) f(\mathrm{t}, \mathbf{x}, \mathbf{k}') - S(\mathbf{k}, \mathbf{k}') f(\mathrm{t}, \mathbf{x}, \mathbf{k}) \right] d\mathbf{k}', \tag{2.10}$$

where $S(\mathbf{k}, \mathbf{k}')$ is the scattering kernel, representing non-local interactions of electrons with a background density distribution.

In the case of silicon, for example, one of the most important collision mechanisms are electron-phonon scatterings due to lattice vibrations of the crystal, which are modeled by acoustic (assumed elastic) and optical (non-elastic) non-polar modes, the latter with a single frequency ω_p, given by

$$\begin{aligned} S(\mathbf{k}, \mathbf{k}') &= (n_q + 1)\, K\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p) \\ &\quad + n_q\, K\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) - \hbar\omega_p) + K_0\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}))\,, \end{aligned} \tag{2.11}$$

with K, K_0 constants for silicon.

The symbol δ indicates the usual Dirac delta distribution corresponding to the well known Fermi's Golden Rule [18]. The constant n_q is related to the phonon occupation factor

$$\mathsf{n}_q = \left[\exp\left(\frac{\hbar\omega_p}{k_B T_L} \right) - 1 \right]^{-1},$$

where k_B is the Boltzmann constant and $T_L = 300K$ is the constant lattice temperature.

In the Poisson Eq. (4.17), the parameter ϵ_0 is the dielectric constant in a vacuum, $\epsilon_r(\mathbf{x})$ labels the relative dielectric function which depends on the material. $\rho(\mathrm{t}, \mathbf{x})$, the electron charge density, is given by the integral over the domain in the $\mathbf{k}$-space $\Omega_{\mathbf{k}}$

$$\rho(\mathrm{t}, \mathbf{x}) = \int_{\Omega_{\mathbf{k}}} f(\mathrm{t}, \mathbf{x}, \mathbf{k})\, d\mathbf{k}\,, \tag{2.12}$$

and $N_D(\mathbf{x})$ is the doping profile, representing an external fixed density of positive charge carriers.

The Boltzmann Eq. (2.8) can be generalized to more bands ε_i by replacing f with a vector array of pdf's f_i, and including the related scattering terms in the collisional operator. The associated BP systems of *pdf*'s would have the form

$$\frac{\partial f_i}{\partial \mathrm{t}} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\, \varepsilon_i \cdot \nabla_{\mathbf{x}} f_i + \frac{q_i}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f_i = \sum_j Q_{i,j}\,, \tag{2.13}$$

$$-\nabla_{\mathbf{x}} \cdot (\epsilon\, \nabla_{\mathbf{x}} V) = qN(\mathbf{x}) + \sum_i q_i \rho_i, \quad \mathbf{E} = -\nabla_{\mathbf{x}} V\,. \tag{2.14}$$

In this case, each $f_i(\mathrm{t}, \mathbf{x}, \mathbf{k})$ is the probability density function over the phase space $(\mathbf{x}, \mathbf{k})$ of a carrier in the i-th energy band/valley in position $\mathbf{x}$, with crystal momentum $\hbar\,\mathbf{k}$ at time t. The collision operators $Q_{i,j}(f_i, f_j)$ model i-th and j-th carrier recombinations, generation effects, or intra-band scatterings when $i = j$. $\mathbf{E}(\mathrm{t}, \mathbf{x})$ is the electric field, $\mathcal{E}_i(\mathbf{k})$ is the i-th energy band surface,

the i-th charge density $\rho_i(\mathrm{t}, \mathbf{x})$ is the integral over all possible $\mathbf{k}$-states of f_i, q_i are their respective electric charges, and $N(\mathbf{x})$ is the doping profile.

2.1.3 Mathematical Formulation of the Boltzmann-Poisson Problem

2.1.3.1 Classical Formulation of the BP IVP with BC for a single conduction band

We consider the probability density function (*pdf*) for electrons along a single conduction band, denoting it by $f(t, \mathbf{x}, \mathbf{k})$ We denote by $\Omega_{\mathbf{x}}$ the physical domain in the $\mathbf{x}$-space. To solve the Boltzmann Eq. (2.8) coupled with the Poisson Eq. (4.17) requires to assign an initial value for f and suitable boundary conditions both for f and the electric potential V. Following [17], we recall the *classical (strong) formulation of the initial value problem for the BP system with boundary conditions, for a pdf of electrons on a single conduction band*

Find $f : \mathbb{R}^+ \times \Omega_{\mathbf{x}} \times \Omega_{\mathbf{k}} \to \mathbb{R}, \quad f(\mathrm{t}, \mathbf{x}, \mathbf{k}) \geq 0$ and $V(t, \mathbf{x}) : \mathbb{R}^+ \times \Omega_{\mathbf{x}} \to \mathbb{R}$, such that the Boltzmann equation

$$\frac{\partial f}{\partial \mathrm{t}} + \frac{1}{\hbar} \nabla_{\mathbf{k}}\, \varepsilon(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar} \mathbf{E}(\mathrm{t}, \mathbf{x}) \cdot \nabla_{\mathbf{k}} f = Q(f)\,, \tag{2.15}$$

with the linear collision operator $Q(f)$, defined by

$$Q(f) = \int_{\Omega_{\mathbf{k}}} [S(\mathbf{k}', \mathbf{k}) f(\mathrm{t}, \mathbf{x}, \mathbf{k}') - S(\mathbf{k}, \mathbf{k}') f(\mathrm{t}, \mathbf{x}, \mathbf{k})]\, d\mathbf{k}'\,,$$

$$S(\mathbf{k}, \mathbf{k}') = (n_q{+}1)\, K\, \delta(\varepsilon(\mathbf{k}'){-}\varepsilon(\mathbf{k}){+}\hbar\omega_p){+}n_q\, K\, \delta(\varepsilon(\mathbf{k}'){-}\varepsilon(\mathbf{k}){-}\hbar\omega_p){+}K_0\, \delta(\varepsilon(\mathbf{k}'){-}\varepsilon(\mathbf{k}))\,,$$

and the Poisson equation

$$\nabla_{\mathbf{x}} \cdot [\epsilon_r(\mathbf{x})\, \nabla_{\mathbf{x}} V(\mathrm{t}, \mathbf{x})] = \frac{q}{\epsilon_0} [\rho(\mathrm{t}, \mathbf{x}) - N_D(\mathbf{x})]\,, \quad \mathbf{E}(\mathrm{t}, \mathbf{x}) = -\nabla_{\mathbf{x}} V(\mathrm{t}, \mathbf{x})\,, \tag{2.16}$$

subject to the initial condition

$$f(0, \mathbf{x}, \mathbf{k}) = f_0(\mathbf{x}, \mathbf{k}) \quad \forall\, (\mathbf{x}, \mathbf{k}) \in \Omega_{\mathbf{x}} \times \Omega_{\mathbf{k}},\, t = 0\,,$$

and suitable boundary conditions for f on $\partial\Omega_{\mathbf{x}} \times \Omega_{\mathbf{k}}$ and $\Omega_{\mathbf{k}} \times \partial\Omega_{\mathbf{x}}$, and for V on $\partial\Omega_{\mathbf{x}}$ are satisfied. The boundary $\partial\Omega_{\mathbf{x}}$ is usually split for the Poisson Equation in Dirichlet $\partial\Omega_{\mathbf{x}}^D$, Neumann $\partial\Omega_{\mathbf{x}}^N$, and Interface boundaries $\partial\Omega_{\mathbf{x}}^I$, such that $\partial\Omega_{\mathbf{x}} = \partial\Omega_{\mathbf{x}}^D \cup \partial\Omega_{\mathbf{x}}^N \cup \partial\Omega_{\mathbf{x}}^I$.

Examples of boundary conditions used for the Boltzmann Equation include [17]

- Charge neutrality [51], [26], [33], [34]

  $$f_{out}(\mathrm{t}, \mathbf{x}, \mathbf{k}) = \frac{N_D(\mathbf{x})\, f_{in}(\mathrm{t}, \mathbf{x}, \mathbf{k})}{\rho_{in}(\mathrm{t}, \mathbf{x})} \qquad \mathrm{t} \geq 0,\, x \in \partial\Omega_{\mathbf{x}}^D,\, \mathbf{k} \in \Omega_{\mathbf{k}}\,. \tag{2.17}$$

  This condition is usually employed at the device contacts (Dirichlet boundaries $\partial\Omega_{\mathbf{x}}^D$).

- Null $\mathbf{x}$-flux

  $$\mathbf{n}(\mathbf{x}) \cdot \nabla_{\mathbf{x}} f(\mathrm{t}, \mathbf{x}, \mathbf{k}) = 0 \qquad \mathrm{t} \geq 0, x \in \partial\Omega_{\mathbf{x}}^N,\, \mathbf{k} \in \Omega_{\mathbf{k}}, \tag{2.18}$$

  where $\mathbf{n}(\mathbf{x})$ is the normal to the surface $\partial\Omega_{\mathbf{x}}^N$ at the point $\mathbf{x}$. This condition is imposed on the part of the physical domain with an insulating layer (Neumann boundaries $\partial\Omega_{\mathbf{x}}^N$).

- Vanishing boundary conditions in the $\mathbf{k}$-space

$$f(\mathrm{t}, \mathbf{x}, \mathbf{k}) = 0 \qquad \mathrm{t} \geq 0,\, \mathbf{x} \in \Omega_{\mathbf{x}},\, \mathbf{k} \in \partial\Omega_{\mathbf{k}}. \tag{2.19}$$

  These conditions correspond to negligible densities for large energy values. We use these vanishing conditions for the Boltzmann Equation in our work. We will just mention that, if we had chosen $\Omega_{\mathbf{k}}$ as the first Brillouin zone, then periodic boundary conditions in the $\mathbf{k}$-space would be the correct physical conditions. However, it is difficult to apply these conditions on the complex shape of the boundary of a truncated octahedron, which is the shape of the first Brillouin zone for Silicon and Germanium crystals.

  Boundary conditions related to the Poisson Equation could be

- Applied potential (bias)

$$V(\mathrm{t}, \mathbf{x}) = V_0(\mathrm{t}, \mathbf{x}) \qquad \mathrm{t} \geq 0,\, \mathbf{x} \in \partial\Omega_{\mathbf{x}}^D\ . \tag{2.20}$$

  This condition is imposed where we have device contacts (Dirichlet boundaries).

- Neumann boundary conditions for the electric potential

$$\mathbf{n}(\mathbf{x}) \cdot \nabla_{\mathbf{x}} V(\mathrm{t}, \mathbf{x}) = 0 \qquad \mathrm{t} \geq 0\,, \mathbf{x} \in \partial\Omega_{\mathbf{x}}^N\,, \tag{2.21}$$

  where $\mathbf{n}(\mathbf{x})$ is the normal to the surface $\partial\Omega_{\mathbf{x}}^N$ at the point $\mathbf{x}$. This condition is imposed on the part of the physical domain with an insulating layer, which is a Neumann boundary.

It is important to mention that the contact boundaries $\partial\Omega_{\mathbf{x}}^{D}$ for the Boltzmann and Poisson equations must be the same.

2.1.4 Properties of the Boltzmann Linear Collision Operator for Electron Scattering in Silicon Semiconductors

We will study in this section the properties of the Linear Collision Operator for our problem of hot electron transport under a low density approximation regime

$$Q(f) = \int_{\Omega_{\mathbf{k}}} \left[S(\mathbf{k}', \mathbf{k}) f(\mathrm{t}, \mathbf{x}, \mathbf{k}') - S(\mathbf{k}, \mathbf{k}') f(\mathrm{t}, \mathbf{x}, \mathbf{k}) \right] d\mathbf{k}' \,, \tag{2.22}$$

$$S(\mathbf{k}, \mathbf{k}') = (n_q{+}1)\, K\, \delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})+\hbar\omega_p)+n_q\, K\, \delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})-\hbar\omega_p)+K_0\, \delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k}))\,.$$

As mentioned in the previous section, the scattering kernel $S(\mathbf{k}, \mathbf{k}')$ models electron - phonon collisions in silicon, which cause energy jumps of $\hbar\omega_p$ for optical electron-phonon scattering, and which are approximated as elastic for acoustic electron - phonon scattering.

2.1.4.1 Mass Conservation

The integral of the collision term over the momentum space is zero

$$\int_{\Omega_{\mathbf{k}}} Q(f) d\mathbf{k} = \int_{\Omega_{\mathbf{k}}} \int_{\Omega_{\mathbf{k}}} \left[S(\mathbf{k}', \mathbf{k}) f(\mathrm{t}, \mathbf{x}, \mathbf{k}') - S(\mathbf{k}, \mathbf{k}') f(\mathrm{t}, \mathbf{x}, \mathbf{k}) \right] d\mathbf{k}' d\mathbf{k} = 0\,. \tag{2.23}$$

This is an important property since we can use it to derive an equation of mass conservation. If we define the particle density ρ and the current $\mathbf{J}$ as

$$\rho(\mathbf{x},\mathrm{t}) = \int_{\Omega_\mathbf{k}} f(\mathbf{x},\mathbf{k},\mathrm{t})\, d\mathbf{k}, \tag{2.24}$$

$$\mathbf{J}(\mathbf{x},\mathrm{t}) = \int_{\Omega_\mathbf{k}} f(\mathbf{x},\mathbf{k},\mathrm{t})\, \frac{\nabla_\mathbf{k}\, \varepsilon(\mathbf{k})}{\hbar}\, d\mathbf{k}\,, \tag{2.25}$$

we have that

$$\begin{aligned} \frac{d\rho}{d\mathrm{t}} &= \frac{d}{d\mathrm{t}} \int_{\Omega_\mathbf{k}} f d\mathbf{k} = \int_{\Omega_\mathbf{k}} \frac{df}{d\mathrm{t}} d\mathbf{k} = \int_{\Omega_\mathbf{k}} Q(f) d\mathbf{k}, \\ \int_{\Omega_\mathbf{k}} Q(f) d\mathbf{k} &= \int_{\Omega_\mathbf{k}} \frac{\partial f}{\partial \mathrm{t}} d\mathbf{k} + \int_{\Omega_\mathbf{k}} \frac{\nabla_\mathbf{k}\, \varepsilon}{\hbar} \cdot \nabla_\mathbf{x} f d\mathbf{k} - \int_{\Omega_\mathbf{k}} \frac{q}{\hbar} \mathbf{E} \cdot \nabla_\mathbf{k} f d\mathbf{k}\,. \end{aligned}$$

The last term related to the electric field will vanish due to the either periodic, cut-off, or vanishing boundary conditions of f in $\partial\Omega_\mathbf{k}$ after applying the divergence theorem. Using the fact that the integral of the collision operator over the momentum space is zero we obtain our equation of mass conservation

$$\begin{aligned} \frac{d\rho}{d\mathrm{t}} &= \frac{\partial}{\partial \mathrm{t}} \int_{\Omega_\mathbf{k}} f d\mathbf{k} + \nabla_\mathbf{x} \cdot \int_{\Omega_\mathbf{k}} \frac{\nabla_\mathbf{k}\, \varepsilon}{\hbar} f d\mathbf{k} - \frac{q}{\hbar} \int_{\Omega_\mathbf{k}} \nabla_\mathbf{k} \cdot (f\mathbf{E}) d\mathbf{k} = \int_{\Omega_\mathbf{k}} Q(f) d\mathbf{k}, \\ \frac{d\rho}{d\mathrm{t}} &= \frac{\partial \rho(\mathbf{x},\mathrm{t})}{\partial \mathrm{t}} + \nabla_\mathbf{x} \cdot \mathbf{J}(\mathbf{x},\mathrm{t}) + 0 = \int_{\Omega_\mathbf{k}} Q(f) d\mathbf{k} = 0\,. \end{aligned} \tag{2.26}$$

2.1.4.2 Moments of the Boltzmann pdf

We introduce as well the following notation for the moment of the pdf for a function $g(\mathbf{x},\mathbf{k},t)$

$$\langle g \rangle\,(\mathbf{x},\mathrm{t}) = \int_{\Omega_\mathbf{k}} f(\mathbf{x},\mathbf{k},\mathrm{t})\, g(\mathbf{x},\mathbf{k},\mathrm{t})\, d\mathbf{k} = \langle f,\, g \rangle_{\mathbf{L}^2(\Omega_\mathbf{k})}\,. \tag{2.27}$$

Under this definition, we have the following mass, velocity and energy moments

$$\langle 1 \rangle = \int_{\Omega_{\mathbf{k}}} f(\mathbf{x}, \mathbf{k}, \mathrm{t}) \cdot 1 \, d\mathbf{k} = \rho(\mathbf{x}, \mathrm{t}), \tag{2.28}$$

$$\langle \mathbf{v} \rangle = \int_{\Omega_{\mathbf{k}}} f(\mathbf{x}, \mathbf{k}, \mathrm{t}) \, \frac{\nabla_{\mathbf{k}} \, \varepsilon(\mathbf{k})}{\hbar} \, d\mathbf{k} = \mathbf{J}(\mathbf{x}, \mathrm{t}), \tag{2.29}$$

$$\langle \varepsilon \rangle = \int_{\Omega_{\mathbf{k}}} f(\mathbf{x}, \mathbf{k}, \mathrm{t}) \, \varepsilon(\mathbf{k}) \, d\mathbf{k} = \langle f, \, \varepsilon \rangle_{\mathbf{L}^2(\Omega_{\mathbf{k}})} \, . \tag{2.30}$$

They are analogous to the zeroth, first, and second moments about the origin, being proportional to them for the case of a parabolic band model $\varepsilon(\mathbf{k}) = \hbar^2 \mathbf{k}^2 / 2m^*$, for which the velocity is then $\mathbf{v}(\mathbf{k}) = \hbar \mathbf{k} / m^*$.

We will omit the subscript $\mathbf{L}^2(\Omega_{\mathbf{k}})$ from our notation for the inner product. If needed, we will clarify in which space the inner product is taken in the subsequent development of the thesis.

2.1.4.3 Collision Operator Structure & Detailed Balance Principle

We will study in this section the structure of our linear collision operator for electron - phonon collisions in silicon. First, we notice that

$$\begin{aligned}
Q(f) &= \int_{\Omega_{\mathbf{k}}} \left[S(\mathbf{k}',\mathbf{k})f(\mathrm{t},\mathbf{x},\mathbf{k}') - S(\mathbf{k},\mathbf{k}')f(\mathrm{t},\mathbf{x},\mathbf{k})\right] d\mathbf{k}' = \langle S(\mathbf{k}',\mathbf{k}), f'\rangle - \langle S(\mathbf{k},\mathbf{k}'), f\rangle \\
&= \langle (n_q+1)\, K\, \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') + \hbar\omega_p) + n_q\, K\, \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') - \hbar\omega_p), f'\rangle \\
&- \langle (n_q+1)\, K\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p) + n_q\, K\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) - \hbar\omega_p), f\rangle \\
&+ \langle K_0\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})), f' - f\rangle \\
&= K\, \langle \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') + \hbar\omega_p), (n_q+1)f' - n_q f\rangle \\
&- K\, \langle \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p), (n_q+1)f - n_q f'\rangle \\
&+ K_0\, \langle\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})), f' - f\rangle\ .
\end{aligned}$$

We remember that the phonon distribution follows the Bose-Einstein statistics, $n_q = \left[\exp\left(\frac{\hbar\omega_p}{k_B T_L}\right) - 1\right]^{-1}$, therefore we have that

$$\frac{n_q+1}{n_q} = n_q^{-1} + 1 = \exp\left(\frac{\hbar\omega_p}{k_B T_L}\right). \tag{2.31}$$

The Collision Operator acting on f can be written then as

$$\begin{aligned}
Q(f) &= K n_q \left\langle \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') + \hbar\omega_p), e^{\frac{\hbar\omega_p}{k_B T_L}} f' - f \right\rangle \\
&- K n_q \left\langle \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p), e^{\frac{\hbar\omega_p}{k_B T_L}} f - f' \right\rangle \\
&+ K_0\, \langle\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})), f' - f\rangle\ .
\end{aligned}$$

We observe by means of this structure of the collision operator that the

energy dependent Maxwellian

$$M(\mathbf{k}) = e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}} = M(\varepsilon(\mathbf{k})) \tag{2.32}$$

is an equilibrium distribution in the Kernel of our collision operator, as

$$\begin{aligned} Q\left(e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}}\right) &= K n_q \left\langle \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') + \hbar\omega_p),\, e^{\frac{\hbar\omega_p}{k_B T_L}} e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} - e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}} \right\rangle \\ &- K n_q \left\langle \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p),\, e^{\frac{\hbar\omega_p}{k_B T_L}} e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}} - e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} \right\rangle \\ &+ K_0 \left\langle \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})),\, e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} - e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}} \right\rangle = 0\,, \end{aligned}$$

since each of these terms vanishes individually by the shift in energies due to the Dirac deltas.

Moreover, the structure of this collision operator is related to the more general Detailed Balance Principle. We have that

$$S(\mathbf{k},\mathbf{k}') = n_q\, K \left[e^{\frac{\hbar\omega_p}{k_B T_L}} \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p) + \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) - \hbar\omega_p) \right] + K_0\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}))\,.$$

Using the formula above, we have then that

$$\begin{aligned} S(\mathbf{k},\mathbf{k}') e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}} &= n_q\, K \left[e^{\frac{\hbar\omega_p}{k_B T_L}} \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) + \hbar\omega_p) + \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) - \hbar\omega_p) \right] e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}} \\ &+ K_0\, \delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k})) e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}}\,, \end{aligned}$$

and

$$\begin{aligned} S(\mathbf{k}',\mathbf{k}) e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} &= n_q\, K \left[e^{\frac{\hbar\omega_p}{k_B T_L}} \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') + \hbar\omega_p) + \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') - \hbar\omega_p) \right] e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} \\ &+ K_0\, \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}')) e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}}\,. \end{aligned}$$

Therefore, we have that

$$
\begin{aligned}
& S(\mathbf{k}',\mathbf{k})e^{-\frac{\varepsilon(\mathbf{k}')}{k_BT_L}} - S(\mathbf{k},\mathbf{k}')e^{-\frac{\varepsilon(\mathbf{k})}{k_BT_L}} = \\
& Kn_q\left[\delta(\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}')+\hbar\omega_p)\left(e^{\frac{\hbar\omega_p-\varepsilon(\mathbf{k}')}{k_BT_L}} - e^{-\frac{\varepsilon(\mathbf{k})}{k_BT_L}}\right)\right] \\
- \quad & Kn_q\left[\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})+\hbar\omega_p)\left(e^{\frac{\hbar\omega_p-\varepsilon(\mathbf{k})}{k_BT_L}} - e^{-\frac{\varepsilon(\mathbf{k}')}{k_BT_L}}\right)\right] \\
+ \quad & K_0\,\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k}))\left(e^{-\frac{\varepsilon(\mathbf{k}')}{k_BT_L}} - e^{-\frac{\varepsilon(\mathbf{k})}{k_BT_L}}\right),
\end{aligned}
$$

and we can conclude that there is a Detailed Balance Principle satisfied by our particular scattering, but distributionally, since

$$
\begin{aligned}
& \left\langle S(\mathbf{k}',\mathbf{k})e^{-\frac{\varepsilon(\mathbf{k}')}{k_BT_L}} - S(\mathbf{k},\mathbf{k}')e^{-\frac{\varepsilon(\mathbf{k})}{k_BT_L}},\, g\right\rangle = \\
& \left\langle Kn_q\left[\delta(\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}')+\hbar\omega_p)\left(e^{\frac{\hbar\omega_p-\varepsilon(\mathbf{k}')}{k_BT_L}} - e^{-\frac{\varepsilon(\mathbf{k})}{k_BT_L}}\right)\right],\, g\right\rangle \\
- \quad & \left\langle Kn_q\left[\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})+\hbar\omega_p)\left(e^{\frac{\hbar\omega_p-\varepsilon(\mathbf{k})}{k_BT_L}} - e^{-\frac{\varepsilon(\mathbf{k}')}{k_BT_L}}\right)\right],\, g\right\rangle \\
+ \quad & \left\langle K_0\,\delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k}))\left(e^{-\frac{\varepsilon(\mathbf{k}')}{k_BT_L}} - e^{-\frac{\varepsilon(\mathbf{k})}{k_BT_L}}\right),\, g\right\rangle \;=\; 0\,,
\end{aligned}
$$

as each of the terms above vanishes individually on a distributional sense. Therefore, the following term operates as a zero distribution,

$$
S(\mathbf{k}',\mathbf{k})e^{-\frac{\varepsilon(\mathbf{k}')}{k_BT_L}} - S(\mathbf{k},\mathbf{k}')e^{-\frac{\varepsilon(\mathbf{k})}{k_BT_L}} = 0\,. \tag{2.33}
$$

We obtain then a Detailed Balance Principle in a distributional sense

$$
S(\mathbf{k}',\mathbf{k})e^{-\frac{\varepsilon(\mathbf{k}')}{k_BT_L}} = S(\mathbf{k},\mathbf{k}')e^{-\frac{\varepsilon(\mathbf{k})}{k_BT_L}}\,, \tag{2.34}
$$

which defines the following symmetric distribution $\sigma(\mathbf{k}',\mathbf{k})$ below

$$
\sigma(\mathbf{k}',\mathbf{k}) = S(\mathbf{k}',\mathbf{k})e^{-\frac{\varepsilon(\mathbf{k}')}{k_BT_L}} = S(\mathbf{k},\mathbf{k}')e^{-\frac{\varepsilon(\mathbf{k})}{k_BT_L}} = \sigma(\mathbf{k},\mathbf{k}')\,. \tag{2.35}
$$

This Detailed Balance Principle is a distributional yet local equality showing that the energy dependent Maxwellian is in the kernel of the collision operator. We can write the collision operator in the following way then,

$$\begin{aligned} Q(f) &= \int_{\Omega_{\mathbf{k}}} \left[S(\mathbf{k}',\mathbf{k}) e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} f(\mathrm{t},\mathbf{x},\mathbf{k}') e^{\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} - S(\mathbf{k},\mathbf{k}') e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}} f(\mathrm{t},\mathbf{x},\mathbf{k}) e^{\frac{\varepsilon(\mathbf{k})}{k_B T_L}} \right] d\mathbf{k}' \\ &= \int_{\Omega_{\mathbf{k}}} S(\mathbf{k}',\mathbf{k}) e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} \left(\frac{f(\mathrm{t},\mathbf{x},\mathbf{k}')}{e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}}} - \frac{f(\mathrm{t},\mathbf{x},\mathbf{k})}{e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}}} \right) d\mathbf{k}' \qquad (2.36) \\ &= \left\langle \sigma(\mathbf{k}',\mathbf{k}),\ \frac{f'}{M'} - \frac{f}{M} \right\rangle , \qquad (2.37) \end{aligned}$$

with

$$\begin{aligned} &\sigma(\mathbf{k}',\mathbf{k}) = \sigma(\mathbf{k},\mathbf{k}') = e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} \left[K_0\, \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}')) + \right. \qquad (2.38) \\ &\left. n_q\, K \left(e^{\frac{\hbar\omega_p}{k_B T_L}} \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') + \hbar\omega_p) + \ \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') - \hbar\omega_p) \right) \right] . \end{aligned}$$

2.1.4.4 Collision Invariants, Dissipative property, Entropy Inequalities, Energy & Momentum Transfer Theorems

We obtain the following identity using symmetry arguments and the Detailed Balance Principle

$$\begin{aligned} \int_{\Omega_{\mathbf{k}}} Q(f) g d\mathbf{k} &= \int_{\Omega_{\mathbf{k}}} \int_{\Omega_{\mathbf{k}}} S(\mathbf{k}',\mathbf{k}) e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} \left(\frac{f(\mathrm{t},\mathbf{x},\mathbf{k}')}{e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}}} - \frac{f(\mathrm{t},\mathbf{x},\mathbf{k})}{e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}}} \right) g(\mathbf{x},\mathbf{k},\mathrm{t}) d\mathbf{k}' d\mathbf{k} \\ &= \int_{\Omega_{\mathbf{k}}} \int_{\Omega_{\mathbf{k}}} S(\mathbf{k},\mathbf{k}') e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}} \left(\frac{f(\mathrm{t},\mathbf{x},\mathbf{k})}{e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}}} - \frac{f(\mathrm{t},\mathbf{x},\mathbf{k}')}{e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}}} \right) g(\mathbf{x},\mathbf{k}',\mathrm{t}) d\mathbf{k}' d\mathbf{k} \\ &= \int_{\Omega_{\mathbf{k}}} \int_{\Omega_{\mathbf{k}}} S(\mathbf{k}',\mathbf{k}) e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} \left(\frac{f(\mathrm{t},\mathbf{x},\mathbf{k})}{e^{-\frac{\varepsilon(\mathbf{k})}{k_B T_L}}} - \frac{f(\mathrm{t},\mathbf{x},\mathbf{k}')}{e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}}} \right) g(\mathbf{x},\mathbf{k}',\mathrm{t}) d\mathbf{k}' d\mathbf{k} \\ &= \int_{\Omega_{\mathbf{k}}} \int_{\Omega_{\mathbf{k}}} \frac{\sigma(\mathbf{k}',\mathbf{k})}{2} \left(\frac{f'}{M(\mathbf{k}')} - \frac{f}{M(\mathbf{k})} \right) \left(g(\mathbf{x},\mathbf{k},\mathrm{t}) - g(\mathbf{x},\mathbf{k}',\mathrm{t}) \right) d\mathbf{k}' d\mathbf{k} . \end{aligned}$$

We can derive so called entropy inequalities for collision operators like ours when considering functions $g\left(f(\mathbf{x},\mathbf{k},\mathrm{t})/M(\mathbf{k})\right)$ that have a monotone dependence on their argument. That is, since

$$\begin{aligned}\int_{\Omega_{\mathbf{k}}} Q(f)\, g\, d\mathbf{k} &= -\frac{1}{2}\int_{\Omega_{\mathbf{k}}}\int_{\Omega_{\mathbf{k}}} S(\mathbf{k}',\mathbf{k}) e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}} \left(\frac{f'}{M'}-\frac{f}{M}\right)(g'-g)\, d\mathbf{k}' d\mathbf{k} \\ &= -\frac{1}{2}\int_{\Omega_{\mathbf{k}}}\int_{\Omega_{\mathbf{k}}} \sigma(\mathbf{k}',\mathbf{k}) \left(\frac{f'}{M'}-\frac{f}{M}\right)(g'-g)\, d\mathbf{k}' d\mathbf{k}\,, \quad (2.39)\end{aligned}$$

and since $S(\mathbf{k},\mathbf{k}') = (n_q+1)\, K\, \delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})+\hbar\omega_p) + n_q\, K\, \delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k})-\hbar\omega_p) + K_0\, \delta(\varepsilon(\mathbf{k}')-\varepsilon(\mathbf{k}))$ is a sum of positive point mass distributions, we have that, if $g\left(\frac{f}{M}\right)$ is monotone increasing ,

$$\int_{\Omega_{\mathbf{k}}} Q(f) g\left(\frac{f}{M}\right) d\mathbf{k} = \int_{\Omega_{\mathbf{k}}}\int_{\Omega_{\mathbf{k}}} \frac{\sigma(\mathbf{k}',\mathbf{k})}{2}\left(\frac{f'}{M'}-\frac{f}{M}\right)\left(g\left(\frac{f}{M}\right)-g\left(\frac{f'}{M'}\right)\right) d\mathbf{k}' d\mathbf{k} \le 0.$$

Collision Invariants are the physical observable quantities conserved by $Q(f)$, that is, functions $g(\mathbf{x},\mathbf{k},\mathrm{t})$ such that

$$0 = \int_{\Omega_{\mathbf{k}}} Q(f)\, g(\mathbf{x},\mathbf{k},\mathrm{t})\, d\mathbf{k} = \langle Q(f),\, g\rangle\ . \quad (2.40)$$

The only family of functions that are both monotone decreasing and monotone increasing at the same time are the family of constant functions $g = C, \quad C \in \mathbf{R}$, for which

$$0 \le \int_{\Omega_{\mathbf{k}}} Q(f)\cdot C\, d\mathbf{k} = C\int_{\Omega_{\mathbf{k}}} Q(f)\, d\mathbf{k} \le 0\,. \quad (2.41)$$

The conservation of mass follows from choosing the element $g = 1$ in the family of collision invariant constant functions, as

$$\frac{d\rho}{d\mathrm{t}} = \frac{\partial\rho}{\partial\mathrm{t}} + \nabla_{\mathbf{x}}\cdot\mathbf{J} = \int_{\Omega_{\mathbf{k}}} Q(f)\cdot 1\, d\mathbf{k} = 0\,. \quad (2.42)$$

The energy $\varepsilon(\mathbf{k})$ or the velocity $\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})/\hbar$ are not monotone functions of the argument f/M. However, we can obtain transfer of energy & momentum conservation theorems using the collision structure studied before. We can derive the following Kinetic Energy-Work Theorem, keeping in mind that integrals at the boundary $\partial\Omega_{\mathbf{k}}$ will vanish due to the boundary conditions of f at $\partial\Omega_{\mathbf{k}}$,

$$\begin{aligned}
\int_{\Omega_{\mathbf{k}}} Q(f)\,\varepsilon(\mathbf{k})d\mathbf{k} &= \int_{\Omega_{\mathbf{k}}} \left[\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} f \cdot \frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar} - \frac{q\mathbf{E}}{\hbar}\cdot\nabla_{\mathbf{k}} f\right] \varepsilon(\mathbf{k})d\mathbf{k} \\
\int_{\Omega_{\mathbf{k}}} Q(f)\,\varepsilon(\mathbf{k})d\mathbf{k} &= \frac{\partial}{\partial \mathrm{t}}\int_{\Omega_{\mathbf{k}}} f\,\varepsilon(\mathbf{k})d\mathbf{k} + \nabla_{\mathbf{x}}\cdot\int_{\Omega_{\mathbf{k}}} f\,\frac{\varepsilon(\mathbf{k})\nabla_{\mathbf{k}}\varepsilon}{\hbar}d\mathbf{k} + q\mathbf{E}\cdot\int_{\Omega_{\mathbf{k}}} f\,\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\,d\mathbf{k} \\
\int_{\Omega_{\mathbf{k}}} Q(f)\,\varepsilon(\mathbf{k})d\mathbf{k} &= \frac{\partial\,\langle\varepsilon\rangle}{\partial \mathrm{t}} + \nabla_{\mathbf{x}}\cdot\left\langle\frac{\varepsilon\nabla_{\mathbf{k}}\varepsilon}{\hbar}\right\rangle + q\mathbf{E}\cdot\mathbf{J}(\mathbf{x},t)\,, \qquad (2.43) \\
\int_{\Omega_{\mathbf{k}}} Q(f)\,\varepsilon(\mathbf{k})d\mathbf{k} &= \int_{\Omega_{\mathbf{k}}}\int_{\Omega_{\mathbf{k}}} \frac{S(\mathbf{k}',\mathbf{k})e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}}}{2}\left(\frac{f'}{M'} - \frac{f}{M}\right)(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}'))\,d\mathbf{k}'d\mathbf{k}\,.
\end{aligned}$$

We can derive as well a Conservation Theorem of Momentum Transfer

$$\begin{aligned}
\int_{\Omega_{\mathbf{k}}} Q(f)\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}d\mathbf{k} &= \frac{\partial}{\partial \mathrm{t}}\int_{\Omega_{\mathbf{k}}} f\,\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}d\mathbf{k} + \nabla_{\mathbf{x}}\cdot\int_{\Omega_{\mathbf{k}}} f\,\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}d\mathbf{k} - q\int_{\Omega_{\mathbf{k}}}\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\frac{\nabla_{\mathbf{k}}\cdot f\mathbf{E}}{\hbar}\,d\mathbf{k} \\
\int_{\Omega_{\mathbf{k}}} Q(f)\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}d\mathbf{k} &= \frac{\partial\mathbf{J}}{\partial \mathrm{t}} + \nabla_{\mathbf{x}}\cdot\left\langle\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\right\rangle + q\mathbf{E}\int_{\Omega_{\mathbf{k}}} f\frac{\nabla^2_{\mathbf{k}}\varepsilon}{\hbar^2}\,d\mathbf{k} = \frac{d\mathbf{J}}{d\mathrm{t}} \qquad (2.44) \\
\int_{\Omega_{\mathbf{k}}} Q(f)\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}d\mathbf{k} &= \int_{\Omega_{\mathbf{k}}}\int_{\Omega_{\mathbf{k}}} \frac{S(\mathbf{k}',\mathbf{k})e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}}}{2}\left(\frac{f'}{M'} - \frac{f}{M}\right)\left(\frac{\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})}{\hbar} - \frac{\nabla_{\mathbf{k}'}\varepsilon(\mathbf{k}')}{\hbar}\right)d\mathbf{k}'d\mathbf{k}\,.
\end{aligned}$$

For example, in the case of a parabolic band model $\varepsilon(\mathbf{k}) = \hbar^2\mathbf{k}^2/2m^*$, we have that $\int_{\Omega_{\mathbf{k}}} f\,\nabla^2_{\mathbf{k}}\varepsilon/\hbar^2\,d\mathbf{k} = \int_{\Omega_{\mathbf{k}}} f\,3/m^*\,d\mathbf{k} = 3\,\rho/m^*$, as this average is a measure of the curvature of the energy band in the momentum space.

Back to the structure of our collision operator

$$\int_{\Omega_{\mathbf{k}}} Q(f)\, g\, d\mathbf{k} \;=\; -\int_{\Omega_{\mathbf{k}}}\int_{\Omega_{\mathbf{k}}} \frac{S(\mathbf{k}',\mathbf{k})e^{-\frac{\varepsilon(\mathbf{k}')}{k_B T_L}}}{2}\left(\frac{f'}{M'}-\frac{f}{M}\right)(g'-g)\, d\mathbf{k}' d\mathbf{k}\,,$$

we recognize that our collision operator has a family of entropy functionals, associated to the family of functions $g(f/M)$ monotone in the argument f/M, from which a family of entropy inequalities can be derived.

There are two monotone functions g of interest. The first one is $g\,(f/M) = f/M$. In this case, we have

$$\int_{\Omega_{\mathbf{k}}} Q(f)\,\frac{f}{M}\, d\mathbf{k} \;=\; -\int_{\Omega_{\mathbf{k}}}\int_{\Omega_{\mathbf{k}}} \frac{\sigma(\mathbf{k}',\mathbf{k})}{2}\left(\frac{f'}{M'}-\frac{f}{M}\right)^2 d\mathbf{k}' d\mathbf{k} \le 0. \quad (2.45)$$

This entropy inequality is important because it defines a norm of f in which our pdf is decreasing

$$\begin{aligned}
0 \;&\ge\; \int_{\Omega_{\mathbf{k}}} Q(f)\,\frac{f}{M}\, d\mathbf{k} = \int_{\Omega_{\mathbf{k}}} \frac{\partial f}{\partial \mathrm{t}}\frac{f}{M} d\mathbf{k} + \int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{x}} f\cdot\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\frac{f}{M}\, d\mathbf{k} - \frac{q}{\hbar}\int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{k}} f\cdot\mathbf{E}\frac{f}{M}\, d\mathbf{k}\\
0 \;&\ge\; \int_{\Omega_{\mathbf{k}}} \frac{df}{d\mathrm{t}}\frac{f}{M} d\mathbf{k} = \frac{1}{2}\left[\frac{\partial}{\partial \mathrm{t}}\int_{\Omega_{\mathbf{k}}}\frac{f^2}{M} d\mathbf{k} + \nabla_{\mathbf{x}}\cdot\int_{\Omega_{\mathbf{k}}}\frac{f^2}{M}\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\, d\mathbf{k} - \frac{q}{\hbar}\mathbf{E}\cdot\int_{\Omega_{\mathbf{k}}}\frac{\nabla_{\mathbf{k}} f^2}{M}\, d\mathbf{k}\right]\\
0 \;&\ge\; \int_{\Omega_{\mathbf{k}}} \frac{df}{d\mathrm{t}}\frac{f}{M} d\mathbf{k} = \frac{1}{2}\int_{\Omega_{\mathbf{k}}}\frac{df^2}{d\mathrm{t}} M^{-1} d\mathbf{k}\,. \qquad (2.46)
\end{aligned}$$

This entropy inequality defines a natural Maxwellian-weighted $\mathbf{L}^2$-norm in $\mathbf{k}$ in which f is decreasing. Therefore, we define the following Maxwellian-weighted dot product

$$\langle f, g\rangle_{\mathbf{B}^2(\Omega_{\mathbf{k}})} = \int_{\Omega_{\mathbf{k}}} f\, g\, M^{-1} d\mathbf{k}\,, \qquad (2.47)$$

which defines then the following Maxwellian-weighted $\mathbf{L}^2$-norm

$$\|f\|_{\mathbf{B}^2(\Omega_{\mathbf{k}})} = \left(\int_{\Omega_{\mathbf{k}}}\frac{f^2}{M}\, d\mathbf{k}\right)^{1/2}. \qquad (2.48)$$

Using this notation, we can express the previously found entropy inequality for $g = f/M$ as

$$0 \;\geq\; \left\langle f, \frac{df}{d\mathrm{t}} \right\rangle_{\mathbf{B}^2(\Omega_{\mathbf{k}})} = \frac{1}{2}\frac{\partial}{\partial \mathrm{t}} \|f\|^2_{\mathbf{B}^2(\Omega_{\mathbf{k}})} + \frac{1}{2}\nabla_{\mathbf{x}} \cdot \left\langle f^2 \,,\, \frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar} \right\rangle_{\mathbf{B}^2(\Omega_{\mathbf{k}})} - \frac{q}{\hbar}\mathbf{E} \cdot \langle f, \nabla_{\mathbf{k}} f \rangle_{\mathbf{B}^2(\Omega_{\mathbf{k}})} \,.$$

The second monotone function to be considered is $g\,(f/M) = \log\,(f/M)$. We have that

$$\int_{\Omega_{\mathbf{k}}} Q(f)\, \log \frac{f}{M}\, d\mathbf{k} = -\int_{\Omega_{\mathbf{k}}}\int_{\Omega_{\mathbf{k}}} \frac{\sigma(\mathbf{k}', \mathbf{k})}{2} \left(\frac{f'}{M'} - \frac{f}{M}\right)\left(\log \frac{f'}{M'} - \log \frac{f}{M}\right) d\mathbf{k}' d\mathbf{k} \leq 0\,.$$

We can derive then the following associated entropy inequality for f

$$0 \;\geq\; \int_{\Omega_{\mathbf{k}}} \frac{\partial f}{\partial \mathrm{t}} \log \frac{f}{M} d\mathbf{k} + \int_{\Omega_{\mathbf{k}}} \frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar} \cdot \nabla_{\mathbf{x}} f \log \frac{f}{M}\, d\mathbf{k} - \frac{q}{\hbar}\mathbf{E} \cdot \int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{k}} f \log \frac{f}{M}\, d\mathbf{k}\,.$$

In order to express this entropy inequality in a clearer way, we notice that

$$\log \frac{f}{M}\partial f = \log f \partial f - \log M \partial f = \partial\left[f\,(\log f - 1)\right] + \frac{\varepsilon(\mathbf{k})}{k_B T_L}\partial f\,, \qquad (2.49)$$

so, if we define the following relative local entropy as

$$H = f\left(\log f - 1 + \frac{\varepsilon(\mathbf{k})}{k_B T_L}\right) = f\,(\log f - 1 - \log M) = f \log \frac{f}{Me}\,, \qquad (2.50)$$

then

$$\partial H = \log \frac{f}{M}\partial f + f\frac{\partial\, \varepsilon(\mathbf{k})}{k_B T_L}\,. \qquad (2.51)$$

Therefore, we can express our entropy inequality as

$$0 \;\geq\; \int_{\Omega_{\mathbf{k}}} \frac{\partial H}{\partial \mathrm{t}} d\mathbf{k} + \int_{\Omega_{\mathbf{k}}} \frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar} \cdot \nabla_{\mathbf{x}} H\, d\mathbf{k} - \frac{q}{\hbar}\mathbf{E} \cdot \int_{\Omega_{\mathbf{k}}} \left(\nabla_{\mathbf{k}} H - f\frac{\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})}{k_B T_L}\right) d\mathbf{k}$$

$$0 \;\geq\; \frac{\partial}{\partial \mathrm{t}} \left\langle \log \frac{f}{Me} \right\rangle + \nabla_{\mathbf{x}} \cdot \left\langle \mathbf{v} \log \frac{f}{Me} \right\rangle - \frac{q}{\hbar}\mathbf{E} \cdot \int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{k}} H\, d\mathbf{k} + \frac{q}{\hbar}\mathbf{E} \cdot \frac{\hbar\,\langle \mathbf{v} \rangle}{k_B T_L}\,.$$

We can consider a couple more monotone functions $g(f/M)$ that let us find stability and positivity properties of the solution f of our Boltzmann Equation.

Consider the function $g(f/M) = \mathrm{sgn}(f/M)$, which is discontinuous yet monotone increasing. We have that

$$\int_{\Omega_{\mathbf{k}}} Q(f)\,\mathrm{sgn}\frac{f}{M}\,d\mathbf{k} \;=\; -\int_{\Omega_{\mathbf{k}}}\int_{\Omega_{\mathbf{k}}} \frac{\sigma(\mathbf{k}',\mathbf{k})}{2}\left(\frac{f'}{M'}-\frac{f}{M}\right)\left(\mathrm{sgn}\frac{f'}{M'}-\mathrm{sgn}\frac{f}{M}\right)d\mathbf{k}'d\mathbf{k} \le 0\,.$$

Substituting the collision operator for the transport term of the Boltzmann Equation, we have that

$$0 \ge \int_{\Omega_{\mathbf{k}}} \mathrm{sgn}\frac{f}{M}\frac{df}{d\mathrm{t}}d\mathbf{k} = \int_{\Omega_{\mathbf{k}}} \mathrm{sgn}\frac{f}{M}\frac{\partial f}{\partial \mathrm{t}}d\mathbf{k} + \int_{\Omega_{\mathbf{k}}} \mathrm{sgn}\frac{f}{M}\nabla_{\mathbf{x}} f\cdot\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\,d\mathbf{k} - \frac{q}{\hbar}\int_{\Omega_{\mathbf{k}}} \mathrm{sgn}\frac{f}{M}\,\nabla_{\mathbf{k}} f\cdot\mathbf{E}\,d\mathbf{k}\,,$$

and since we have as well that

$$\mathrm{sgn}\frac{f}{M}\partial f = \mathrm{sgn} f\,\partial f = \partial G, \quad G = \int \mathrm{sgn}\frac{f}{M}\partial f = \int \mathrm{sgn} f\,\partial f = |f|\;, \quad (2.52)$$

we can rewrite our inequality in the form

$$\begin{aligned} 0 \;&\ge\; \int_{\Omega_{\mathbf{k}}} \frac{d|f|}{dt}d\mathbf{k} = \int_{\Omega_{\mathbf{k}}} \frac{\partial|f|}{\partial \mathrm{t}}d\mathbf{k} + \int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{x}}|f|\cdot\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\,d\mathbf{k} - \frac{q}{\hbar}\int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{k}}|f|\cdot\mathbf{E}\,d\mathbf{k} \\ 0 \;&\ge\; \frac{d}{dt}\int_{\Omega_{\mathbf{k}}} |f|d\mathbf{k} = \frac{\partial}{\partial \mathrm{t}}\int_{\Omega_{\mathbf{k}}} |f|d\mathbf{k} + \nabla_{\mathbf{x}}\cdot\int_{\Omega_{\mathbf{k}}} |f|\frac{\nabla_{\mathbf{k}}\varepsilon}{\hbar}\,d\mathbf{k} - \frac{q}{\hbar}\mathbf{E}\cdot\int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{k}}|f|\,d\mathbf{k}\,. \end{aligned}$$

Therefore, we have just proved that the solution f to our Boltzmann Equation is L^1-stable, since its L^1 norm decreases on time.

We can prove the positivity of f using a shifted version of the previous monotone function. We consider now the function

$$g\left(\frac{f}{M}\right) = \left(\mathrm{sgn}\frac{f}{M} - 1\right) = \mathrm{sgn} f - 1, \quad (2.53)$$

which is monotone increasing too, so

$$0 \geq \int_{\Omega_{\mathbf{k}}} Q(f) \left(\mathrm{sgn} \frac{f}{M} - 1 \right) d\mathbf{k} = \int_{\Omega_{\mathbf{k}}} \frac{df}{d\mathrm{t}} \left(\mathrm{sgn} f - 1 \right) d\mathbf{k} \,, \tag{2.54}$$

and, since we have that

$$\left(\mathrm{sgn} f - 1 \right) \partial f = \partial G, \quad G = \int \left(\mathrm{sgn} f - 1 \right) \partial f = |f| - f \geq 0 \,, \tag{2.55}$$

we derive that

$$0 \geq \int_{\Omega_{\mathbf{k}}} \frac{d(|f| - f)}{d\mathrm{t}} d\mathbf{k} = \frac{d}{d\mathrm{t}} \int_{\Omega_{\mathbf{k}}} (|f| - f) d\mathbf{k}. \tag{2.56}$$

Therefore, the function of time on the right hand side is decreasing, so

$$\int_{\Omega_{\mathbf{k}}} (|f| - f)|_{\mathrm{t}=0} \, d\mathbf{k} \geq \int_{\Omega_{\mathbf{k}}} (|f| - f)|_{\mathrm{t}} \, d\mathbf{k} \geq 0 \,. \tag{2.57}$$

We can conclude that the solution of our Boltzmann Equation preserves its positivity over time. If our initial condition was a non-negative function $f|_{t=0} \geq 0$, then at any subsequent time it holds that

$$0 = \int_{\Omega_{\mathbf{k}}} (|f| - f)|_{\mathrm{t}=0} \, d\mathbf{k} \geq \int_{\Omega_{\mathbf{k}}} (|f| - f)|_{\mathrm{t}} \, d\mathbf{k} \geq 0 \,.$$

Therefore we have that

$$0 = \int_{\Omega_{\mathbf{k}}} (|f| - f)|_{\mathrm{t}} \, d\mathbf{k} \,,$$

and, since $|f| - f \geq 0$, the only possible way this can happen is if a.e. on the domain $\Omega_{\mathbf{k}}$ we have

$$f(\mathbf{x}, \mathbf{k}, \mathrm{t}) = |f|(\mathbf{x}, \mathbf{k}, \mathrm{t}) \geq 0 \,, \tag{2.58}$$

for any time $\mathrm{t} \geq 0,\ \mathbf{x} \in \Omega_{\mathbf{x}}$.

For a general monotone increasing function $g(f/M)$, we can try to derive similar entropy inequalities noticing that

$$0 \geq \int_{\Omega_{\mathbf{k}}} Q(f) g\left(\frac{f}{M}\right) d\mathbf{k} = \int_{\Omega_{\mathbf{k}}} g\left(\frac{f}{M}\right) \left[\frac{\partial f}{\partial \mathrm{t}} + \nabla_{\mathbf{x}} f \cdot \frac{\nabla_{\mathbf{k}} \varepsilon}{\hbar} - \nabla_{\mathbf{k}} f \cdot \frac{q\mathbf{E}}{\hbar}\right] d\mathbf{k}\,,$$

so, provided that we are able to find a function G such that

$$g\left(\frac{f}{M}\right) \partial f = \partial G, \quad G(f, M) = \int g\left(\frac{f}{M}\right) \partial f\ , \tag{2.59}$$

for $\partial = \partial_t,\ \nabla_{\mathbf{x}},\ \nabla_{\mathbf{k}},\ d_t$, we obtain the inequality

$$0 \geq \int_{\Omega_{\mathbf{k}}} g\left(\frac{f}{M}\right) \frac{df}{d\mathrm{t}} d\mathbf{k} = \int_{\Omega_{\mathbf{k}}} \frac{dG}{d\mathrm{t}}\, d\mathbf{k}\,, \tag{2.60}$$

which yields

$$\begin{aligned}
0 \ &\geq \ \int_{\Omega_{\mathbf{k}}} \frac{dG}{d\mathrm{t}} d\mathbf{k} = \int_{\Omega_{\mathbf{k}}} \frac{\partial G}{\partial \mathrm{t}} d\mathbf{k} + \int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{x}} G \cdot \frac{\nabla_{\mathbf{k}} \varepsilon}{\hbar}\, d\mathbf{k} - \frac{q}{\hbar} \int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{k}} G \cdot \mathbf{E}\, d\mathbf{k} \\
0 \ &\geq \ \frac{d}{d\mathrm{t}} \int_{\Omega_{\mathbf{k}}} G d\mathbf{k} = \frac{\partial}{\partial \mathrm{t}} \int_{\Omega_{\mathbf{k}}} G d\mathbf{k} + \nabla_{\mathbf{x}} \cdot \int_{\Omega_{\mathbf{k}}} G \frac{\nabla_{\mathbf{k}} \varepsilon}{\hbar}\, d\mathbf{k} - \frac{q}{\hbar} \mathbf{E} \cdot \int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{k}} G\, d\mathbf{k}\,.
\end{aligned}$$

If $G(f, M) = fP(f, M)$, then we have that

$$\begin{aligned}
0 \ &\geq \ \frac{d}{d\mathrm{t}} \int_{\Omega_{\mathbf{k}}} fP d\mathbf{k} = \frac{\partial}{\partial \mathrm{t}} \int_{\Omega_{\mathbf{k}}} fP d\mathbf{k} + \nabla_{\mathbf{x}} \cdot \int_{\Omega_{\mathbf{k}}} fP \frac{\nabla_{\mathbf{k}} \varepsilon}{\hbar}\, d\mathbf{k} - \frac{q}{\hbar} \mathbf{E} \cdot \int_{\Omega_{\mathbf{k}}} \nabla_{\mathbf{k}} (fP)\, d\mathbf{k} \\
0 \ &\geq \ \frac{d}{d\mathrm{t}} \langle P \rangle = \frac{\partial}{\partial \mathrm{t}} \langle P \rangle + \nabla_{\mathbf{x}} \cdot \langle P\, \mathbf{v} \rangle - \frac{q}{\hbar} \mathbf{E} \cdot \left\langle \frac{\nabla_{\mathbf{k}} (fP)}{f} \right\rangle\,,
\end{aligned}$$

with

$$P(f, M) = \frac{G(f, M)}{f} = \frac{1}{f} \int g\left(\frac{f}{M}\right) \partial f\,. \tag{2.61}$$

One particular set of monotone functions of f/M is the family of polynomials $g(f/M) = (f/M)^{\alpha}$, $\alpha \neq -1$, which is monotone, $f/M \geq 0$.

For the polynomials $(f/M)^\alpha$ we have that

$$\begin{aligned} g\left(\frac{f}{M}\right) &= \left(\frac{f}{M}\right)^\alpha \\ G(f,M) &= \int \left(\frac{f}{M}\right)^\alpha \partial f = \frac{f}{\alpha+1}\left(\frac{f}{M}\right)^\alpha - \int \frac{f^{\alpha+1}}{\alpha+1}\partial M^{-\alpha} \\ G(f,M) &= \frac{f}{\alpha+1}\left(\frac{f}{M}\right)^\alpha - \frac{\alpha}{\alpha+1}\int f\left(\frac{f}{M}\right)^\alpha \frac{\partial\varepsilon(\mathbf{k})}{k_B T_L}\,, \end{aligned} \tag{2.62}$$

so the associated set of entropy equations for $\alpha \geq 0$ are of the form

$$0 \geq \frac{\partial}{\partial \mathrm{t}}\left\langle \left(\frac{f}{M}\right)^\alpha \right\rangle + \nabla_{\mathbf{x}} \cdot \left\langle \left(\frac{f}{M}\right)^\alpha \mathbf{v} \right\rangle + \frac{q\alpha}{k_B T_L}\mathbf{E} \cdot \left\langle \left(\frac{f}{M}\right)^\alpha \frac{\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})}{\hbar} \right\rangle ,$$

and for the monotone decreasing functions s.t. $0 \geq \alpha \neq -1$ we have

$$0 \leq \frac{\partial}{\partial \mathrm{t}}\left\langle \left(\frac{f}{M}\right)^\alpha \right\rangle + \nabla_{\mathbf{x}} \cdot \left\langle \left(\frac{f}{M}\right)^\alpha \mathbf{v} \right\rangle + \frac{q\alpha}{k_B T_L}\mathbf{E} \cdot \left\langle \left(\frac{f}{M}\right)^\alpha \frac{\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})}{\hbar} \right\rangle ,$$

in both cases integrating by parts and using the boundary conditions of f in $\partial\Omega_{\mathbf{k}}$ (for the vanishing at infinity BC case, we also assume that f decays at a Maxwellian rate $f/M \to O(1)$).

The case $\alpha = 0$ is the monotone case that is both decreasing and increasing, giving then an equality that is the well known mass conservation equation

$$0 = \frac{\partial}{\partial \mathrm{t}}\langle 1 \rangle + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} \rangle \ .$$

For the singular case $\alpha = -1$ we have the decreasing function

$$\begin{aligned} g(f/M) &= \left(\frac{f}{M}\right)^{-1} = \frac{M}{f}, \\ G(f,M) &= \int g(f/M)\partial f = \int \frac{M\partial f}{f} = M\log f - \int \log f \partial M, \\ G(f,M) &= M\log f + \frac{1}{k_B T_L}\int M\log f \partial\varepsilon(\mathbf{k})\,, \end{aligned}$$

with the entropy inequality

$$0 \leq \frac{\partial}{\partial \mathrm{t}} \left\langle \frac{M}{f} \log f \right\rangle + \nabla_{\mathbf{x}} \cdot \left\langle \frac{M}{f} \log f \mathbf{v} \right\rangle + \frac{q}{k_B T_L} \mathbf{E} \cdot \left\langle \frac{M}{f} \log f \frac{\nabla_{\mathbf{k}} \varepsilon(\mathbf{k})}{\hbar} \right\rangle .$$

2.2 Physics of Electron Transport in Semiconductors

2.2.1 Semiconductor Physics: Energy Bands and Conductivity

The physical phenomena we are interested is the charge transport in semiconductors. We proceed then to describe the physics behind why a material is a semiconductor, as opposed to a a metal or an insulator. The difference in conductivity between these 3 different kind of materials can be explained in terms of the separation of their energy band gaps. The charge carriers, electrons, are fermions, obeying then the Fermi Statistics in equilibrium, which gives the occupancy probability f of finding a fermion in terms of the single particle (assuming there is no degeneracy) energy state ε

$$f(\varepsilon) = \frac{1}{1 + \exp((\varepsilon - \varepsilon_F)/K_B T)},$$

$$\varepsilon_F \quad \text{s.t.} \quad f(\varepsilon_F) = 1/2$$

ε_F is called the Fermi Level. K_B is the Boltzmann's constant and T is the temperature in Kelvins. The filling of the bands determines the conductivity of the material, which can then be classified according to 3 different categories.

- Metals: High Conductivity Their Fermi Level ε_F is within one or more energy bands. There are many occupied states above ε_F, and many unoccupied states below. This results in a high conductive material.

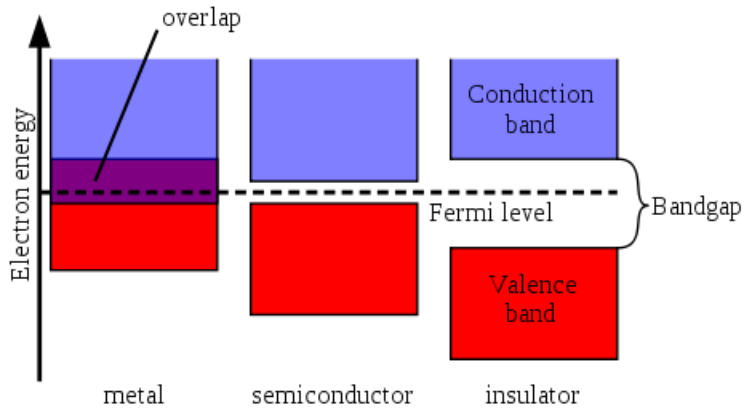


Figure 2.1: Difference between Semiconductors, Metals & Insulators. Energy Band Gaps

- Insulators: Very Low Conductivity ε_F is within a large band gap between the conduction and valence bands. There are extremely few electrons and vacancies (holes). This results in very low conductivity.

- Semiconductors: Low to Intermediate Conductivity ε_F lies within the moderate size band gap between conduction and valence bands. There are only a few electrons and vacancies (holes). This results in low to intermediate conductivity.

As mentioned in [11], the advantage of semiconductors is that we can control the electron and hole concentrations and thus, e.g., conductivity, via addition of impurities, externally imposed fields, light, etc.

2.2.2 Semiconductors with Periodic Crystal Structure

We consider in our study semiconductor materials classified as crystals, a periodic array of atoms. This crystal structure is defined by a lattice (a periodic array of mathematical points in space) and an atomic basis (a fixed array of one or more atoms associated with each lattice point). The lattice has a translational symmetry. The translation vectors T that leave the lattice invariant under translations are given by a basis of vectors $\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3}$, so that any two lattice points are connected by a translational vector of the form

$$T = i\mathbf{a_1} + j\mathbf{a_2} + k\mathbf{a_3}, \quad \text{where} \quad i, j, k \quad \text{are integers.}$$

The lattice periodicity in the position $\mathbf{x}$-space translates in an associated periodicity in the Fourier $\mathbf{k}$-space. We have then a reciprocal lattice as well in $\mathbf{k}$-space. The reciprocal lattice vectors are generated by a basis $\mathbf{b_1}, \mathbf{b_2}, \mathbf{b_3}$, related to the basis of the lattice vectors in $\mathbf{x}$-space by the property

$$\mathbf{b_i} \cdot \mathbf{a_j} = 2\pi\delta_{ij},$$

where i, j are integers, and δ_{ij} is the Kronecker delta.

The reciprocal lattice is invariant under translations by vectors G of the form

$$G = i\mathbf{b_1} + j\mathbf{b_2} + k\mathbf{b_3}, \quad \text{where} \quad i, j, k \quad \text{are integers.}$$

The vectors G are called reciprocal lattice vectors.

A cell related to the translational symmetry of the lattice is called a unit cell. It is called a primitive unit cell when it can't be reduced to a smaller

cell. A Wigner - Seitz unit cell is the primitive unit cell that best displays the symmetry of a lattice. The Brillioun Zone (BZ) is defined then as the Wigner-Seitz unit cell of the reciprocal lattice.

2.2.3 Quantum Mechanics: Schrodinger Equation, Energy Eigenvalues & Bloch functions

Quantum Mechanics is the physical theory that gives the energy bands which explain the conductivity behaviour of a semiconductor material. We obtain these energy values by solving the Eigenvalue Problem of Schrödinger Equation

$$\varepsilon\Psi(\mathbf{x}) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right]\Psi(\mathbf{x}),$$

where ε is the energy eigenvalue associated to the eigenstate function $\Psi(\mathbf{x})$, $\mathbf{x}$ is the position vector, $V(\mathbf{x})$ is the related atomic potential of the system, $\hbar$ is Planck's constant, and m is the electron mass. Since our material is periodic, we can assume that the related atomic potential $V(\mathbf{x})$ is periodic as well. Then, using the lattice vectors related to the translational symmetry of the reciprocal lattice, we express the potential in a Fourier Series in terms of the reciprocal lattice vectors G, in the form

$$V(\mathbf{x}) = \sum_G C_G\, e^{iG\cdot\mathbf{x}}\,.$$

The eigenfunctions related to this problem are called Bloch functions. So, for $\mathbf{k}$ in the BZ, and α being an Energy Band index, we have

$$\Psi_{\alpha,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}u_{\alpha,\mathbf{k}}(\mathbf{x}), \quad \text{where} \quad u_{\alpha,\mathbf{k}}(\mathbf{x}) = \sum_G a_{\alpha,\mathbf{k}+G}\, e^{iG\cdot\mathbf{x}}.$$

The energy eigenvalues $\varepsilon_\alpha(\mathbf{k})$ of Schrödinger Equation are given by the determinant

$$\Big|\Big(\frac{\hbar^2\|\mathbf{k}+G\|^2}{2m} - \varepsilon_\alpha(\mathbf{k})\Big)\delta_{G,G'} + C_{G,G'}\Big| = 0\,.$$

The reciprocal lattice vectors G, G' are used for indexing the matrix above, understanding that they were defined before in terms of 3 integers, so $G = G(i,j,k)$, $G = G'(i',j',k')$. The unit matrix is then represented by $\delta_{G,G'}$, and we also define $C_{G,G'} = C_{G-G'}$, where $C_{G-G'}$ is the Fourier expansion coefficient of the potential $V(\mathbf{x})$ corresponding to the lattice vector $G - G'$. The Dispersion Relation $\varepsilon_\alpha(\mathbf{k})$ appearing in this Quantum Mechanical problem is called the energy band structure.

2.2.4 Electronic Band Structure and the Empirical Pseudopotential Method (EPM)

The Empirical Pseudopotential Methods (EPM) [37] give a full electronic band structure in $\mathbf{k}$-space. In these methods, the Lattice Potential $V(\mathbf{x})$ is approximated as the sum of potentials $w(\mathbf{x})$ due to individual atoms and associated electrons. For the case of Silicon, with a 2 atom basis, V can be expressed as

$$V(\mathbf{x}) = \sum_G C_G\, e^{iG\cdot\mathbf{x}}, \quad C_G = S_G\, W_G, \quad \text{where}$$

$$S_G = e^{iG\cdot T} + e^{iG\cdot T} = 2\cos(G\cdot T), \quad T = a(\hat{x}+\hat{y}+\hat{z})/8,$$

$$\text{and} \quad W_G = \frac{\int_\Omega w(\mathbf{x}) e^{-iG\cdot\mathbf{x}} d\mathbf{x}}{\int_{\Omega_\mathbf{x}} d\mathbf{x}}\,,$$

where S_G is called the structure factor, and W_G is the form factor.

The **Pseudo-potential** part of the method means that the atom potential is assumed symmetric & isotropic, so $W_G = W(|G|)$. The Fourier Expansion of $V(\mathbf{x})$ is truncated

$$V(\mathbf{x}) = \sum_{|G| \leq |G|_{max}} S_G \, W_G e^{iG \cdot \mathbf{x}}$$

The energy values $\varepsilon_\alpha(\mathbf{k})$ are given by the determinant (in terms of the finite set of lattice vectors s.t. $|G|$, $|G'| \leq |G|_{max}$)

$$\left| \Big(\frac{\hbar^2 \|\mathbf{k} + G\|^2}{2m} - \varepsilon_\alpha(\mathbf{k}) \Big) \delta_{G,G'} + S_{G-G'} W_{G-G'} \right| = 0 \, .$$

This determinant is solved for $\varepsilon_\alpha(\mathbf{k})$ as a function of $W(|G|)$. The **Empirical** aspect of the method consists in choosing the $W(|G|)$ parameters to fit experimental data such as band types, gaps, optical absorption rates, etc. More information about EPM can be found in [11], [38].

2.2.5 Conduction Energy Band - Carrier Velocity Models

The Quantum Mechanical Wavefunction associated to our charge transport problem has the form

$$\Psi_{\alpha,\mathbf{k}}(\mathbf{x}, \mathrm{t}) = \sum_{\mathbf{k},\alpha} A_{\mathbf{k},\alpha} \left[e^{i\mathbf{k} \cdot G} \sum_G a_{\alpha,\mathbf{k}+G} \; e^{iG \cdot \mathbf{x} - w_\alpha(\mathbf{k})\mathrm{t}} \right] .$$

It is natural then to use as a model for the charge carrier velocity along a desired band the group velocity of the quantum mechanical wave function

$$\frac{\partial w}{\partial \mathbf{k}} = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}}(\mathbf{k}) \, .$$

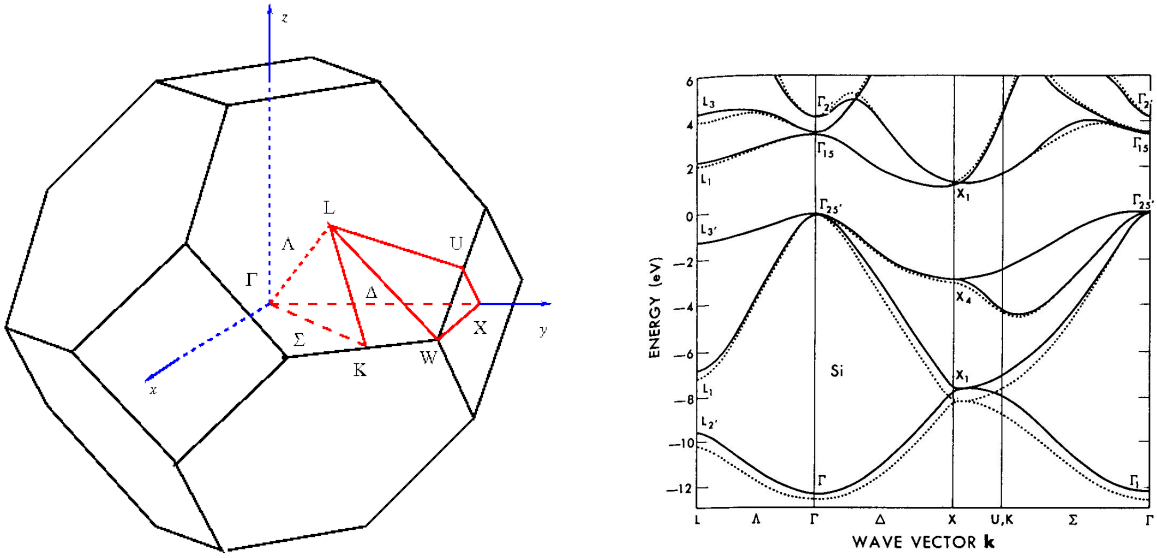


Figure 2.2: Brillouin Zone & Electronic Energy Band structure for Silicon. Electronic Structure and Optical Properties of Semiconductors (Cohen and Chelikowsky [38])

Some analytic band models are commonly used to describe the electronic bands that give as well a carrier velocity model on the conduction band. For example, the Parabolic Band Model is a reasonable fit on conduction energy band valleys. It is basically a 2nd order Taylor fit to a local minimum $\varepsilon(\mathbf{k}_0)$ of the conduction band.

$$\varepsilon(\mathbf{k}) \approx \sum_{i=1}^{3} \frac{\hbar^2 \left(k_i - k_{0,i}\right)^2}{2m_i^*}, \quad m_i^* = \hbar^2 \left(\frac{\partial^2 \varepsilon(\mathbf{k}_0)}{\partial k_i^2} \right)^{-1}.$$

The Effective mass approximation m_i^* is related to the 2nd Order Taylor Coefficients as above. It is commmon in the Boltzmann community to use a Parabolic Band model in which a single effective mass parameter m^* is the same used for the 3 orthogonal directions. On the other hand, the Kane Band Model [4] can be considered as a first order correction of the parabolic model,

with a non-parabolicity factor α

$$\varepsilon(1+\alpha\varepsilon) = \frac{\hbar^2(\mathbf{k}-\mathbf{k}_0)^2}{2m^*}\,.$$

The Kane Model has a validity limited up to energies of 1-2 eV [18] , which limits is validity as well in applying it to model high-field transport.

2.3 Discontinuous Galerkin Method

2.3.1 Introduction to the DG Method - 1D Linear Hyperbolic Equation

Discontinuous Galerkin (DG) Methods are a class of finite element methods using discontinuous basis functions, which are usually chosen as piecewise continuous polynomials. The DG method was first designed as an effective numerical method for solving hyperbolic conservation laws, which may have discontinuous solutions. It was introduced in 1973 by Reed and Hill [3] in the framework of neutron transport, modeled by a time independent linear hyperbolic equation. We recommend the reference [1] for a review of the method on a 2D case (we will follow their presentation on the next section). This introductory session to the DG Method is based on [9].

Since the basis functions on the DG method can be discontinuous, these methods have the flexibility which is not shared by typical finite element methods, such as the allowance of arbitrary triangulation with hanging nodes, complete freedom in changing the polynomial degrees in each element independent of that in the neighbors (p adaptivity), and extremely local data structure, (elements only communicate with immediate neighbors regardless

of the order of accuracy of the scheme) resulting in a high parallel efficiency (usually more that 99% for a fixed mesh, and more than 80% for a dynamic load balancing with adaptive meshes which change often during time evolution, as commented in [1]).

In this section we will focus on the method of lines DG methods, that is, we do not discretize the time variable. We consider then a semi-discrete formulation of DG. To set up some basic ideas about how the Discontinuous Galerkin Method works, we present as an example problem a Transport Equation in 1D of 1st Order with constant coefficients. We have then

$$u_t + u_x = 0.$$

To make a weak formulation of this problem, we multiply our equation by a test function v

$$u_t v + u_x v = 0,$$

and we integrate over the considered cell in the domain, the interval $I = (x_L, x_R)$

$$\int_I u_t v dx + \int_I u_x v = 0, \quad \text{on} \quad I = (x_L, x_R),$$

integrating by parts on the x-domain to pass the derivative in x from the solution living in the trial space to the test function

$$\int_I u_t v dx - \int_I u v_x + uv(x_R) - uv(x_L) = 0.$$

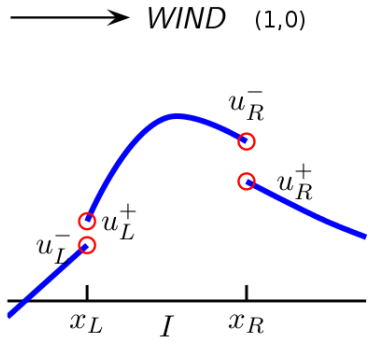
The DG Method for solving our problem (which is a weak formulation) is defined as follows. Find $u \in V_h$, the trial function space, such that for any test function v in the test space V_h (in this case the test function space is the same as the trial space), it holds that

$$\int_I u_t v dx - \int_I u v_x + \hat{u} v^-(x_R) - \hat{u} v^+(x_L) = 0.$$

In this case, $v^-(x_0) = \lim_{x \to x_0^-}$, $v^+(x_0) = \lim_{x \to x_0^+}$, which is a useful notation since our functions could be discontinuous at the boundaries between intervals (cells). $\hat{u}$ is called the numerical flux, which is a single valued function defined at the cell boundary. It depends on the values of the numerical solution u of the DG Method, which is discontinuous precisely on those boundaries. There are several (function) rules to define the numerical flux $\hat{u}$. One of them is the upwind rule.

For example, for this particular problem, according to the upwind rule we would have that $\hat{u} = u^-$ if the direction of the transport vector (wind) is $(1, 0)$ and $\hat{u} = u^+$ if its direction $(-1, 0)$.

The upwind flux rule tries to follow the physics of the transport phenomena it describes by taking in the boundary the value of u 'carried' by the 'wind direction' associated to the hyperbolic equation, that is, the vector $(1, 0)$, as if this value was transported from one cell to the neighboring one by the transport process. On the other hand, the values of the test function taken in these boundary integrals (point evaluations for this 1D problem) are the values of v on the interior of the cell $I = (x_L, X_R)$, that is, $v^+(x_L)$, $v^-(x_R)$, which



Find $u \in V_h$= piecewise polynomial space, s.t. for any $v \in V_h$,

$$\int_I u_t v \, dx - \int_I u v_x \, dx + \hat{u}v^-(x_R) - \hat{u}v^+(x_L) = 0.$$

makes sense since v is a test function. After applying a semi-discrete DG formulation in x, we would obtain a system of ODEs for the coefficients related to the test function. Assuming, for example, that V_h is the space of piecewise constant polynomials, we would then obtain the ODE $du_I/dt = L(u_I, u_{I-1})$, where u_I is the value of the constant value inside the cell I.

To mention briefly the issue of time discretization in the DG method, we must mention that for hyperbolic problems or convection dominated problems, a class of high order nonlinearly stable Runge-Kutta time discretizations is often used. It is distinctive from them that they are convex combinations of first order forward Euler steps, which makes them maintain strong stability properties in any semi-norm (total variation semi-norm, maximum norm, entropy condition, etc.) of the forward Euler step. It is only needed then to prove nonlinear stability for the first order forward Euler step, which is

relatively easy in many situations, such as the TVD schemes, and the same strong stability property is automatically obtained for the higher order time discretization in this class. One of the most popular schemes in this class is the following 3rd Order Runge-Kutta method for solving $u_t = L(u,t)$, where $L(u,t)$ is a spatial discretization operator (it does not need to be, and it is often not, linear)

$$u^{(1)} = u^n + \Delta t L(u^n, t^n)\,,$$
$$u^{(2)} = \frac{3}{4}u^n + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)}, t^n + \Delta t)\,,$$
$$u^{(n+1)} = \frac{1}{3}u^n + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)}, t^n + \frac{1}{2}\Delta t)\,.$$

We refer to the survey paper [8] for more details.

Chapter 3

DG Deterministic Solvers for BP Models of Electron Transport incorporating EPM

3.1 Boltzmann equation in spherical coordinates for the k-vector

We show here the Boltzmann equation with the momentum $\mathbf{k}$ in spherical coordinates presented in [35]. As opposed to the previous work in [34], the coordinate transformation based on the Kane analytic band relation proposed in [21] can no longer be used for an energy band that does not assume this analytic Kane band model and that takes into account anisotropy for $\varepsilon(\mathbf{k})$. The spherical coordinate system is used in $\mathbf{k}$ space instead of Cartesian coordinates because of the higher resolution demands near the conduction band minimum (chosen as the origin $\mathbf{k} = 0$), and large cells in $\mathbf{k}$-space are sufficient for describing the tail of the distribution function accurately.

We introduce a change of variables to obtain the dimensionless quantities

$$t = \frac{\mathrm{t}}{t_*}\,, \quad (\vec{x}, z) = \frac{\mathbf{x}}{\ell_*}\,, \quad \mathbf{k} = \frac{\sqrt{2m^* k_B T_L}}{\hbar}\sqrt{r}\left(\mu, \sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi\right)$$

with $r \geq 0\,, \mu \in [-1, 1]\,, \varphi \in [-\pi, \pi]$.

$$\mathcal{E}(r, \mu, \varphi) = \frac{1}{k_B T_L}\varepsilon(\mathbf{k})\,,$$

$$\Psi(t,x,y,z) = \frac{V(t_*\,t, \ell_*\,x, \ell_*\,y, \ell_*\,z)}{V_*}, \quad \mathbf{E} = -c_v \nabla_{\mathbf{x}} V\,,$$

with $c_v = \dfrac{V_*}{\ell_* E_*}$ and $E_* = 0.1\, V_*\, \ell_*^{-1}$.

where the spherical coordinate transformation maps the $\mathbf{k}$-domain $\Omega_{\mathbf{k}}$ onto the set Ω of the (r, μ, φ) space. Typical values for length, time and voltage are given by $\ell_* = 10^{-6}\, m$, $t_* = 10^{-12}\, s$ and $V_* = 1\,\text{Volt}$, respectively.

Thus, a new unknown "weighted" *pdf* function Φ is obtained by multiplying the *pdf* f by the Jacobian of the spherical $\mathbf{k}$-transformation

$$\Phi(t,x,y,z,r,\mu,\varphi) = \frac{\sqrt{r}}{2}\, f(t,x,y,z,r,\mu,\varphi)\,, \tag{3.1}$$

which can be interpreted as the probability density function of an electron being in the neighborhood of the phase-space state $(x, y, z, r, \mu, \varphi)$ at time t.

Hence, writing the collisional integral in spherical coordinates and multiplying the Boltzmann equation by the Jacobian associated to the $\mathbf{k}$-spherical transformation, yields the following Transformed Boltzmann Equation (TBE) for the unknown Φ

$$\frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial x}\,(a_1\,\Phi) + \frac{\partial}{\partial y}\,(a_2\,\Phi) + \frac{\partial}{\partial z}\,(a_3\,\Phi) + \frac{\partial}{\partial r}\,(a_4\,\Phi) + \frac{\partial}{\partial \mu}\,(a_5\,\Phi) + \frac{\partial}{\partial \varphi}\,(a_6\,\Phi) = C(\Phi)\,, \tag{3.2}$$

with the transport vector $\vec{a} = (a_1, a_2, a_3, a_4, a_5, a_6)^T$ with components

$$a_1(\cdot) = c_D \left(2\sqrt{r}\,\mu \frac{\partial \mathcal{E}}{\partial r} + \frac{1-\mu^2}{\sqrt{r}} \frac{\partial \mathcal{E}}{\partial \mu} \right),$$

$$a_2(\cdot) = c_D \left(2\sqrt{r}\,\sqrt{1-\mu^2}\,\cos\varphi \frac{\partial \mathcal{E}}{\partial r} - \frac{\mu\sqrt{1-\mu^2}\,\cos\varphi}{\sqrt{r}} \frac{\partial \mathcal{E}}{\partial \mu} - \frac{\sin\varphi}{\sqrt{r}\,\sqrt{1-\mu^2}} \frac{\partial \mathcal{E}}{\partial \varphi} \right),$$

$$a_3(\cdot) = c_D \left(2\sqrt{r}\,\sqrt{1-\mu^2}\,\sin\varphi \frac{\partial \mathcal{E}}{\partial r} - \frac{\mu\sqrt{1-\mu^2}\,\sin\varphi}{\sqrt{r}} \frac{\partial \mathcal{E}}{\partial \mu} + \frac{\cos\varphi}{\sqrt{r}\,\sqrt{1-\mu^2}} \frac{\partial \mathcal{E}}{\partial \varphi} \right),$$

$$a_4(\cdot) = -2\,c_E\,\sqrt{r} \left[\mu\,E_x(t,x,y,z) + \sqrt{1-\mu^2}\,(\cos\varphi\,E_y(t,x,y,z) + \sin\varphi\,E_z(t,x,y,z)) \right],$$

$$a_5(\cdot) = -c_E \left[\frac{1-\mu^2}{\sqrt{r}}\,E_x(t,x,y,z) - \frac{\mu\sqrt{1-\mu^2}}{\sqrt{r}}\,(\cos\varphi\,E_y(t,x,y,z) + \sin\varphi\,E_z(t,x,y,z)) \right],$$

$$a_6(\cdot) = -c_E\,\frac{1}{\sqrt{r}\,\sqrt{1-\mu^2}}\,[\,-\sin\varphi\,E_y(t,x,y,z) + \cos\varphi\,E_z(t,x,y,z)]\,,$$

and the linear collision operator

$$C(\Phi)(t,x,y,z,r,\mu,\varphi) = \frac{\sqrt{r}}{2} \int_\Omega \mathcal{S}(r',\mu',\varphi',r,\mu,\varphi)\,\Phi(t,x,y,z,r',\mu',\varphi')\,dr'\,d\mu' d\varphi'$$
$$- \Phi(t,x,y,z,r,\mu,\varphi) \int_\Omega \mathcal{S}(r,\mu,\varphi,r',\mu',\varphi')\,\frac{\sqrt{r'}}{2}\,dr'\,d\mu' d\varphi'\,, \tag{3.3}$$

where the scattering kernel is

$$\mathcal{S}(r,\mu,\varphi,r',\mu',\varphi') = c_+\,\delta(\mathcal{E}(r',\mu',\varphi') - \mathcal{E}(r,\mu,\varphi) + \alpha_p)$$
$$+\,c_-\,\delta(\mathcal{E}(r',\mu',\varphi') - \mathcal{E}(r,\mu,\varphi) - \alpha_p) + c_0\,\delta(\mathcal{E}(r',\mu',\varphi') - \mathcal{E}(r,\mu,\varphi)),$$

accounting for acoustic and optical electron-phonon interaction, the main scattering mechanisms in silicon. The constants above are defined as

$$c_D = \frac{t_*}{\ell_*}\sqrt{\frac{k_B T_L}{2\,m^*}}\,, \quad c_E = \frac{t_* q E_*}{\sqrt{2m^* k_B T_L}}\,, \quad \alpha_p = \frac{\hbar\omega_p}{k_B T_L}\,,$$
$$(c_+, c_-, c_0) = \frac{2m^*\,t_*}{\hbar^3}\sqrt{2\,m^*\,k_B T_L}\,[(n_q+1)K, n_q K, K_0]\,.$$

The dimensionless Poisson equation is

$$\frac{\partial}{\partial x}\left(\epsilon_r \frac{\partial \Psi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\epsilon_r \frac{\partial \Psi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\epsilon_r \frac{\partial \Psi}{\partial z}\right) = c_p \left[\rho(t,x,y,z,t) - \mathcal{N}_D(x,y,z)\right] , \tag{3.4}$$

where

$$\mathcal{N}_D(x,y,z) = \left(\frac{\sqrt{2\, m^* k_B T_L}}{\hbar}\right)^{-3} N_D(\ell_* x, \ell_* y, \ell_* z), \quad c_p = \left(\frac{\sqrt{2\, m^* k_B T_L}}{\hbar}\right)^{3} \frac{\ell_*^2 q}{\epsilon_0\, V_*},$$
$$\rho(t,x,y,z) = \int_\Omega \Phi(t,x,y,z,r',\mu',\varphi')\, dr'\, d\mu' d\varphi' .$$

3.1.1 Geometrical interpretation of the force terms in the TBE

Although the terms (a_1, a_2, a_3) related to the transport in the **x**-space due to the electron group velocity in the TBE can be easily interpreted as just the gradient $\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})$ expressed in spherical coordinates, the terms (a_4, a_5, a_6) related to the transport in the **k**-space due to the electric field might be more obscure to understand. A simple expression for them can be identified.

$$a_4 \;=\; -2\, c_E \sqrt{r}\left(\mu, \sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi\right)\cdot \mathbf{E} = -2\, c_E \sqrt{r}\, \hat{e}_r \cdot \mathbf{E}, \tag{3.5}$$

$$a_5 \;=\; -c_E \frac{\sqrt{1-\mu^2}}{\sqrt{r}}\left(\sqrt{1-\mu^2}, -\mu\cos\varphi, -\mu\sin\varphi\right)\cdot \mathbf{E} = -c_E \frac{\sqrt{1-\mu^2}}{\sqrt{r}}\, \hat{e}_\mu \cdot \mathbf{E}, \tag{3.6}$$

$$a_6 \;=\; -c_E \frac{1}{\sqrt{r}\sqrt{1-\mu^2}}\,(0, -\sin\varphi, \cos\varphi)\cdot \mathbf{E} = -c_E \frac{1}{\sqrt{r}\sqrt{1-\mu^2}}\, \hat{e}_\varphi \cdot \mathbf{E}. \tag{3.7}$$

These transport terms express the acceleration field induced by **E** in spherical coordinates, as they are related to the negatives of the directional cosines of

E with respect to the unit vectors $\hat{e}_r$, $\hat{e}_\mu$, $\hat{e}_\varphi$. Hence, the TBE (3.2) is written in conservative, divergence form, as a flow in the **k**-space due to the electric field decomposed in each of the orthogonal components of the spherical **k**-coordinates. This can be easily derived from the expression for the divergence in general curvilinear coordinates, applied to the particular case of spherical coordinates $\mathbf{k}(r, \mu, \varphi)$. This calculation is performed below in the following section.

3.1.2 TBE in Divergence Form for k in Spherical Coordinates

The divergence in **k** in the standard spherical coordinates $(|\mathbf{k}|, \theta, \varphi)$ for a vector field $A(\mathbf{x}, \mathbf{k}, t) = (A_1, A_2, A_3) = A_{|\mathbf{k}|}\hat{e}_{|\mathbf{k}|} + A_\theta \hat{e}_\theta + A_\varphi \hat{e}_\varphi$ has the expression

$$\nabla_{\mathbf{k}} \cdot A = \frac{1}{|\mathbf{k}|^2}\frac{\partial(|\mathbf{k}|^2 A_{|\mathbf{k}|})}{\partial|\mathbf{k}|} + \frac{1}{|\mathbf{k}|\sin\theta}\frac{\partial\left(A_\theta \sin\theta\right)}{\partial\theta} + \frac{1}{|\mathbf{k}|\sin\theta}\frac{\partial A_\varphi}{\partial\varphi}\,. \tag{3.8}$$

The divergence of A, with a respective orthogonal decomposition $A = A_r\hat{e}_r + A_\mu\hat{e}_\mu + A_\varphi\hat{e}_\varphi$, in terms of the modified spherical coordinates (r, μ, φ) used in the TBE is obtained from (3.8) by taking into account $|\mathbf{k}|^2 = (2m^* k_B T_L/\hbar^2)r$, $\mu = \cos\theta$. Therefore $\dfrac{dr}{d|\mathbf{k}|} = \dfrac{\hbar}{\sqrt{2m^* k_B T_L}}\,2\sqrt{r}\,,\ \dfrac{d\mu}{d\theta} = -\sqrt{1-\mu^2}$, following that $\hat{e}_\mu = -\hat{e}_\theta$, $A_\mu = -A_\theta$, and $\hat{e}_{|\mathbf{k}|} = \hat{e}_r$, $A_{|\mathbf{k}|} = A_r$. We have then

$$\begin{aligned}
\nabla_{\mathbf{k}} \cdot A &= \frac{1}{r}\frac{\partial(rA_r)}{\partial r}\frac{dr}{d|\mathbf{k}|} + \frac{\hbar}{\sqrt{2m^* k_B T_L}}\left(\frac{1}{\sqrt{r}\sin\theta}\frac{\partial(A_\theta\sin\theta)}{\partial\mu}\frac{d\mu}{d\theta} + \frac{1}{\sqrt{r}\sin\theta}\frac{\partial A_\varphi}{\partial\varphi}\right) \\
&= \frac{\hbar}{\sqrt{2m^* k_B T_L}}\cdot\frac{2}{\sqrt{r}}\left[\frac{\partial}{\partial r}\left(rA_r\right) + \frac{\partial}{\partial\mu}\left(-\frac{\sqrt{1-\mu^2}}{2}A_\theta\right) + \frac{\partial}{\partial\varphi}\left(\frac{1}{2\sqrt{1-\mu^2}}A_\varphi\right)\right].
\end{aligned}$$

We obtain then the divergence in the modified spherical coordinates used in this work, since

$$\frac{\sqrt{r}}{2}\,\nabla_{\mathbf{k}}\cdot A = \left(\frac{\hbar}{\sqrt{2m^{*}k_{B}T_{L}}}\right)\left[\frac{\partial}{\partial r}\left(rA_{r}\right)+\frac{\partial}{\partial\mu}\left(\frac{\sqrt{1-\mu^{2}}}{2}A_{\mu}\right)+\frac{\partial}{\partial\varphi}\left(\frac{1}{2\sqrt{1-\mu^{2}}}A_{\varphi}\right)\right]. \tag{3.9}$$

So, the **k**-transport term in the TBE (3.2) can be expressed in the divergence form (3.9) by using

$$\frac{\sqrt{r}}{2}\left(\frac{-q\,\mathbf{E}(t,\mathbf{x})}{\hbar}\cdot\nabla_{\mathbf{k}}f\right)=\frac{\sqrt{r}}{2}\nabla_{\mathbf{k}}\cdot\left(\frac{-q\,\mathbf{E}(t,\mathbf{x})}{\hbar}f\right)=\frac{\sqrt{r}}{2}\nabla_{\mathbf{k}}\cdot A \tag{3.10}$$

for the vector field

$$A=\frac{-q\,\mathbf{E}(t,\mathbf{x})}{\hbar}f=\frac{-q\,\mathbf{E}(t,\mathbf{x})}{\hbar}\frac{\Phi}{\sqrt{r}/2}\,. \tag{3.11}$$

The formula (3.9) mentioned above for A can be interpreted geometrically as a flow of electric field in the orthogonal directions of the spherical coordinate geometry used, since by definition,

$$A_{r}=A\cdot\hat{e}_{r},\quad A_{\mu}=A\cdot\hat{e}_{\mu},\quad A_{\varphi}=A\cdot\hat{e}_{\varphi}. \tag{3.12}$$

We can express the Boltzmann Equation transformed to our coordinate system to the momentum as

$$\frac{\partial\Phi}{\partial t}+c_{D}\partial_{(x,y,z)}\cdot(\Phi\vec{v})-c_{E}\partial_{(r,\mu,\varphi)}\cdot\left(M\cdot\mathbf{E}\,\Phi/\sqrt{r}/2\right)=C(\Phi)\,, \tag{3.13}$$

with

$$c_{D}\vec{v}=(a_{1},a_{2},a_{3}),\quad M(r,\mu,\varphi)=\left(r\hat{e}_{r}\left|\frac{\sqrt{1-\mu^{2}}}{2}\hat{e}_{\mu}\right|\frac{1}{2\sqrt{1-\mu^{2}}}\hat{e}_{\varphi}\right). \tag{3.14}$$

3.2 DG formulation for the TBE and the Poisson equation

An important point is to keep in mind that, in the DG formulation used for the problem, a numerical flux is imposed in the surface integrals. So, when applying the upwind rule to the TBE in the scheme, the value of the approximated *pdf* must depend on the sign of terms of the form of components $\hat{e}_r \cdot \mathbf{E}$, etc. Therefore, the upwind rule to be applied is a condition that models the physics of electron transport in the new phase space $(x, y, z, r, \mu, \varphi)$ due to the mean electric field force acting over the charge carriers. The details of the discussion about the scheme and numerical fluxes can be found in Section 3.2.2.

3.2.1 Domain and Finite Element Space

Let's consider a $2\,D$ rectangular domain in the physical space and a rectangular domain $\Omega_{\mathbf{k}}$ in momentum space. We use simple rectangular cells

$$\Omega_{ijkmn} = \left[x_{i-\frac{1}{2}},\, x_{i+\frac{1}{2}}\right] \times \left[y_{j-\frac{1}{2}},\, y_{j+\frac{1}{2}}\right] \times K_{kmn}\,,$$

where

$$K_{kmn} = \left[r_{k-\frac{1}{2}},\, r_{k+\frac{1}{2}}\right] \times \left[\mu_{m-\frac{1}{2}},\, \mu_{m+\frac{1}{2}}\right] \times \left[\varphi_{n-\frac{1}{2}},\, \varphi_{n+\frac{1}{2}}\right]\,,$$

with

$$x_{i\pm\frac{1}{2}} = x_i \pm \frac{\Delta x_i}{2},\; y_{j\pm\frac{1}{2}} = y_j \pm \frac{\Delta y_j}{2},\; r_{k\pm\frac{1}{2}} = r_k \pm \frac{\Delta r_k}{2} \cdots\,,$$

and $i = 1, ..., N_x$, $j = 1, ..., N_y$, $k = 1, ...N_r$, $m = 1, ...N_\mu$, $n = 1, ..., N_\varphi$.

The test functions $\psi(x, y, r, \mu, \varphi)$ belong to the linear function space

$$V_h^1 = \left\{ v : v|_{\Omega_{ijkmn}} \in P^1(\Omega_{ijkmn}) \right\},$$

where $P^1(\Omega_{ijkmn})$ is the set of polynomials of degree at most 1 on the cell Ω_{ijkmn}.

A set of piecewise linear basis functions for V_h^1 in the open cell $\mathring{\Omega}_{ijkmn}$ is given by

$$\left\{ 1,\, 2\,\frac{(x - x_i)}{\Delta x_i},\, 2\,\frac{(y - y_j)}{\Delta y_j},\, 2\,\frac{(r - r_k)}{\Delta r_k},\, 2\,\frac{(\mu - \mu_m)}{\Delta \mu_m},\, 2\,\frac{(\varphi - \varphi_n)}{\Delta \varphi_n} \right\} \tag{3.15}$$

Hence, in the cell $\mathring{\Omega}_{ijkmn}$, we approximate our weighted-*pdf* Φ by a piecewise polynomial Φ_h of first degree in V_h^1,

$$\begin{aligned} \Phi_h(t, x, y, r, \mu, \varphi) &= T_{ijkmn}(t) + X_{ijkmn}(t)\,\frac{(x - x_i)}{\Delta x_i/2} + Y_{ijkmn}(t)\,\frac{(y - y_j)}{\Delta y_j/2} \\ &+ R_{ijkmn}(t)\,\frac{(r - r_k)}{\Delta r_k/2} + M_{ijkmn}(t)\,\frac{(\mu - \mu_m)}{\Delta \mu_m/2} + P_{ijkmn}(t)\,\frac{(\varphi - \varphi_n)}{\Delta \varphi_n/2} \end{aligned} \tag{3.16}$$

The charge density on $\left[x_{i-\frac{1}{2}},\, x_{i+\frac{1}{2}}\right] \times \left[y_{j-\frac{1}{2}},\, y_{j+\frac{1}{2}}\right]$ under this piecewise linear approximation is

$$\rho_h = \sum_{k=1}^{N_r} \sum_{m=1}^{N_\mu} \sum_{n=1}^{N_\varphi} \left[T_{ijkmn}(t) + X_{ijkmn}(t)\,\frac{(x - x_i)}{\Delta x_i/2} + Y_{ijkmn}(t)\,\frac{(y - y_j)}{\Delta y_j/2} \right] \Delta r_k \Delta \mu_m\, \Delta \varphi_n\,. \tag{3.17}$$

The problem is then reduced to find, by means of our numerical scheme, the unknowns

$$T_{ijkmn}(t),\, X_{ijkmn}(t),\, Y_{ijkmn}(t),\, R_{ijkmn}(t),\, M_{ijkmn}(t),\, P_{ijkmn}(t). \tag{3.18}$$

3.2.2 Discontinuous Galerkin Formulation for the TBE

The corresponding weak DG formulation and its corresponding approximation consists on finding $\Phi_h \in V_h^1$, such that for any test function $v_h \in V_h^1$ and a generic cell K of the decomposition of $\Omega_{\mathbf{x}} \times \Omega_{\mathbf{k}}$, solves

$$\begin{aligned}
&\int_K \frac{\partial \Phi_h}{\partial t}\, v_h d\sigma - \int_K \frac{\partial v_h}{\partial x}\,(a_1\,\Phi_h)\,d\sigma - \int_K \frac{\partial v_h}{\partial y}\,(a_2\,\Phi_h)\,d\sigma - \qquad (3.19)\\
&\int_K \frac{\partial v_h}{\partial r}\,(a_4\,\Phi_h)\,d\sigma - \int_K \frac{\partial v_h}{\partial \mu}\,(a_5\,\Phi_h)\,d\sigma - \int_K \frac{\partial v_h}{\partial \varphi}\,(a_6\,\Phi_h)\,d\sigma +\\
&F_x^+ - F_x^- + F_y^+ - F_y^- + F_r^+ - F_r^- + F_\mu^+ - F_\mu^- + F_\varphi^+ - F_\varphi^- = \int_K C(\Phi_h) v_h\, d\sigma,
\end{aligned}$$

where v_h is a test function in V_h^1, $d\sigma = dx\,dy\,dr\,d\mu\,d\varphi$, and where the $F^{\pm}$'s terms are boundary integrals over four-dimensional boundary surfaces associated to each 5-dimensional volume element Ω_{ijkmn}, that is,

$$\begin{aligned}
F_x^{\pm} &= \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_1 \hat{\Phi}_h v_h^{\mp}\Big|_{x_{i\pm\frac{1}{2}}}\, dydrd\mu d\varphi\\
F_y^{\pm} &= \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_2 \hat{\Phi}_h v_h^{\mp}\Big|_{y_{j\pm\frac{1}{2}}}\, dxdrd\mu d\varphi\\
F_r^{\pm} &= \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_4 \hat{\Phi}_h v_h^{\mp}\Big|_{r_{k\pm\frac{1}{2}}}\, dxdyd\mu d\varphi\\
F_\mu^{\pm} &= \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_5 \hat{\Phi}_h v_h^{\mp}\Big|_{\mu_{m\pm\frac{1}{2}}}\, dxdydrd\varphi\\
F_\varphi^{\pm} &= \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} a_6 \hat{\Phi}_h v_h^{\mp}\Big|_{\varphi_{n\pm\frac{1}{2}}}\, dxdydrd\mu \quad .
\end{aligned}$$

The values for $v_h^{\mp}$ are the ones for the function v_h on the interior of the considered cell. The upwind numerical flux $\hat{\Phi}_h$ defines the value of Φ_h at the boundary. That means Φ_h might be discontinuous at the boundary.

The collisional terms

$$\int_K C(\Phi_h) v_h \, d\sigma$$

become a linear combination, with numerical constant coefficients, of the the unknowns (3.18) which are precomputed and stored. The Poisson equation can be solved by either an integral formula, projecting the solution to the electric field into the space V_h^1, for the 1D device case, or by means of a LDG method, for higher dimensional cases. A Runge Kutta method is applied for the time evolution of the time dependent coefficients (3.18) for the piecewise linear approximation $\Phi_h \in V_h^1$.

3.2.3 Transport and Collision terms in the DG formulation

We consider now the details of the DG scheme for $5D$ plus time.

3.2.3.1 Collision terms

Denote by $K_{kmn} = \left[r_{k-\frac{1}{2}},\, r_{k+\frac{1}{2}}\right] \times \left[\mu_{m-\frac{1}{2}},\, \mu_{m+\frac{1}{2}}\right] \times \left[\varphi_{n-\frac{1}{2}},\, \varphi_{n+\frac{1}{2}}\right]$ the rectangular cells in the spherical coordinates for **k**-space. Because the collisional operators only perform integrations in **k**-space, it is convenient to write the basis functions in (3.15) as the product of two functions $\eta_{i,j}^p(x,y)$ and $\xi_{k,m,n}^p(r,\mu,\varphi)$, which are given in $\Omega_{ijkmn} = \Omega_I$ by

$$\left\{\eta_{i,j}^p(\vec{x})\right\}_{p=0,1,..,5} = \left\{1,\, 1,\, 1,\, 1\,,\, \frac{2(x-x_i)}{\Delta x_i},\, \frac{2(y-y_j)}{\Delta y_j}\right\}, \tag{3.20}$$

$$\left\{\xi_{k,m,n}^p(\vec{r})\right\}_{p=0,1,..,5} = \left\{1,\, \frac{2(r-r_k)}{\Delta r_k},\, \frac{2(\mu-\mu_m)}{\Delta \mu_m},\, \frac{2(\varphi-\varphi_n)}{\Delta \varphi_n},\, 1,\, 1\right\} \tag{3.21}$$

where we define

$$\vec{x} = (x, y)\,, \quad \vec{r} = (r, \mu, \varphi)\,, \quad \vec{r}\,' = (r', \mu', \varphi')\,, \quad d\,\vec{r} = dr\, d\mu\, d\varphi\,, \tag{3.22}$$

$$I = (i, j, k, m, n)\,, \tag{3.23}$$

$$\chi_I = \chi_I(\vec{x}, \vec{r}) = \begin{cases} 1 & \text{if } (\vec{x}, \vec{r}) \in \mathring{\Omega}_I, \\ 0 & \text{otherwise.} \end{cases} \tag{3.24}$$

and

$$W_I^0(t) := T_I(t)\,, \quad W_I^1(t) := R_I(t)\,, \quad W_I^2(t) := M_I(t)\,, \quad W_I^3(t) := P_I(t)\,, \tag{3.25}$$

$$W_I^4(t) := X_I(t)\,, \quad W_I^5(t) := Y_I(t)\,. \tag{3.26}$$

Then, in a piecewise continuous linear approximation of Φ, we have (almost everywhere), that

$$\Phi(t, \vec{x}, \vec{r}) = \sum_I \chi_I(\vec{x}, \vec{r}) \left[\sum_{p=0}^{5} W_I^p(t)\, \eta_{i,j}^p(\vec{x})\, \xi_{k,m,n}^p(\vec{r}) \right] \tag{3.27}$$

Because the phonon collision scatterings only consider the Fermi Golden Rule [18] and the spherical coordinates localize the negative part operator, there is a natural split of the collision operator in gain and loss terms of probability density rates.

Gain Term of the collisional operator. The **gain term**, when using the piecewise linear function (3.27), becomes

$$\frac{\sqrt{r}}{2}\int_0^\infty\int_{-1}^1\int_{-\pi}^\pi d\vec{r}\,'\,\mathcal{S}(\vec{r}\,',\vec{r})\sum_I \chi_I(\vec{x},\vec{r}\,')\sum_{p=0}^5 W_I^p(t)\eta_{i,j}^p(\vec{x})\xi_{k,m,n}^p(\vec{r}\,') \;\approx$$

$$\sum_I \frac{\sqrt{r}}{2}\int_{K_{kmn}} \mathcal{S}(\vec{r}\,',\vec{r})\,\chi_I(\vec{x},\vec{r}\,')\sum_{p=0}^5 W_I^p(t)\,\eta_{i,j}^p(\vec{x})\,\xi_{k,m,n}^p(\vec{r}\,')d\vec{r}\,' \;=$$

$$\sum_I\sum_{p=0}^5 \frac{\sqrt{r}}{2}\,\chi_{ij}(\vec{x})\,W_I^p(t)\,\eta_{i,j}^p(\vec{x})\int_{K_{kmn}} \mathcal{S}(\vec{r}\,',\vec{r})\,\xi_{k,m,n}^p(\vec{r}\,')\,d\vec{r}\,'\,,$$

with χ_I and W_I^p from (3.24 - 3.26)

$$\chi_{ij}(\vec{x}) = \begin{cases} 1 & \text{if } (x,y)\in\left[x_{i-\frac{1}{2}},\,x_{i+\frac{1}{2}}\right]\times\left[y_{j-\frac{1}{2}},\,y_{j+\frac{1}{2}}\right] \\ 0 & \text{otherwise}\end{cases}\quad.$$

In the weak formulation, the gain term is multiplied by the test function $\eta_{\bar{i},\bar{j}}^q(\vec{x})\,\xi_{\bar{k},\bar{m},\bar{n}}^q(\vec{r})$ and an integral over the domain $\Omega_{\bar{I}}$, $\bar{I}=(\bar{i},\bar{j},\bar{k},\bar{m},\bar{n})$, with respect to $(\vec{x},\vec{r})$ is performed, obtaining

$$\int_{\Omega_{\bar{I}}}\sum_I\sum_{p=0}^5 \frac{\sqrt{r}}{2}\,\chi_{ij}(\vec{x})\,W_I^p(t)\,\eta_{i,j}^p(\vec{x})\int_{K_{kmn}} \mathcal{S}(\vec{r}\,',\vec{r})\,\xi_{k,m,n}^p(\vec{r}\,')d\vec{r}\,' \quad \eta_{\bar{i},\bar{j}}^q(\vec{x})\,\xi_{\bar{k},\bar{m},\bar{n}}^q(\vec{r})d\vec{x}\,d\vec{r}, \tag{3.28}$$

or

$$\sum_I\sum_{p=0}^5 W_I^p(t)\int_{K_{\bar{k}\bar{m}\bar{n}}}\frac{\sqrt{r}}{2}\int_{K_{kmn}} \mathcal{S}(\vec{r}\,',\vec{r})\xi_{k,m,n}^p(\vec{r}\,')d\vec{r}\,'\xi_{\bar{k},\bar{m},\bar{n}}^q(\vec{r})d\vec{r}\int_{x_{\bar{i}-\frac{1}{2}}}^{x_{\bar{i}+\frac{1}{2}}}\int_{y_{\bar{j}-\frac{1}{2}}}^{y_{\bar{j}+\frac{1}{2}}}\chi_{ij}\,\eta_{i,j}^p(\vec{x})\,\eta_{\bar{i},\bar{j}}^q(\vec{x})d\vec{x}\,. \tag{3.29}$$

The integration with respect to x and y gives

$$\int_{x_{\bar{i}-\frac{1}{2}}}^{x_{\bar{i}+\frac{1}{2}}}\int_{y_{\bar{j}-\frac{1}{2}}}^{y_{\bar{j}+\frac{1}{2}}}\chi_{ij}(\vec{x})\,\eta_{i,j}^p(\vec{x})\,\eta_{\bar{i},\bar{j}}^q(\vec{x})\,dx\,dy = \delta_{i\bar{i}}\,\delta_{j\bar{j}}\,\beta_{pq}\,\Delta x_{\bar{i}}\,\Delta y_{\bar{j}}\,,$$

where the matrix β_{pq} is given by

$$(\beta_{pq}) = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{3} \end{pmatrix}.$$

Then, equation (3.29) is reduced to

$$\sum_{k,m,n}\sum_{p=0}^{5} W^p_{\bar{i}\bar{j}kmn}(t)\beta_{pq}\Delta x_{\bar{i}}\Delta y_{\bar{j}} \times \int_{K_{\bar{k}\bar{m}\bar{n}}} \left[\frac{\sqrt{r}}{2}\int_{K_{kmn}} \mathcal{S}(\vec{r}\,',\vec{r})\,\xi^p_{k,m,n}(\vec{r}\,')\,d\vec{r}\,'\right] \xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r})d\vec{r}. \tag{3.30}$$

Loss Term of the collisional operator. The weak formulation of the loss term of the collisional operator gives

$$\int_{\Omega_{\bar{I}}} \Phi(t,\vec{x},\vec{r}) \int_0^{+\infty} dr' \int_{-1}^{1} d\mu' \int_{-\pi}^{\pi} d\varphi'\, \mathcal{S}(\vec{r},\vec{r}\,')\frac{\sqrt{r'}}{2}\,\eta^q_{\bar{i},\bar{j}}(\vec{x})\,\xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r})\,d\vec{x}d\vec{r} \approx$$

$$\int_{\Omega_{\bar{I}}} \Phi(t,\vec{x},\vec{r}) \left[\sum_{k,m,n}\int_{K_{kmn}} \frac{\sqrt{r'}}{2}\mathcal{S}(\vec{r},\vec{r}\,')d\vec{r}\,'\right] \eta^q_{\bar{i},\bar{j}}(\vec{x})\xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r})\,d\vec{x}d\vec{r}. \tag{3.31}$$

Using the linear approximation of Φ given by (3.27), integral (3.31) becomes

$$\int_{\Omega_{\bar{I}}} \left[\sum_I \chi_I(\vec{x},\vec{r})\sum_{p=0}^{5} W^p_I(t)\,\eta^p_{i,j}(\vec{x})\,\xi^p_{k,m,n}(\vec{r})\right] \left[\sum_{k,m,n}\int_{K_{kmn}} \frac{1}{2}\sqrt{r'}\,\mathcal{S}(\vec{r},\vec{r}\,')\,d\vec{r}\,'\right] \eta^q_{\bar{i},\bar{j}}(\vec{x})\,\xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r})\,d\vec{x}\,d\vec{r}$$

$$= \sum_{p=0}^{5} W^p_{\bar{I}}(t)\int_{\Omega_{\bar{I}}} \eta^p_{\bar{i},\bar{j}}(\vec{x})\xi^p_{\bar{k},\bar{m},\bar{n}}(\vec{r}) \left[\sum_{k,m,n}\int_{K_{kmn}} \frac{\sqrt{r'}}{2}\mathcal{S}(\vec{r},\vec{r}\,')d\vec{r}\,'\right] \eta^q_{\bar{i},\bar{j}}(\vec{x})\xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r})\,d\vec{x}d\vec{r}\,.$$

Therefore, equation (3.31) reduces to

$$\sum_{p=0}^{5} W^p_{\bar{I}}(t)\beta_{pq}\Delta x_{\bar{i}}\Delta y_{\bar{j}} \sum_{k,m,n}\int_{K_{\bar{k}\bar{m}\bar{n}}} \left[\int_{K_{kmn}} \frac{\sqrt{r'}}{2}\,\mathcal{S}(\vec{r},\vec{r}\,')\,d\vec{r}\,'\right] \xi^p_{\bar{k},\bar{m},\bar{n}}(\vec{r})\,\xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r})\,d\vec{r}. \tag{3.32}$$

3.2.3.2 Transport terms

The following notation for boundary terms will be needed. We denote

$$\begin{aligned}
\hat{\Phi}_{i\pm\frac{1}{2}} &= \hat{\Phi}(t, x_{i\pm\frac{1}{2}}, y, r, \mu, \varphi)\,, \quad \hat{\Phi}_{j\pm\frac{1}{2}} = \hat{\Phi}(t, x, y_{j\pm\frac{1}{2}}, r, \mu, \varphi) \qquad (3.33)\\
\hat{\Phi}_{k\pm\frac{1}{2}} &= \hat{\Phi}(t, x, y, r_{k\pm\frac{1}{2}}, \mu, \varphi)\,, \quad \hat{\Phi}_{m\pm\frac{1}{2}} = \hat{\Phi}(t, x, y, r, \mu_{m\pm\frac{1}{2}}, \varphi)\,,\\
\hat{\Phi}_{n\pm\frac{1}{2}} &= \hat{\Phi}(t, x, y, r, \mu, \varphi_{n\pm\frac{1}{2}})\,,\\
\eta^p_{i\pm1,j}|_{i\pm\frac{1}{2}} &= \eta^p_{i\pm1,j}(x_{i\pm\frac{1}{2}}, y)\,, \quad \eta^p_{i,j}|_{i\pm\frac{1}{2}} = \eta^p_{i,j}(x_{i\pm\frac{1}{2}}, y)\,, \qquad (3.34)\\
\eta^p_{i,j\pm1}|_{j\pm\frac{1}{2}} &= \eta^p_{i,j\pm1}(x, y_{j\pm\frac{1}{2}})\,, \quad \eta^p_{i,j}|_{j\pm\frac{1}{2}} = \eta^p_{i,j}(x, y_{j\pm\frac{1}{2}})\,, \quad p \in \{0,\, 1,\, \cdots, 5\}.\\
\xi^p_{k,m,n}|_{k\pm\frac{1}{2}} &= \xi^p_{k,m,n}(r_{k\pm\frac{1}{2}}, \mu, \varphi)\,, \quad \xi^p_{k,m,n}|_{m\pm\frac{1}{2}} = \xi^p_{k,m,n}(r, \mu_{m\pm\frac{1}{2}}, \varphi)\,,\\
\xi^p_{k,m,n}|_{n\pm\frac{1}{2}} &= \xi^p_{k,m,n}(r, \mu, \varphi_{n\pm\frac{1}{2}})\\
\xi^p_{k\pm1,m,n}|_{k\pm\frac{1}{2}} &= \xi^p_{k\pm1,m,n}(r_{k\pm\frac{1}{2}}, \mu, \varphi)\,, \quad \xi^p_{k,m\pm1,n}|_{m\pm\frac{1}{2}} = \xi^p_{k,m\pm1,n}(r, \mu_{m\pm\frac{1}{2}}, \varphi)\,,\\
\xi^p_{k,m,n\pm1}|_{n\pm\frac{1}{2}} &= \xi^p_{k,m,n\pm1}(r, \mu, \varphi_{n\pm\frac{1}{2}})\,, \quad p \in \{0,\, 1,\, \cdots, 5\}. \qquad (3.35)
\end{aligned}$$

We consider first the weak formulation of the transport terms in space, namely $\frac{\partial}{\partial x}\,(a_1\Phi)$ and $\frac{\partial}{\partial y}\,(a_2\Phi)$, related to the advection in $\mathbf{x}$, where the first cartesian component a_1 of the electron group velocity is involved. Because their discretization forms are similar we only present the one for $\frac{\partial}{\partial x}\,(a_1\Phi)$.

$$\begin{aligned}
(A_1) &= \int_{\Omega_I} \frac{\partial}{\partial x}\left[a_1(r,\mu,\varphi)\,\Phi(t,\vec{x},\vec{r})\right]\psi(\vec{x},\vec{r})\,d\vec{x}\,d\vec{r} =\\
&= \frac{1}{\Delta x_i}\int_{\Omega_I} a_1(\vec{r})\left[\hat{\Phi}_{i+\frac{1}{2}}\psi_{i+\frac{1}{2}} - \hat{\Phi}_{i-\frac{1}{2}}\psi_{i-\frac{1}{2}}\right]d\vec{x}d\vec{r} - \int_{\Omega_I} a_1(\vec{r})\Phi(t,\vec{x},\vec{r})\frac{\partial}{\partial x}\psi(\vec{x},\vec{r})d\vec{x}d\vec{r}.
\end{aligned}$$

Due to the upwind flux rule, we have to consider two cases depending on the sign of a_1. In the sequel, the symbol $\approx$ will denote the approximation of given integral terms.

If $a_1(\vec{r}) > 0$ in K_{kmn}, for $q = 0, ..., 5$, one obtains

$$
\begin{aligned}
(A_1) \;\approx\; & \sum_{p=0}^{5} \frac{W_I^p(t)}{\Delta x_i} \int_{\Omega_I} a_1(\vec{r}) \eta_{i,j}^p|_{i+\frac{1}{2}} \xi_{k,m,n}^p(\vec{r}) \eta_{i,j}^q|_{i+\frac{1}{2}} \xi_{k,m,n}^q(\vec{r}) d\vec{x} d\vec{r} \\
- \; & \sum_{p=0}^{5} \frac{W_{i-1\,jkmn}^p(t)}{\Delta x_i} \int_{\Omega_I} a_1(\vec{r}) \eta_{i-1,j}^p|_{i-\frac{1}{2}} \xi_{k,m,n}^p(\vec{r}) \eta_{i,j}^q|_{i-\frac{1}{2}} \xi_{k,m,n}^q(\vec{r}) d\vec{x} d\vec{r} \\
- \; & \sum_{p=0}^{5} W_I^p(t) \int_{\Omega_I} a_1(\vec{r})\, \eta_{i,j}^p(\vec{x})\, \xi_{k,m,n}^p(\vec{r})\, \frac{2\,\delta_{q4}}{\Delta x_i}\, \xi_{k,m,n}^q(\vec{r})\, d\vec{x}\, d\vec{r} \\
= \; & \sum_{p=0}^{5} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \eta_{i,j}^p|_{i+\frac{1}{2}} \eta_{i,j}^q|_{i+\frac{1}{2}} dy \cdot \int_{K_{kmn}} a_1(\vec{r}) \xi_{k,m,n}^p(\vec{r}) \xi_{k,m,n}^q(\vec{r}) d\vec{r} \cdot W_I^p(t) \\
- \; & \sum_{p=0}^{5} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \eta_{i-1,j}^p|_{i-\frac{1}{2}} \eta_{i,j}^q|_{i-\frac{1}{2}} dy \int_{K_{kmn}} a_1(\vec{r}) \xi_{k,m,n}^p(\vec{r}) \xi_{k,m,n}^q(\vec{r}) d\vec{r} \cdot W_{i-1\,jkmn}^p(t) \\
- \; & \sum_{p=0}^{5} \left[\frac{2\,\delta_{q4}}{\Delta x_i} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \eta_{i,j}^p(\vec{x})\, d\vec{x} \right] \left[\int_{K_{kmn}} a_1(\vec{r}) \xi_{k,m,n}^p(\vec{r}) \xi_{k,m,n}^q(\vec{r})\, d\vec{r} \right] \cdot W_I^p(t)\,.
\end{aligned}
$$

If $a_1(\vec{r}) < 0$ in K_{kmn}, for $q = 0, ..., 5$,

$$
\begin{aligned}
(A_1) \;\approx\; & \sum_{p=0}^{5} \frac{W_{i+1\,jkmn}^p(t)}{\Delta x_i} \int_{\Omega_I} a_1(\vec{r}) \eta_{i+1,j}^p|_{i+\frac{1}{2}} \xi_{k,m,n}^p(\vec{r}) \eta_{i,j}^q|_{i+\frac{1}{2}} \xi_{k,m,n}^q(\vec{r})\, d\vec{x} d\vec{r} \\
- \; & \frac{1}{\Delta x_i} \sum_{p=0}^{5} W_I^p(t) \int_{\Omega_I} a_1(\vec{r}) \eta_{i,j}^p|_{i-\frac{1}{2}} \xi_{k,m,n}^p(\vec{r}) \eta_{i,j}^q|_{i-\frac{1}{2}} \xi_{k,m,n}^q(\vec{r})\, d\vec{x} d\vec{r} \\
- \; & \sum_{p=0}^{5} W_I^p(t) \int_{\Omega_I} a_1(\vec{r})\, \eta_{i,j}^p(\vec{x})\, \xi_{k,m,n}^p(\vec{r})\, \frac{2\,\delta_{q4}}{\Delta x_i}\, \xi_{k,m,n}^q(\vec{r})\, d\vec{x}\, d\vec{r} \\
= \; & \sum_{p=0}^{5} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \eta_{i+1,j}^p|_{i+\frac{1}{2}} \eta_{i,j}^q|_{i+\frac{1}{2}} dy \int_{K_{kmn}} a_1(\vec{r}) \xi_{k,m,n}^p(\vec{r}) \xi_{k,m,n}^q(\vec{r}) d\vec{r}\, W_{i+1\,jkmn}^p(t) \\
- \; & \sum_{p=0}^{5} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \eta_{i,j}^p|_{i-\frac{1}{2}} \eta_{i,j}^q|_{i-\frac{1}{2}} dy \int_{K_{kmn}} a_1(\vec{r}) \xi_{k,m,n}^p(\vec{r}) \xi_{k,m,n}^q(\vec{r}) d\vec{r}\, W_I^p(t) \\
- \; & \sum_{p=0}^{5} \frac{2\,\delta_{q4}}{\Delta x_i} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \eta_{i,j}^p(\vec{x})\, dx\, dy \int_{K_{kmn}} a_1(\vec{r})\, \xi_{k,m,n}^p(\vec{r})\, \xi_{k,m,n}^q(\vec{r})\, d\vec{r}\, W_I^p(t)\,.
\end{aligned}
$$

We consider now the weak formulation for the transport terms in momentum space $\frac{\partial}{\partial r}\left(a_4\,\Phi\right)+\frac{\partial}{\partial \mu}\left(a_5\,\Phi\right)+\frac{\partial}{\partial \varphi}\left(a_6\,\Phi\right)$ advected by the electric field. It can be noticed in Eq. 3.2 that all the terms a_4, a_5, a_6 are the sum of terms of the form $a_*(\vec{r})\,E_*(t,\vec{x})$, where $E_*(t,\vec{x})$ is a cartesian component of the electric field.

The r-derivative including a_4 can be split as a sum of terms as the following

$$\begin{aligned}
(A_{4*}) &= \int_{\Omega_I}\frac{\partial}{\partial r}\left[a_*(\vec{r})\,E_*(t,\vec{x})\,\Phi(t,\vec{x},\vec{r})\right]\psi(\vec{x},\vec{r})\,d\vec{x}\,d\vec{r}\\
&= \frac{1}{\Delta r_k}\int_{\Omega_I} a_*|_{k+\frac{1}{2}}\,E_*(t,\vec{x})\,\hat{\Phi}_{k+\frac{1}{2}}\,\psi_{k+\frac{1}{2}}\,d\vec{x}\,d\vec{r}-\frac{1}{\Delta r_k}\int_{\Omega_I} a_*|_{k-\frac{1}{2}}\,E_*(t,\vec{x})\,\hat{\Phi}_{k-\frac{1}{2}}\,\psi_{k-\frac{1}{2}}\,d\vec{x}\,d\vec{r}\\
&- \int_{\Omega_I} a_*(\vec{r})\,E_*(t,\vec{x})\,\Phi(t,\vec{x},\vec{r})\frac{\partial}{\partial r}\psi(\vec{x},\vec{r})\,d\vec{x}\,d\vec{r}.
\end{aligned}$$

By the Upwind Flux Rule, if $a_*(\vec{r})\,E_*(t,\vec{x})>0$ in $\partial_r^{\pm}\Omega_I$, for $q=0,...,5$,

$$\begin{aligned}
(A_{4*}) \approx & \sum_{p=0}^{5}\frac{W_I^p}{\Delta r_k}\int_{\Omega_I} a_*|_{k+\frac{1}{2}}E_*(t,\vec{x})\eta_{i,j}^p(\vec{x})\xi_{k,m,n}^p|_{k+\frac{1}{2}}\eta_{i,j}^q(\vec{x})\xi_{k,m,n}^q|_{k+\frac{1}{2}}d\vec{x}d\vec{r}\\
- & \sum_{p=0}^{5}\frac{W_{ijk-1mn}^p}{\Delta r_k}\int_{\Omega_I} a_*|_{k-\frac{1}{2}}E_*\eta_{i,j}^p(\vec{x})\xi_{k-1,m,n}^p|_{k-\frac{1}{2}}\eta_{i,j}^q(\vec{x})\xi_{k,m,n}^q|_{k-\frac{1}{2}}d\vec{x}d\vec{r}\\
- & \sum_{p=0}^{5}W_I^p(t)\int_{\Omega_I} a_*(\vec{r})\,E_*(t,\vec{x})\,\eta_{i,j}^p(\vec{x})\,\xi_{k,m,n}^p(\vec{r})\,\frac{2\,\delta_{q1}}{\Delta r_k}\,\eta_{i,j}^q(\vec{x})\,d\vec{x}\,d\vec{r}\\
= & \sum_{p=0}^{5}\left[\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}}E_*(t,\vec{x})\eta_{i,j}^p(\vec{x})\eta_{i,j}^q(\vec{x})dxdy\right]\left\{\left[\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}}\int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}}a_*|_{k+\frac{1}{2}}\xi_{k,m,n}^p|_{k+\frac{1}{2}}\xi_{k,m,n}^q|_{k+\frac{1}{2}}d\mu d\varphi\right.\right.\\
- & \left.\frac{2\,\delta_{q1}}{\Delta r_k}\int_{K_{kmn}}a_*(\vec{r})\,\xi_{k,m,n}^p(\vec{r})\,d\vec{r}\right]W_I^p\\
- & \left.\left[\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}}\int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}}a_*|_{k-\frac{1}{2}}\,\xi_{k-1,m,n}^p|_{k-\frac{1}{2}}\,\xi_{k,m,n}^q|_{k-\frac{1}{2}}\,d\mu\,d\varphi\right]W_{ijk-1mn}^p\right\}.
\end{aligned}$$

If $a_*(\vec{r})\, E_*(t,\vec{x}) < 0$ in $\partial_r^{\pm}\Omega_I$, $q = 0, ..., 5$,

$$
\begin{aligned}
(A_{4*}) \;\approx\; & \frac{1}{\Delta r_k}\sum_{p=0}^{5} W^p_{ijk+1mn}(t)\int_{\Omega_I} a_*|_{k+\frac{1}{2}}\, E_*(t,\vec{x})\,\eta^p_{i,j}(\vec{x})\,\xi^p_{k+1,m,n}|_{k+\frac{1}{2}}\eta^q_{i,j}(\vec{x})\,\xi^q_{k,m,n}|_{k+\frac{1}{2}}\,d\vec{x}\,d\vec{r} \\
- \;& \sum_{p=0}^{5}\frac{W^p_I}{\Delta r_k}\int_{\Omega_I} a_*|_{k-\frac{1}{2}} E_*\eta^p_{i,j}(\vec{x})\xi^p_{k,m,n}|_{k-\frac{1}{2}}\eta^q_{i,j}(\vec{x})\xi^q_{k,m,n}|_{k-\frac{1}{2}}d\vec{x}d\vec{r} \\
- \;& \sum_{p=0}^{5} W^p_I(t)\int_{\Omega_I} a_*(\vec{r})\, E_*(t,\vec{x})\,\eta^p_{i,j}(\vec{x})\,\xi^p_{k,m,n}(\vec{r})\,\frac{2\,\delta_{q1}}{\Delta r_k}\,\eta^q_{i,j}(\vec{x})\,d\vec{x}\,d\vec{r} \\
= \;& \sum_{p=0}^{5}\left[\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} E_*(t,\vec{x})\,\eta^p_{i,j}(\vec{x})\,\eta^q_{i,j}(\vec{x})\,dx\,dy\right] \\
& \times\left\{\left[\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}}\int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_*|_{k+\frac{1}{2}}\,\xi^p_{k+1,m,n}|_{k+\frac{1}{2}}\,\xi^q_{k,m,n}|_{k+\frac{1}{2}}\,d\mu\,d\varphi\right] W^p_{ijk+1mn}(t)\right. \\
& -\left[\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}}\int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_*|_{k-\frac{1}{2}}\,\xi^p_{k,m,n}|_{k-\frac{1}{2}}\,\xi^q_{k,m,n}|_{k-\frac{1}{2}}\,d\mu\,d\varphi\right. \\
& \left.\left.+\,\frac{2\,\delta_{q1}}{\Delta r_k}\int_{K_{kmn}} a_*(\vec{r})\,\xi^p_{k,m,n}(\vec{r})\,d\vec{r}\right] W^p_I(t)\right\}.
\end{aligned}
$$

The weak form for the term related to $\frac{\partial}{\partial\mu}\,(a_5\Phi)$ is

$$
(A_{5*}) = \int_{\Omega_I}\frac{\partial}{\partial\mu}\left[a_*(\vec{r})\, E_*(t,\vec{x})\,\Phi(t,\vec{x},\vec{r})\right]\psi(\vec{x},\vec{r})\,d\vec{x}\,d\vec{r}.
$$

By the Upwind Flux rule, if $a_*(\vec{r})\, E_*(t,\vec{x}) > 0$ in $\partial_\mu^{\pm}\Omega_I$, $q = 0, ..., 5$,

$$
\begin{aligned}
(A_{5*}) \;\approx\; & \sum_{p=0}^{5}\left[\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} E_*(t,\vec{x})\,\eta^p_{i,j}(\vec{x})\,\eta^q_{i,j}(\vec{x})\,dx\,dy\right] \\
& \times\left\{\left[\int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}}\int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_*|_{m+\frac{1}{2}}\,\xi^p_{k,m,n}|_{m+\frac{1}{2}}\,\xi^q_{k,m,n}|_{m+\frac{1}{2}}\,dr\,d\varphi\right.\right. \\
& \left.-\frac{2\,\delta_{q2}}{\Delta\mu_m}\int_{K_{kmn}} a_*(\vec{r})\,\xi^p_{k,m,n}(\vec{r})\,d\vec{r}\right] W^p_I(t) \\
& -\left.\left[\int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}}\int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_*|_{m-\frac{1}{2}}\,\xi^p_{k,m-1,n}|_{m-\frac{1}{2}}\,\xi^q_{k,m,n}|_{m-\frac{1}{2}}\,dr\,d\varphi\right] W^p_{ijkm-1n}(t)\right\}.
\end{aligned}
$$

If $a_*(\vec{r})\, E_*(t,\vec{x}) < 0$ in $\partial_\mu^{\pm}\Omega_I$, $q = 0, ..., 5$,

$$
\begin{aligned}
(A_{5*}) \;\approx\; & \sum_{p=0}^{5} \left[\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} E_*(t,\vec{x})\, \eta_{i,j}^{p}(\vec{x})\, \eta_{i,j}^{q}(\vec{x})\, dx\, dy \right] \\
& \times \left\{ \left[\int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_*|_{m+\frac{1}{2}}\, \xi_{k,m+1,n}^{p}|_{m+\frac{1}{2}}\, \xi_{k,m,n}^{q}|_{m+\frac{1}{2}}\, dr\, d\varphi \right] W_{ijkm+1n}^{p}(t) \right. \\
& - \left[\int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} a_*|_{m-\frac{1}{2}}\, \xi_{k,m,n}^{p}|_{m-\frac{1}{2}}\, \xi_{k,m,n}^{q}|_{m-\frac{1}{2}}\, dr\, d\varphi \right. \\
& \left. \left. + \frac{2\,\delta_{q2}}{\Delta\mu_m} \int_{K_{kmn}} a_*(\vec{r})\, \xi_{k,m,n}^{p}(\vec{r})\, d\vec{r} \right] W_I^{p}(t) \right\} .
\end{aligned}
$$

The weak form for the term related to $\frac{\partial}{\partial\varphi}\,(a_6\Phi)$ is

$$
(A_{6*}) \qquad \int_{\Omega_I} \frac{\partial}{\partial\varphi} \left[a_*(\vec{r})\, E_*(t,\vec{x})\, \Phi(t,\vec{x},\vec{r}) \right] \psi(\vec{x},\vec{r})\, d\vec{x}\, d\vec{r} \tag{3.36}
$$

By the Upwind Flux Rule, if $a_*(\vec{r})\, E_*(t,\vec{x}) > 0$ in $\partial_\varphi^{\pm}\Omega_I$, $q = 0, ..., 5$,

$$
\begin{aligned}
(A_{6*}) \;\approx\; & \sum_{p=0}^{5} \left[\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} E_*(t,\vec{x})\, \eta_{i,j}^{p}(\vec{x})\, \eta_{i,j}^{q}(\vec{x})\, dx\, dy \right] \times \\
& \left\{ \left[\int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} a_*|_{n+\frac{1}{2}} \xi_{k,m,n}^{p}|_{n+\frac{1}{2}} \xi_{k,m,n}^{q}|_{n+\frac{1}{2}} dr d\mu \;\; - \frac{2\,\delta_{q3}}{\Delta\varphi_n} \int_{K_{kmn}} a_*(\vec{r}) \xi_{k,m,n}^{p}(\vec{r}) d\vec{r} \right] W_I^{p}(t) \right. \\
& \left. - \left[\int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} a_*|_{n-\frac{1}{2}}\, \xi_{k,m,n-1}^{p}|_{n-\frac{1}{2}}\, \xi_{k,m,n}^{q}|_{n-\frac{1}{2}}\, dr\, d\mu \right] W_{ijkmn-1}^{p}(t) \right\} .
\end{aligned}
$$

If $a_*(\vec{r})\, E_*(t,\vec{x}) < 0$ in $\partial_\varphi^{\pm}\Omega_I$, $q = 0, ..., 5$,

$$
\begin{aligned}
(A_{6*}) \;\approx\; & \sum_{p=0}^{5} \left[\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} E_*(t,\vec{x})\, \eta_{i,j}^{p}(\vec{x})\, \eta_{i,j}^{q}(\vec{x})\, dx\, dy \right] \times \\
& \left\{ \left[\int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} a_*|_{n+\frac{1}{2}}\, \xi_{k,m,n+1}^{p}|_{n+\frac{1}{2}}\, \xi_{k,m,n}^{q}|_{n+\frac{1}{2}}\, dr\, d\mu \right] W_{ijkmn+1}^{p}(t) \right. \\
& - \left[\int_{r_{k-\frac{1}{2}}}^{r_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} a_*|_{n-\frac{1}{2}}\, \xi_{k,m,n}^{p}|_{n-\frac{1}{2}}\, \xi_{k,m,n}^{q}|_{n-\frac{1}{2}}\, dr\, d\mu \right. \\
& \left. \left. + \frac{2\,\delta_{q3}}{\Delta\varphi_n} \int_{K_{kmn}} a_*(\vec{r})\, \xi_{k,m,n}^{p}(\vec{r})\, d\vec{r} \right] W_I^{p}(t) \right\} .
\end{aligned}
$$

3.2.3.3 Computation of Collision Integrals for electron - phonon scattering with radial dependance.

In the case of an energy band function with radial dependance $\varepsilon(r)$,

$$
\begin{aligned}
\mathcal{S}(r,r') &= c_0\, \delta(\mathcal{E}(r') - \mathcal{E}(r)) + c_+\, \delta(\mathcal{E}(r') - \mathcal{E}(r) + \alpha_p) + c_-\, \delta(\mathcal{E}(r') - \mathcal{E}(r) - \alpha_p) \\
&= \sum_{l=-1}^{+1} c_l\, \delta(\mathcal{E}(r') - \mathcal{E}(r) + l\alpha_p) \,. \qquad (3.37)
\end{aligned}
$$

The radial energy band function can be projected on the space of piecewise linear functions of r to obtain

$$
\mathcal{E}_h(r) = \sum_{k=1}^{N_r} \chi_k \left[\mathcal{E}(r_k) + A_k(r - r_k) \right] = \sum_{k=1}^{N_r} \chi_k \left[\, \mathcal{E}(r_k) \, + \, \partial_r \mathcal{E}(r_k)\, (r - r_k) \, \right] , \qquad (3.38)
$$

and, after this projection, we can calculate the collision integrals involving a delta distribution with the piecewise linear function in their argument. The

computation of such collisional integrals are given by

$$\begin{aligned}
\int_K C(\Phi_h) v_h \, d\sigma &= \sum_{k,m,n} \sum_{p=0}^{5} W^p_{\bar{i}\bar{j}kmn} \beta_{pq} \Delta x_{\bar{i}} \Delta y_{\bar{j}} \int_{K_{\bar{k}\bar{m}\bar{n}}} \int_{K_{kmn}} \mathcal{S}(r', r) \, \xi^p_{k,m,n}(\vec{r}\,') \, d\vec{r}\,' \frac{\sqrt{r}}{2} \, \xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r}) \, d\vec{r} \\
&- \sum_{p=0}^{5} W^p_{\bar{I}}(t) \beta_{pq} \Delta x_{\bar{i}} \Delta y_{\bar{j}} \sum_{k,m,n} \int_{K_{kmn}} \left[\int_{K_{\bar{k}\bar{m}\bar{n}}} \mathcal{S}(r, r') \, \xi^p_{\bar{k},\bar{m},\bar{n}}(\vec{r}) \, \xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r}) \, d\vec{r} \right] \frac{\sqrt{r'}}{2} \, d\vec{r}\,' \\
&= \sum_{k,m,n} \sum_{p=0}^{5} W^p_{\bar{i}\bar{j}kmn}(t) \beta_{pq} \Delta x_{\bar{i}} \Delta y_{\bar{j}} \times \qquad (3.39) \\
&\quad \int_{K_{\bar{k}\bar{m}\bar{n}}} \left[\int_{K_{kmn}} \sum_{l=-1}^{+1} c_l \, \delta(\mathcal{E}(r) - \mathcal{E}(r') + l\alpha_p) \, \xi^p_{k,m,n}(\vec{r}\,') \, d\vec{r}\,' \right] \frac{\sqrt{r}}{2} \, \xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r}) \, d\vec{r} \\
&- \sum_{p=0}^{5} W^p_{\bar{I}}(t) \beta_{pq} \Delta x_{\bar{i}} \Delta y_{\bar{j}} \times \\
&\quad \sum_{k,m,n} \int_{K_{kmn}} \left[\int_{K_{\bar{k}\bar{m}\bar{n}}} \sum_{l=-1}^{+1} c_l \, \delta(\mathcal{E}(r') - \mathcal{E}(r) + l\alpha_p) \, \xi^p_{\bar{k},\bar{m},\bar{n}}(\vec{r}) \, \xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r}) \, d\vec{r} \right] \frac{\sqrt{r'}}{2} d\vec{r}\,'.
\end{aligned}$$

In order to perform the integrations involving $\sqrt{r}$ numerically by means of Gaussian quadrature, the change of variables $r = s^2$ is applied, so that the

functions of s to be integrated are just polynomials,

$$\int_K C(\Phi_h) v_h \, d\sigma =$$

$$\sum_{k,m,n} \sum_{p=0}^{5} W^p_{\bar{i}\bar{j}kmn}(t) \beta_{pq} \Delta x_{\bar{i}} \Delta y_{\bar{j}} \int_{K_{\bar{k}\bar{m}\bar{n}}} \frac{s}{2} \, \xi^q_{\bar{k},\bar{m},\bar{n}}(s^2, \mu, \varphi) \, 2s \, \times$$

$$\left[\sum_{l=-1}^{+1} c_l \int_{K_{kmn}} \delta(\mathcal{E}(r_{\bar{k}}) + A_{\bar{k}}(s^2 - r_{\bar{k}}) + l\alpha_p - \mathcal{E}(r_k) - A_k(r' - r_k)) \, \xi^p_{k,m,n}(\vec{r}\,') \, d\vec{r}\,' \right] ds d\mu d\varphi$$

$$- \sum_{p=0}^{5} W^p_{\bar{I}}(t) \beta_{pq} \Delta x_{\bar{i}} \Delta y_{\bar{j}} \sum_{k,m,n} \int_{K_{kmn}} \frac{s'}{2} \, 2s' \, \times$$

$$\left[\sum_{l=-1}^{+1} c_l \int_{K_{\bar{k}\bar{m}\bar{n}}} \delta(\mathcal{E}(s'^2) + l\alpha_p - \mathcal{E}(r_{\bar{k}}) - A_{\bar{k}}(r - r_{\bar{k}})) \, \xi^p_{\bar{k},\bar{m},\bar{n}}(\vec{r}) \, \xi^q_{\bar{k},\bar{m},\bar{n}}(\vec{r}) \, d\vec{r} \right] ds' d\mu' d\varphi'$$

$$= \sum_{k,m,n} \sum_{p=0}^{5} W^p_{\bar{i}\bar{j}kmn}(t) \beta_{pq} \Delta x_{\bar{i}} \Delta y_{\bar{j}} \, \times \tag{3.40}$$

$$\int_{K_{\bar{k}\bar{m}\bar{n}}} \xi^q_{\bar{k},\bar{m},\bar{n}}(s^2, \mu, \varphi) \, \chi_k \left(\frac{\mathcal{E}(r_{\bar{k}}) + A_{\bar{k}}(s^2 - r_{\bar{k}}) + l\alpha_p - \mathcal{E}(r_k) + A_k r_k}{A_k} \right) s^2 ds d\mu d\varphi \, \times$$

$$\left[\sum_{l=-1}^{+1} c_l \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} \xi^p_{k,m,n} \left(\frac{\mathcal{E}(r_{\bar{k}}) + A_{\bar{k}}(s^2 - r_{\bar{k}}) + l\alpha_p - \mathcal{E}(r_k) + A_k r_k}{A_k}, \mu', \varphi' \right) d\mu' d\varphi' \right] -$$

$$\sum_{p=0}^{5} W^p_{\bar{I}}(t) \beta_{pq} \Delta x_{\bar{i}} \Delta y_{\bar{j}} \sum_{k,m,n} \int_{K_{kmn}} d\mu' d\varphi' \, s'^2 \, \chi_{\bar{k}} \left(\frac{\mathcal{E}(r_k) + A_k(s'^2 - r_k) + l\alpha_p - \mathcal{E}(r_{\bar{k}}) + A_{\bar{k}} r_{\bar{k}}}{A_{\bar{k}}} \right)$$

$$\times \left[\sum_{l=-1}^{+1} c_l \int_{\mu_{\bar{m}-\frac{1}{2}}}^{\mu_{\bar{m}+\frac{1}{2}}} \int_{\varphi_{\bar{n}-\frac{1}{2}}}^{\varphi_{\bar{n}+\frac{1}{2}}} \xi^p_{\bar{k},\bar{m},\bar{n}}(r(s), \mu, \varphi) \, \xi^q_{\bar{k},\bar{m},\bar{n}}(r(s), \mu, \varphi) \, d\mu d\varphi \right] \Bigg|_{r(s)} ds' \, ,$$

with $r(s) = \frac{\mathcal{E}(r_k) + A_k(s'^2 - r_k) + l\alpha_p - \mathcal{E}(r_{\bar{k}}) + A_{\bar{k}} r_{\bar{k}}}{A_{\bar{k}}}$.

The integrals above involve only polynomials, which are numerically computed by Gaussian quadrature rules.

3.2.4 The algorithm for time evolution

Starting with given initial and boundary conditions, the algorithm advances from t^n to t^{n+1} in the way described below.

1. Compute the density ρ.
2. Solve the Poisson equation and find the electric field $\mathbf{E}$.
3. Compute the transport terms a_i's.
4. Compute the collision part.
5. Solve the (large) system of ordinary differential equations for the coefficients of the linear approximation of Φ_h (which are obtained from the DG formulation), by using a TVD Runge - Kutta scheme.
6. Repeat the previous steps as needed.

3.2.5 Poisson Equation in 1D

$$-\partial_x^2 \Psi = \frac{c_p}{\epsilon_r} \left[\mathcal{N}_h(x) - \rho_h(t,x) \right] \in V_h^1 \,, \tag{3.41}$$

with Dirichlet BC for $\Psi(x,t)$, to obtain $E(x,t) = -c_v \, \partial_x \Psi(x,t)$. For the 1D case, there is an analytical solution to the Poisson Eq. BVP with Dirichlet

BC, given by the integral formula

$$\begin{aligned}
\Psi(x,t) &= \Psi(0) + \left[\Psi(1) - \Psi(0) + \int_0^1 \frac{c_p}{\epsilon_r}\left[\mathcal{N}_h(x') - \rho_h(t,x')\right](1-x')dx'\right]x \\
&- \int_0^x \frac{c_p}{\epsilon_r}\left[\mathcal{N}_h(x') - \rho_h(t,x')\right](x-x')dx' \qquad (3.42)\\
&= \underbrace{\left[V_0 + \frac{c_p}{\epsilon_r}\int_0^1 \left[\mathcal{N}_h(x') - \rho_h(t,x')\right](1-x')dx'\right]x}_{\in V_h^1} \\
&- \underbrace{\frac{c_p}{\epsilon_r}\int_0^x \left[\mathcal{N}_h(x') - \rho_h(t,x')\right](x-x')dx'}_{\in V_h^3},
\end{aligned}$$

and

$$\begin{aligned}
&E(x,t) = -c_v\,\partial_x\Psi(x,t) = \qquad (3.43)\\
&= -c_v\left(\Psi|_0^1 + \int_0^1 (1-x')\frac{c_p}{\epsilon_r}\left[\mathcal{N}_h(x') - \rho_h(t,x')\right]dx' - \int_0^x \frac{c_p}{\epsilon_r}\left[\mathcal{N}_h(x') - \rho_h(t,x')\right]dx'\right)\\
&= -c_v\underbrace{(V_0 + \frac{c_p}{\epsilon_r}\int_0^1 \left[\mathcal{N}_h(x') - \rho_h(t,x')\right](1-x')dx'}_{\in V_h^0}\underbrace{-\frac{c_p}{\epsilon_r}\int_0^x \left[\mathcal{N}_h(x') - \rho_h(t,x')\right]dx')}_{\in V_h^2}.
\end{aligned}$$

We observe that, if $-\partial_x^2\Psi = \frac{c_p}{\epsilon_r}\left[\mathcal{N}_h(x) - \rho_h(t,x)\right] \in V_h^1$, then the analytical solutions are such that $E(x,t) = -c_v\,\partial_x\Psi(x,t) \in V_h^2$ and $\Psi \in V_h^3$.
This differs from a piecewise constant density approximation for which $-\partial_x^2\Psi = \frac{c_p}{\epsilon_r}\left[\mathcal{N}_h(x) - \rho_h(t,x)\right] \in V_h^0$ implies that $E(x,t) = -c_v\,\partial_x\Psi(x,t) \in V_h^1$, $\Psi \in V_h^2$. We must project then the analytical solution $E(x,t)$ to our Dirichlet BVP in the Finite Element space V_h^1 to find an approximate solution $E_h(x,t)$ that belongs to the appropriate space for our problem, and likewise for Ψ and its respective projection Ψ_h.

$$E(x,t) \to E_h(x,t) = \Pi_h^1 E(x,t) \in V_h^1. \qquad (3.44)$$

Given the analytical solution of the electric field, it is clear that we only need to project the part of $E(x,t)$ that doesn't belong to V_h^1, namely

$$F(x,t) = \int_0^x \left[\mathcal{N}_h(x') - \rho_h(t,x')\right] dx' \to \Pi_h^1 \int_0^x \left[\mathcal{N}_h(x') - \rho_h(t,x')\right] dx'. \quad (3.45)$$

Let's remeber that

$$\left[\mathcal{N}_h(x') - \rho_h(t,x')\right]|_{x'\in[x_i-,x_i+]} = c_i^0(t) + c_i^1(t)\frac{(x'-x_i)}{\Delta x_i/2} \in V_h^1, \quad (3.46)$$

Therefore,

$$\begin{aligned}
F(x)|_{[x_{i_0}-,x_{i_0}+]} &= \int_0^x \left[\mathcal{N}_h(x') - \rho_h(t,x')\right] dx' = \int_0^x \sum_i \chi_i \left[c_i^0(t) + c_i^1(t)\frac{(x'-x_i)}{\Delta x_i/2}\right] dx' \\
&= \sum_{i<i_0} \int_{x_i-}^{x_i+} \left[c_i^0(t) + c_i^1(t)\frac{(x'-x_i)}{\Delta x_i/2}\right] dx' + \int_{x_{i_0}-}^{x} \left[c_{i_0}^0 + c_{i_0}^1\frac{(x'-x_{i_0})}{\Delta x_{i_0}/2}\right] dx', \\
F(x)|_{x_{i_0}-\le x\le x_{i_0}+} &= \sum_{i<i_0} c_i^0(t)\Delta x_i \;+\; c_{i_0}^0(t)(x-x_{i_0-}) \;+\; c_{i_0}^1(t)\left[\frac{(x-x_{i_0})^2}{\Delta x_{i_0}} - \frac{\Delta x_{i_0}}{4}\right].
\end{aligned}$$

The only part of $F(x)$ that doesn't belong to V_h^1 is proportional to $R(x) = \frac{(x-x_{i_0})^2}{\Delta x_{i_0}}$. We project this residual in V_h^1, so

$$\int_{x_{i_0}-}^{x_{i_0}+} 1\cdot R(x)dx = \int_{x_{i_0}-}^{x_{i_0}+} \frac{(x-x_{i_0})^2}{\Delta x_{i_0}}dx = \frac{\Delta x_{i_0}^2}{12},$$

$$\int_{x_{i_0}-}^{x_{i_0}+} \frac{(x-x_{i_0})}{\Delta x_{i_0}/2}\cdot R(x)dx = \int_{x_{i_0}-}^{x_{i_0}+} \frac{(x-x_{i_0})^3}{\Delta x_{i_0}^2/2}dx = 0.$$

The projection of $R(x)$ in V_h^1 gives the piecewise constant approximation $R^0 = \int_{x_{i_0}-}^{x_{i_0}+} 1\cdot R(x)dx/\Delta x_{i_0} = \frac{\Delta x_{i_0}}{12}$. Projecting $F \to \Pi_h^1 F \in V_h^1$,

$$F(x)|_{[x_{i_0}-,x_{i_0}+]} \longrightarrow \Pi_h^1 F(x)\big|_{[x_{i_0}-,x_{i_0}+]} = \sum_{i<i_0} c_i^0\Delta x_i + c_{i_0}^0(x-x_{i_0-}) + c_{i_0}^1\left[\frac{\Delta x_{i_0}}{12} - \frac{\Delta x_{i_0}}{4}\right],$$

with

$$F(x) = \sum_{i_0} \chi_{i_0}\ F(x)\big|_{x_{i_0}-\leq x\leq x_{i_0}+} \longrightarrow \Pi_h^1 F(x) = \sum_{i_0} \chi_{i_0}\ \Pi_h^1 F(x)\big|_{[x_{i_0}-,x_{i_0}+]}\,,$$

$$\Pi_h^1\, F(x,t)\ = \sum_{i_0} \chi_{i_0} \left[\sum_{i<i_0} c_i^0(t)\Delta x_i\ -\ c_{i_0}^1(t)\frac{\Delta x_{i_0}}{6}\ +\ c_{i_0}^0(t)(x - x_{i_0-}) \right]\ . \quad (3.47)$$

The projection of the electric field $E(x,t)$ into V_h^1 is then

$$E_h(x,t) = \Pi_h^1 E(x,t) = -c_v \left(V_0 + \frac{c_p}{\epsilon_r}\int_0^1 \left[\mathcal{N}_h(x') - \rho_h(t,x')\right](1-x')dx' - \frac{c_p}{\epsilon_r}\,\Pi_h^1\, F(x,t) \right)\,,$$

$$E_h(x,t) = -c_v \times$$

$$\left(V_0 + \frac{c_p}{\epsilon_r}\int_0^1 \left[\mathcal{N}_h(x') - \rho_h(t,x')\right](1-x')dx' - \frac{c_p}{\epsilon_r}\sum_{i_0} \chi_{i_0} \left[\sum_{i<i_0} c_i^0\Delta x_i\ -\ c_{i_0}^1\frac{\Delta x_{i_0}}{6}\ +\ c_{i_0}^0(x - x_{i_0-}) \right] \right)$$

or equivalently, $E_h(x,t) = -\frac{c_v\, c_p}{\epsilon_r} \times$

$$\left(\frac{\epsilon_r V_0}{c_p} + \int_0^1 \left[\mathcal{N}_h - \rho_h\right](1-x')dx' - \sum_{i_0} \chi_{i_0} \left[\sum_{i<i_0} c_i^0\Delta x_i\ -\ c_{i_0}^1\frac{\Delta x_{i_0}}{6}\ +\ c_{i_0}^0\frac{\Delta x_{i_0}}{2}\left(\frac{x - x_{i_0}}{\frac{\Delta x_{i_0}}{2}} + 1 \right) \right] \right)\,,$$

understanding that the coefficients $c_i^j(t)$, $c_{i_0}^j(t)$ are time dependant. If we consider in particular the projection of the electric field for $x \in [x_{i_0}-, x_{i_0}+]$ we have that

$$\begin{aligned} E_h(x,t)\big|_{x\in[x_{i_0}-,x_{i_0}+]} \ &=\ -\frac{c_v\, c_p}{\epsilon_r} \times \\ &\left(\frac{\epsilon_r V_0}{c_p} + \int_0^1 \left[\mathcal{N}_h(x') - \rho_h(t,x')\right](1-x')dx' \right. \\ &\left. - \sum_{i<i_0} c_i^0\Delta x_i\ -\ c_{i_0}^1\frac{\Delta x_{i_0}}{6}\ +\ c_{i_0}^0\frac{\Delta x_{i_0}}{2}\ +\ \left(c_{i_0}^0\frac{\Delta x_{i_0}}{2} \right)\frac{x - x_{i_0}}{\frac{\Delta x_{i_0}}{2}} \right)\,, \end{aligned}$$

where the following integral, after being calculated, is

$$\int_0^1 \left[\mathcal{N}_h(x') - \rho_h(t,x')\right](1-x')dx' = \sum_i (1-x_i)c_i^0(t)\Delta x_i - \sum_i c_i^1(t)\frac{\Delta x_i^2}{6}.\ (3.48)$$

Therefore

$$E_h(x,t)|_{x\in[x_{i_0}-,x_{i_0}+]} = -\frac{c_v\, c_p}{\epsilon_r}\times \tag{3.49}$$

$$\left(\frac{\epsilon_r V_0}{c_p} + \sum_i (1-x_i)c_i^0\Delta x_i - \sum_i c_i^1\frac{\Delta x_i^2}{6} - \sum_{i<i_0} c_i^0\Delta x_i \; - \; c_{i_0}^1\frac{\Delta x_{i_0}}{6} \; + \; c_{i_0}^0\frac{\Delta x_{i_0}}{2} \; + \; c_{i_0}^0\frac{\Delta x_{i_0}}{2}\cdot\frac{x-x_{i_0}}{\frac{\Delta x_{i_0}}{2}}\right).$$

On the other hand, the Poisson Eq. BVP with Dirichlet BC in 1D can also be solved approximately by numerical methods. For example, by means of a Local DG Method, obtaining with this method $\Psi \in V_h^1$, $E(x,t) \in V_h^1$.

3.3 The n^+-n-n^+ silicon diode

We consider the symmetric case of a 1D n^+-n-n^+ diode, in which the conduction band energy function is assumed to be of the form $\varepsilon(|\mathbf{k}|) = \varepsilon(r)$. This assumption preserves azimuthal symmetry for the problem if the initial condition is independent of the azimuthal direction φ. Therefore, under these assumptions the problem has azimuthal symmetry in $\mathbf{k}$ for all times $t \geq 0$, so it suffices to consider $\mathbf{k} = \mathbf{k}(r,\mu)$, reducing then the dimensionality of the problem to 1-D in x-space and 2-D in $\mathbf{k} = \mathbf{k}(r,\mu)$, then the problem reduces to a 3-D plus time. Assuming $\mathbf{E}$ has null y and z components, this symmetric case reduces the TBE to

$$\frac{\partial\Phi}{\partial t} + \frac{\partial}{\partial x}\left(a_1\,\Phi\right) + \frac{\partial}{\partial r}\left(a_4\,\Phi\right) + \frac{\partial}{\partial \mu}\left(a_5\,\Phi\right) = C(\Phi), \tag{3.50}$$

where the terms a_1, a_4 and a_5 are now simplified.

The Poisson equation is reduced to

$$\frac{\partial}{\partial x}\left(\epsilon_r\frac{\partial\Psi}{\partial x}\right) = c_p\left[\rho(t,x) - \mathcal{N}_D(x)\right]. \tag{3.51}$$

For this case both the potential and electric field have analytic integral solutions, that are easily computed numerically for the piecewise linear approximation of the density ρ_h. Then, such electric field solution is projected in the V_h^1 space of piecewise linear polynomials.

3.3.1 Device specifics

We consider first a diode of $1\,\mu m$ length, with an n-channel of $400\,nm$ length, doping of $5 \times 10^{23}\,m^{-3}$ in the n^+ region and $2 \times 10^{21}\,m^{-3}$ in the n region. We also consider a $0.25\mu m$ diode with a $50\,nm$ channel with n^+-doping of $5 \times 10^{24}\,m^{-3}$, and n-doping of $1 \times 10^{21}\,m^{-3}$.

3.3.2 Numerical simulations

The space V_h^1 of piecewise linear polynomials in (x, r, μ), with time dependent coefficients, is used as both the trial and test space in our DG scheme. The input data of the numerical simulations is

- **Computational domain:** $x \in [0, 1]$, $r \in [0, r_{max}]$, $\mu \in [-1, 1]$, where r_{max} is taken in the numerical experiments such that $\Phi(t, x, r, \mu) \approx 0$ for $r \approx r_{max}$ (for example, $r_{max} = 36$ for $V_{bias} = 0.5$ Volts in the 400nm channel case).
- **Initial condition:** $\Phi(0, x, r, \mu) = \Pi_h \left\{ C N_D(x) \dfrac{\sqrt{r}}{2} e^{-\varepsilon(r)} \right\}$, where C constant is such that $\rho(x, 0)$ equals the doping $N_D(x)$ at $t = 0$. The initial condition is projected by Π_h into V_h^1.

- **Boundary conditions:** Neutral charges at the endpoints $x_{\frac{1}{2}} = 0$ and $x_{N_x+\frac{1}{2}} = 1$.
  $\Phi(t, 0, r, \mu) = N_D(0)\dfrac{\Phi(t, x_1, r, \mu)}{\rho(t, x_1)}$ and $\Phi(t, 1, r, \mu) = N_D(1)\dfrac{\Phi(t, x_{N_x}, r, \mu)}{\rho(t, x_{N_x})}$.
  Cut-off in the k-space $\Phi(t, x, r_{max}, \mu) = 0$.

- **Applied potential - bias:** $\Psi(t, 0) = 0$ and $\Psi(t, 1) = V_0$.

No boundary conditions are needed on $r = 0$, $\mu = \pm 1$. Upwind fluxes in r and μ are analytically zero at these boundaries, since they are related to points in **k**-space such as the origin and the poles, which are transformed into boundaries when applying the spherical change of coordinates. It is very simple to verify that $a_4 = 0$ at $r = 0$, and $a_5 = 0$ at $\mu = \pm 1$.

3.4 Computation of the spherical average of a local EPM conduction band for silicon

The motivation of this work is to incorporate numerically, in a DG solver of the BP system electronic conduction bands whose values are obtained by the radial averaging of the full band structure given by a local empirical pseudopotential method (EPM) around a local minimum of the conduction band for silicon. This is done as a midpoint between a radial and an anisotropic full energy band models, with the goal of providing a more accurate physical description of the electron group velocity and of the scattering mechanisms by Fermi Golden Rule, and consequently improve the transport and electron - phonon collision phenomena. The approximation of the electron group velocity

is obtained from the numerical values of the derivatives of the conduction band, which are obtained by means of a cubic spline interpolation. The numerical values of the spherically averaged EPM band and the derivatives are obtained as described below.

A local empirical pseudopotential method (EPM) code developed by Chelikowsky et al. [37] is adapted to compute the conduction band structure of silicon in its Brillouin Zone in the **k**-space. The local pseudopotentials are used in this EPM code to mimic a silicon semiconductor with crystal diamond structure [38].

A color plot of the local EPM conduction band on the first octant of the k-space enclosing the Brillouin Zone for silicon is shown in Fig. 3.1.

The calculated EPM band structure $\varepsilon(k_x, k_y, k_z) = \varepsilon(\mathbf{k}(r, \mu, \varphi))$ is then averaged over the **k**-spheres r_k around the local energy minimum point $\mathbf{k}_0 = (0.8562, 0, 0)2\pi/a$ (where a is the lattice constant for silicon) by means of a 10 point Gaussian quadrature on the angular space. Using the symmetry of the silicon conduction band, the integration only needs to be performed in the (μ, φ) domain $[0, 1] \times [0, \pi]$

$$\tilde{\varepsilon}(r_k) = \frac{\displaystyle\int_0^1 \int_0^\pi \varepsilon(r_k, \mu, \varphi)\, d\mu d\varphi}{\displaystyle\int_0^1 \int_0^\pi d\mu\, d\varphi} \approx \sum_{m=1}^{10} \sum_{n=1}^{10} \omega_m\, \omega_n\, \varepsilon(r_k, \mu_m, \varphi_n)\,. \qquad (3.52)$$

The values of the radius of these **k**-spheres are the grid points r_k in the DG-BP simulations. In this way we obtain a band model that has a dependence on r, and at the same time it uses the information of the anisotropic energy

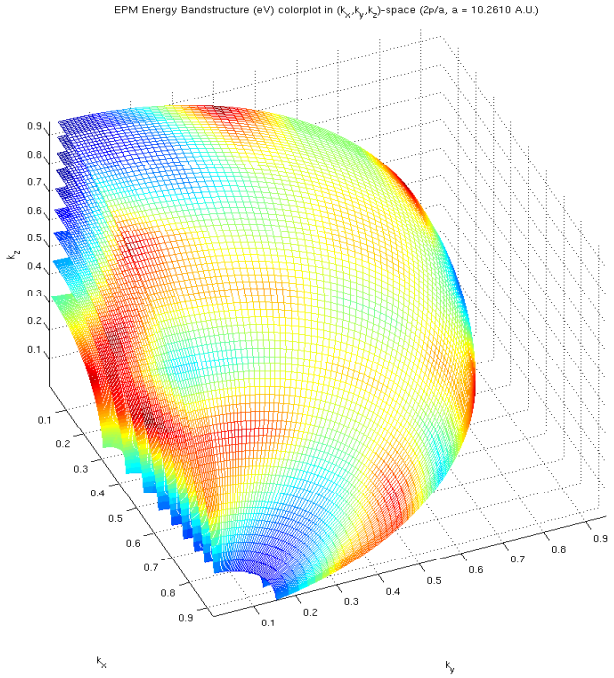


Figure 3.1: Local EPM conduction energy band-structure (ε) color plot in the **k**-space 1^{st} octant enclosing the Silicon Brillouin Zone. Conduction band local minimum: $k_o = (0.8562, 0, 0)(2\pi/a)$

band values in the angular **k**-domain via its numerical average. As a midpoint between a radial band model and a full band anisotropic model, it has the desired advantages of both. A cubic spline interpolation is then performed, using the numerical values of the radial average $\tilde{\varepsilon}(r)$ at the midpoints of the r-cells, and the derivative of this spline interpolation is used to obtain a numerical approximation of the derivative $d\tilde{\varepsilon}/dr$ at these r-midpoints.

The spherical averages of the EPM conduction band $\tilde{\varepsilon}(r)$ vs $r \propto |\mathbf{k}-\mathbf{k}_0|^2$ with the related spline interpolation for Si are shown in Fig. 3.2 (in red). The parabolic (blue), which is a linear function of r, and the Kane (green) analytic conduction band models for silicon are plotted as well.

It can be observed that there is a quantitative difference between the different energy band models. The spherical average of the EPM band is below the Kane band model, which is below the Parabolic band.

We show in Fig. 3.3 the relative l_2 error norm of the spherical average EPM band with respect to the local EPM data $\varepsilon(r, \mu, \varphi)$ as a function of r, given by the formula

$$\frac{\langle[\varepsilon - \tilde{\varepsilon}]^2\rangle}{\langle\varepsilon^2\rangle}(r_k) \approx \frac{\sum_{m=1}^{10}\sum_{n=1}^{10}\omega_m\omega_n\left[\varepsilon(r_k,\mu_m,\varphi_n) - \tilde{\varepsilon}(r_k)\right]^2}{\sum_{m=1}^{10}\sum_{n=1}^{10}\omega_m\omega_n\left[\varepsilon(r_k,\mu_m,\varphi_n)\right]^2}\,.$$

It can be observed in Fig. 3.3 that the relative l_2 error increases with r, which indicates that far away from the local minimum $\mathbf{k}_0$ the anisotropy of the conduction band becomes increasingly more important.

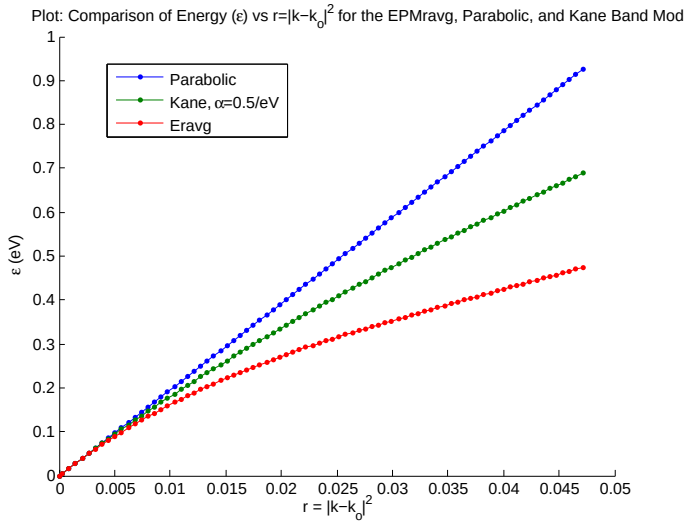


Figure 3.2: Energy (E) vs $r = |\mathbf{k}-\mathbf{k}_0|^2$ for the parabolic, Kane, & symmetrized EPM spherical average band.

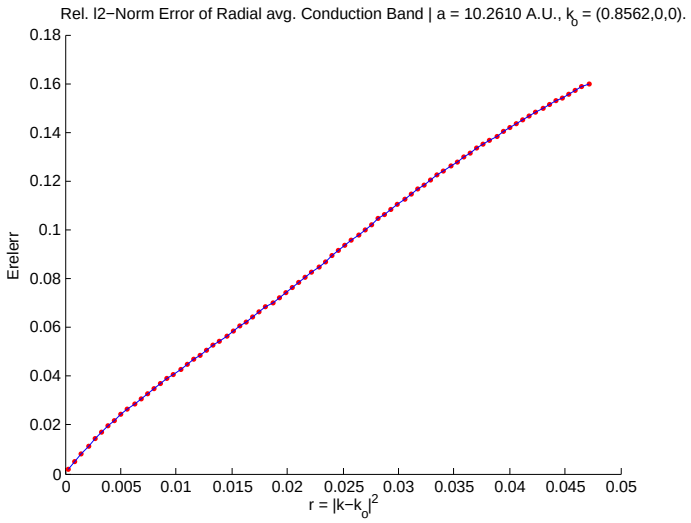


Figure 3.3: Relative l_2-deviation in the angular space of EPM average from the EPM full band for Si, as a function of $r = |\mathbf{k} - \mathbf{k}_0|^2$

3.5 Numerical results

The BP transport along the EPM spherical average energy band is numerically simulated by means of our DG-BP solver, and compared to simulations where the values related to the analytical Parabolic and Kane band models are implemented numerically. We compare simulations for two n^+-n-n^+ silicon diodes with different characteristics. The first one has a length of $1\mu m$, an n-channel length of $400nm$, n^+ doping of $5 \cdot 10^{17} cm^{-3}$, and n doping of $2 \cdot 10^{15} cm^{-3}$. The other one has a device length of $0.25\mu m$, an n-channel length of $50nm$, an n^+ doping of $5 \cdot 10^{18} cm^{-3}$, and n doping of $1 \cdot 10^{15} cm^{-3}$. We show simulations for a potential bias of $V_0 = 0.5\, V$. For the 400 nm channel diode, the number of cells used in the simulations for each of the variables was: $N_x = 120$, $N_r = 80$ and $N_\mu = 24$. The interval size for r is taken as $\Delta r = 0.45$, having then $r_{max} = 36$. We use a mesh as in [34] which gives better resolution close to the first juncture at $x = 0.3\mu m$, and which also has a finer refinement close to the pole in the direction of the electric field. It uses $\Delta x = 0.01$ for the first 20 cells in x-space, $\Delta x = 0.005$ for the next 40 cells, and $\Delta x = 0.01$ for the last 60 cells. Regarding μ, it uses 12 cells for $\mu \in [-1, 0.7]$, and 12 cells for $\mu \in [0.7, 1]$.

For the 50 nm channel diode, the number of cells used in the simulations for each of the variables was: $N_x = 64$, $N_r = 80$ and $N_\mu = 20$. The interval size for r is taken as $\Delta r = 0.8$, having then $r_{max} = 64$. As in [34], we use a mesh intended to give better resolution close to the junctures at $x = 0.1\mu m$ and $x = 0.15\mu m$, and which also has a finer refinement close to the pole in the

direction of the electric field. It uses $\Delta x = 0.01$ for the first 9 cells in x-space, $\Delta x = 0.001$ for the next 20 cells close to the the first juncture at $x = 0.1\mu m$, $\Delta x = 0.005$ for 6 cells at the center of the n-channel, $\Delta x = 0.001$ for the next 20 cells close to the second juncture at $x = 0.15\mu m$, and $\Delta x = 0.01$ for the last 9 cells. Regarding μ, it uses 10 cells for $\mu \in [-1, 0.7]$, and 10 cells for $\mu \in [0.7, 1]$. We let the solver run until $t = 5.0ps$, a time when the simulations are close to a numerical stationary state.

We show plots of the average velocity, the average energy, the momentum (proportional to the current), the electric field and potential, for both the $400nm$ channel and $50nm$ channel diodes. There is a clear quantitative difference, particularly in kinetic moments such as average velocity, average energy, and momentum (current), whose values depend on the energy band model used in each case then. This should be expected since these kinetic moments are averages of quantities related to $\varepsilon(k)$ or its partial derivatives in k-space.

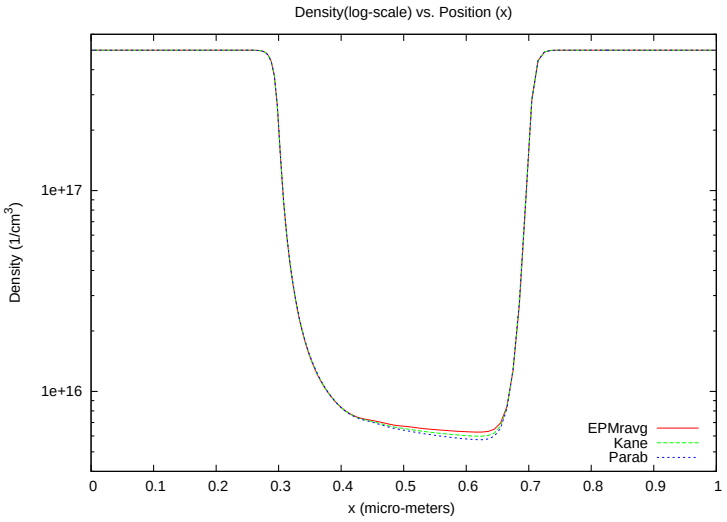


Figure 3.4: Density (ρ, in log-scale) vs. position (x) plots for different conduction band models: parabolic, Kane, EPM average. 400nm channel. $t = 5.0ps$. 0.5 Volts Bias.

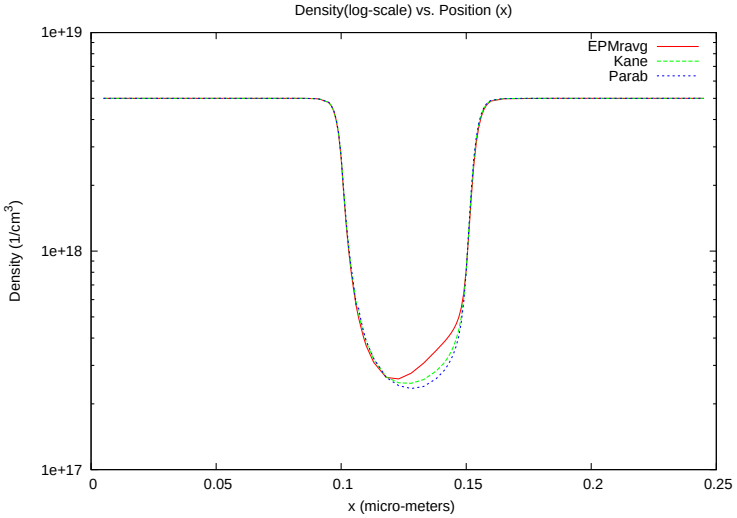


Figure 3.5: Density (ρ, in log-scale) vs. position (x) plots for different conduction band models: parabolic, Kane, EPM average. 50nm channel. $t = 5.0ps$. 0.5 Volts Bias.

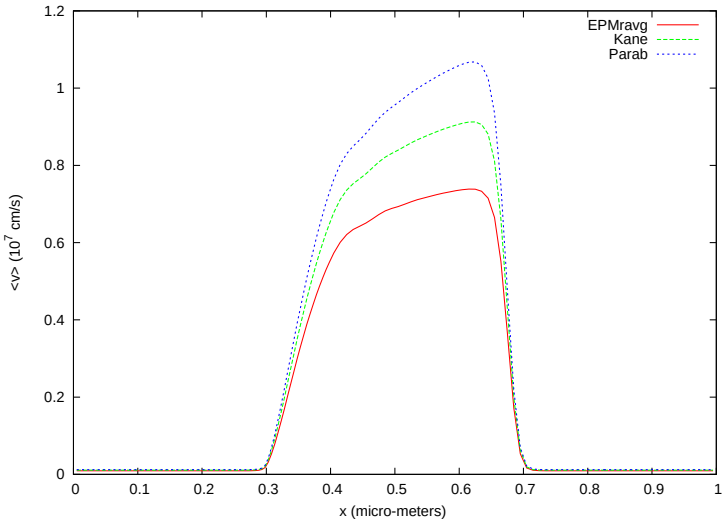


Figure 3.6: Average velocity (v) vs. position (x) plots for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$ 400nm channel. 0.5 Volts Bias

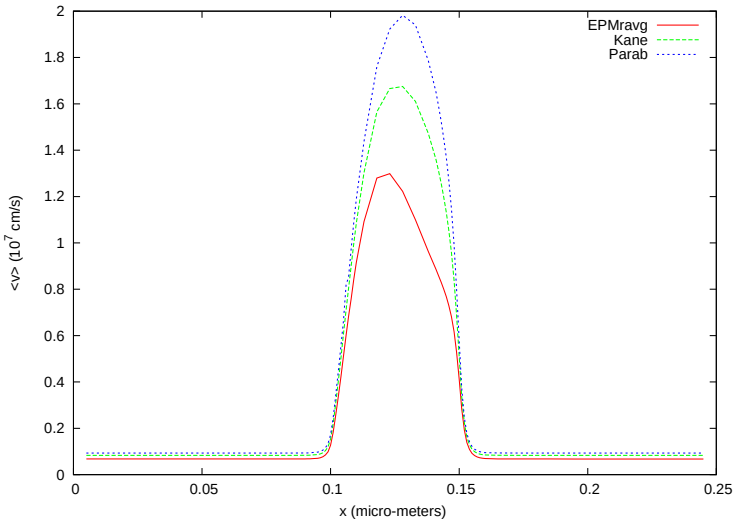


Figure 3.7: Average velocity (v) vs. position (x) plots for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$ 50nm channel. 0.5 Volts Bias

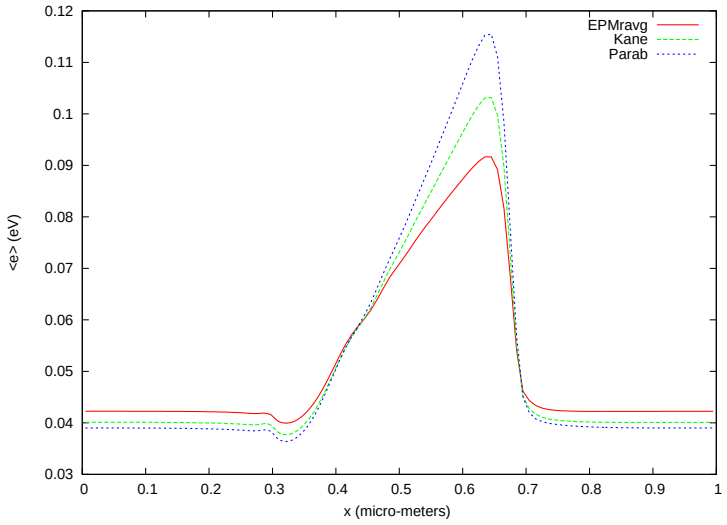


Figure 3.8: Average energy (ε) vs. position (x) for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$. 400nm channel. 0.5 Volts Bias.

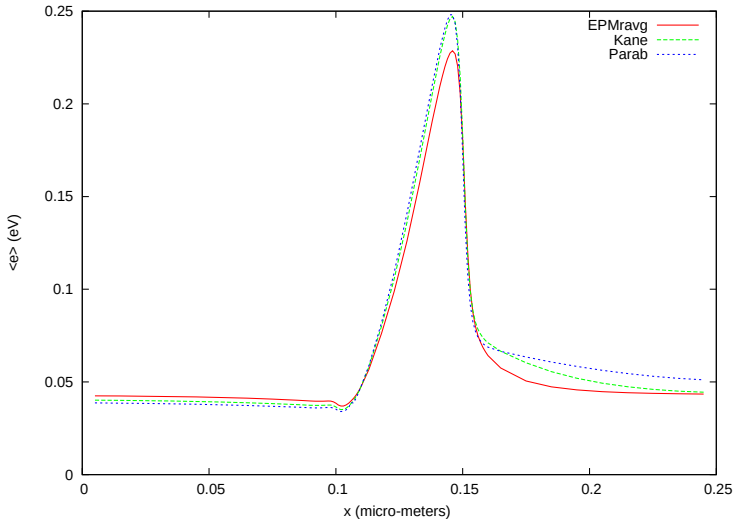


Figure 3.9: Average energy (ε) vs. position (x) for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$. 50nm channel. 0.5 Volts Bias.

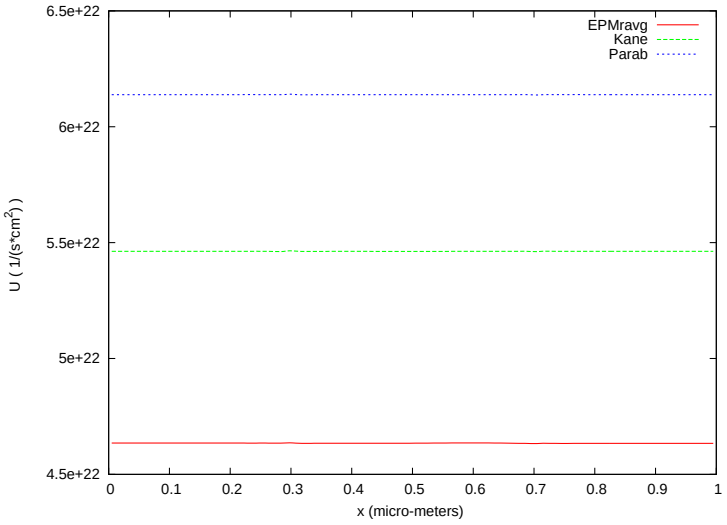


Figure 3.10: Current (Momentum) vs. position (x) for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$. 400nm channel. 0.5 Volts Bias.

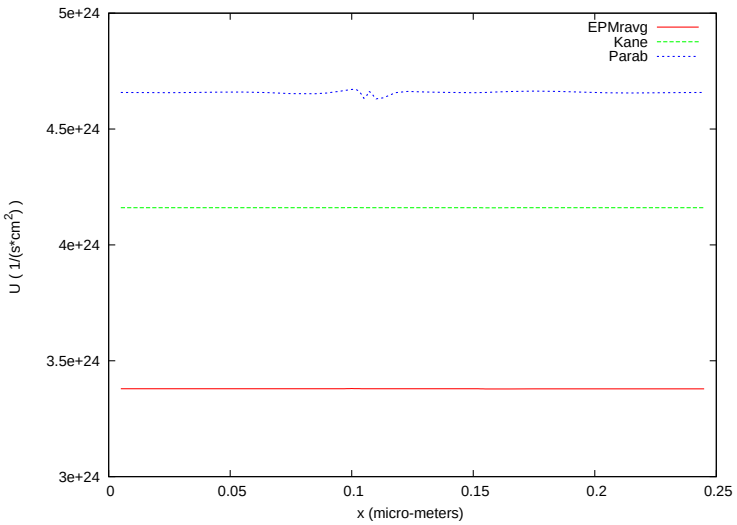


Figure 3.11: Current (Momentum) vs. position (x) for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$. 50nm channel. 0.5 Volts Bias.

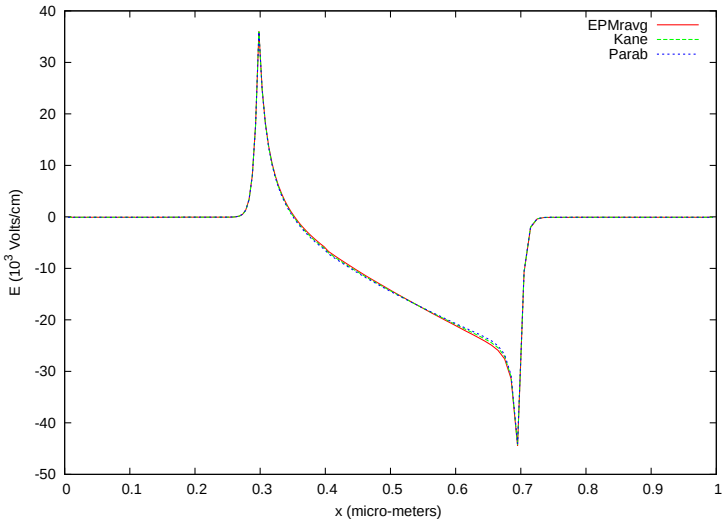


Figure 3.12: Electric field (E) vs. position (x) plots for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$. 400nm channel. 0.5 Volts Bias.

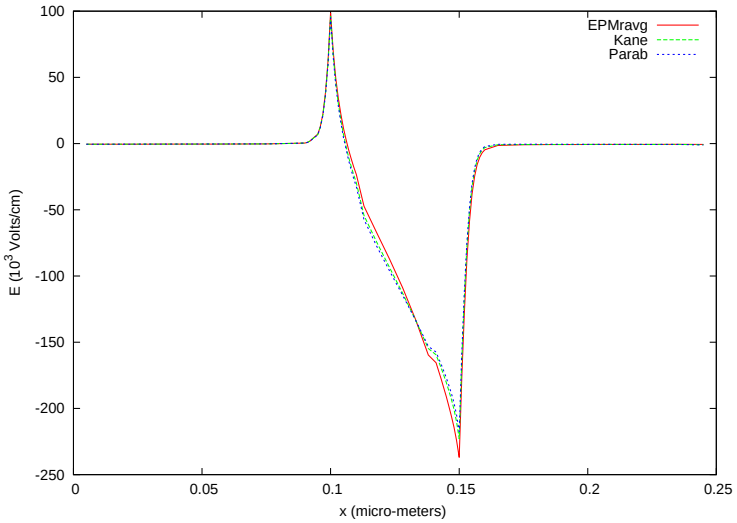


Figure 3.13: Electric field (E) vs. position (x) plots for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$. 50nm channel. 0.5 Volts Bias.

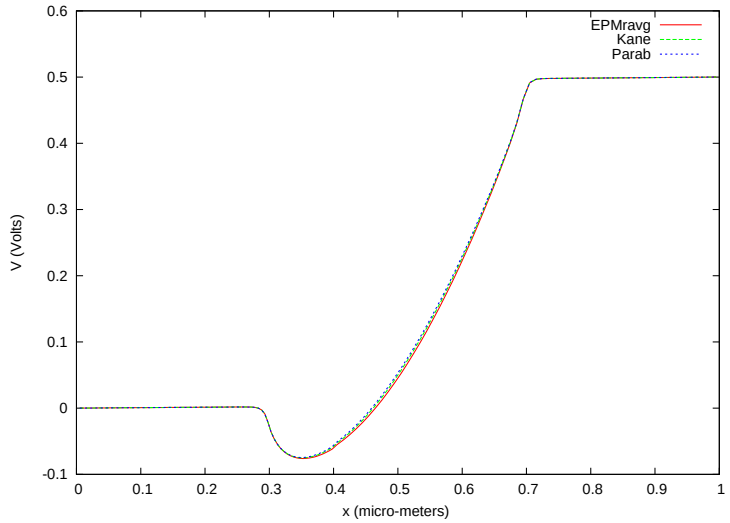


Figure 3.14: Electric Potential (V) vs. position (x) plots for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$. 400nm channel. 0.5 Volts Bias.

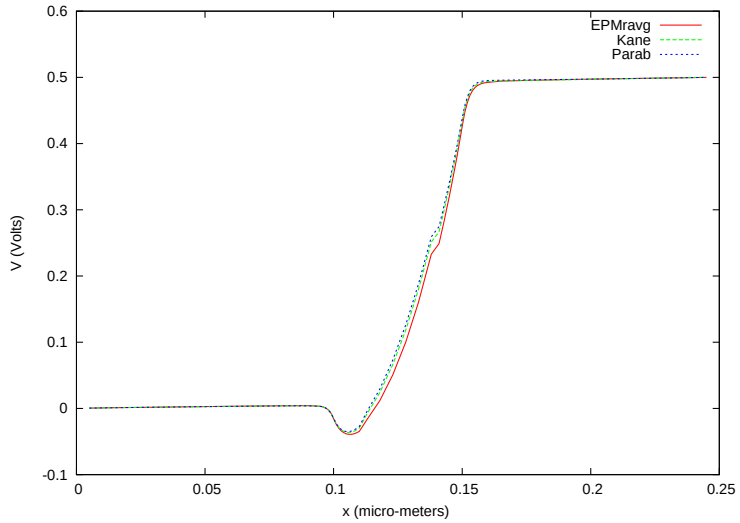


Figure 3.15: Electric Potential (V) vs. position (x) plots for different conduction band models: parabolic, Kane, EPM average. $t = 5.0ps$. 50nm channel. 0.5 Volts Bias.

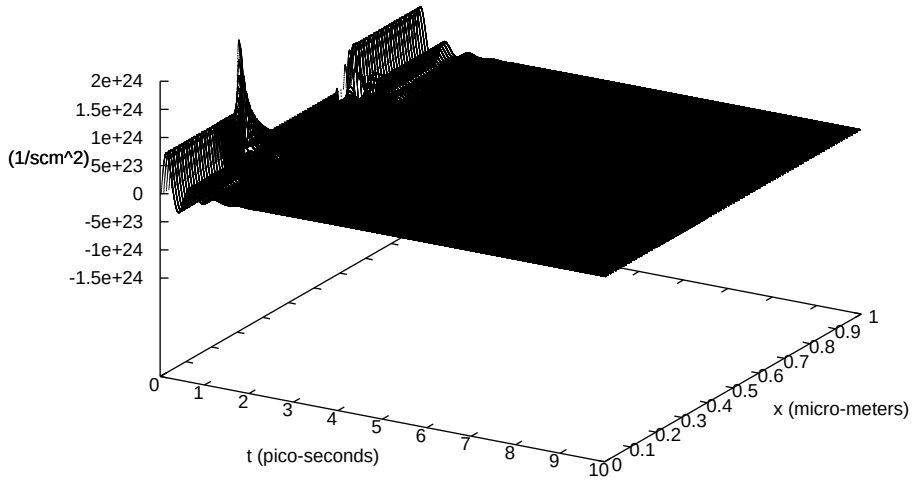


Figure 3.16: Current (Momentum) vs. (t, x) for the 400nm channel diode, using the EPM average band. From initial time to $t = 5.0ps$. 0.5 Volts bias. The initial condition is proportional to the Maxwellian $\exp(-\varepsilon(r))$ times the doping profile $N(x)$. The initial oscillations are produced by the initial state being far from the final steady state.

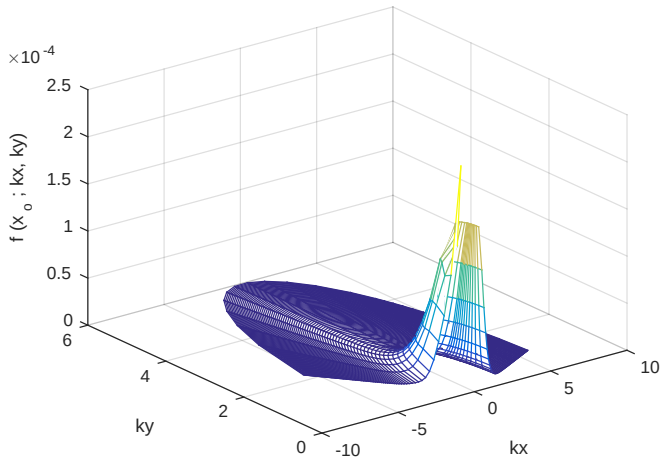


Figure 3.17: PDF $f(r, \mu; t_0, x_0)$ vs. (k_x, k_y) coordinates (Azimuthal symmetry, with $k_z = 0$) at the point $x_0 = 0.3\mu m$ at $t_0 = 5.0ps$, for the $1\mu m$ diode with a $400nm$ channel, using the EPM radial average energy band. 0.5 Volts bias.

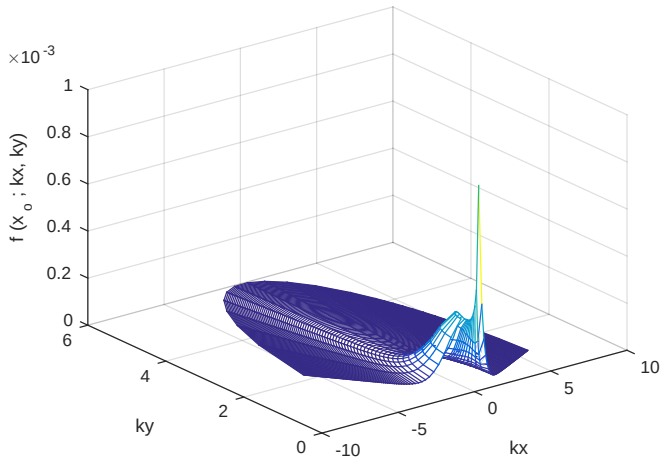


Figure 3.18: PDF $f(r, \mu; t_0, x_0)$ vs. (k_x, k_y) coordinates (Azimuthal symmetry, with $k_z = 0$) at the point $x_0 = 0.7\mu m$ at $t_0 = 5.0ps$, for the $1\mu m$ diode with a $400nm$ channel, using the EPM radial average energy band. 0.5 Volts bias.

Chapter 4

Reflective Boundary Conditions in DG for BP Models of Electron Transport in Semiconductors and Zero Flux Condition for General Mixed Reflection

We discuss in this chapter the use of Discontinuous Galerkin (DG) Finite Element Methods to solve Boltzmann - Poisson (BP) models of electron transport in semiconductor devices at nano scales. We consider the mathematical and numerical modeling of Reflective Boundary Conditions in 2D devices and their implementation in DG-BP schemes. We study the specular, diffusive and mixed reflection BC on physical boundaries of the device, comparing the influence of these different reflection cases in the computational prediction of moments close to the boundaries and their associated scale.

4.1 Introduction

Regarding Boundary Conditions (BC), there are several kinds of BC for BP semiconductor models. They vary according to the considered device and physical situation. For example, in the case of electron transport along a single conduction band, the following BC could arise:

Charge neutrality boundary conditions, given by [54]

$$f_{out}(t,\vec{x},\vec{k})\Big|_{\Gamma} = N_D(\vec{x})\frac{f_{in}(t,\vec{x},\vec{k})}{\rho_{in}(t,\vec{x})}\Bigg|_{\Gamma}, \quad \Gamma \quad \text{subset of} \, \partial\Omega_{\vec{x}}\,. \tag{4.1}$$

This BC is imposed in source and drain boundaries, where electric currents enter or exit the device, to achieve neutral charges there, as $\rho_{out}(\vec{x},t) - N_D(\vec{x}) = 0$.

Reflective BC happen in insulating boundaries, usually defined by a Neumann boundary Γ_N, of 2D and 3D devices. In general, reflective BC can be formulated as the values of the pdf at the inflow boundary being dependent on the outflow boundary values

$$f(\vec{x},\vec{k},t)|_{\Gamma_{N^-}} = F_R\left(f|_{\Gamma_{N^+}}\right), \tag{4.2}$$

where the Neumann Inflow Boundary is defined as

$$\Gamma_N^- = \{(\vec{x},\vec{k}) \,|\, \vec{x} \in \Gamma_N,\, \vec{k} \in \Omega_k,\, \vec{v}(\vec{k}) \cdot \eta(\vec{x}) < 0\}, \tag{4.3}$$

$$\vec{v}(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k})\,, \tag{4.4}$$

$\eta(\vec{x})$ outward unit normal. The Neumann Outflow Boundary is defined as

$$\Gamma_N^+ = \{(\vec{x},\vec{k}) \,|\, \vec{x} \in \Gamma_N,\, \vec{k} \in \Omega_k,\, \vec{v}(\vec{k}) \cdot \eta(\vec{x}) > 0\}\,. \tag{4.5}$$

Specular Reflection BC over the Neumann Inflow Boundary is given by

$$f|_-(\vec{x},\vec{k},t) = F_S(f|_+) = f|_+(\vec{x},\vec{k}',t) \quad \text{for} \quad (\vec{x},\vec{k}) \in \Gamma_N^-, \quad t > 0, \tag{4.6}$$

$$(\vec{x},\vec{k}') \in \Gamma_N^+, \quad \vec{k}' \quad \text{s.t.} \quad \vec{v}(\vec{k}') = \vec{v}(\vec{k}) - 2\,\eta(\vec{x}) \cdot \vec{v}(\vec{k})\,\eta(\vec{x})\,. \tag{4.7}$$

Diffusive reflection is a known condition from kinetic theory, in which the distribution function at the Inflow boundary is proportional to a Maxwellian [52], [2] with $T = T_W = T_W(\vec{x})$ the temperature at the wall

$$f|_-(\vec{x},\vec{k},t) = F_D(f|_+) = C\,\sigma\left\{f|_+\right\}(\vec{x},t)\,e^{-\varepsilon(\vec{k})/K_BT}\,, \quad (\vec{x},\vec{k}) \in \Gamma_N^-\,, \tag{4.8}$$

$$\sigma\left\{f|_+\right\}(\vec{x},t) = \int_{\vec{v}(\vec{k})\cdot\eta>0} \vec{v}(\vec{k})\cdot\eta(\vec{x}) f|_+(\vec{x},\vec{k},t)dk\,. \tag{4.9}$$

Mixed reflection BC models the effect of a physical surface on electron transport in metals and semiconductors, giving the reflected pdf representing the electrons as a linear convex combination of specular and diffuse components, as in the formula

$$\begin{aligned} f|_-(\vec{x},\vec{k},t) &= F_M(f|_+) = p\,F_S(f|_+) + (1-p)\,F_D(f|_+) \\ &= p\,f|_+(\vec{x},\vec{k}',t) \;+\; (1-p)\,C'\,\sigma'\left\{f|_+\right\}(\vec{x},t)\,e^{-\frac{\varepsilon(\vec{k})}{K_BT}}\,, \quad (\vec{x},\vec{k}) \in \Gamma_N^-\,. \end{aligned} \tag{4.10}$$

p is sometimes called specularity parameter. It can either be constant or a function, dependant of the momentum. For example, the work by Soffer [55] studies a statistical model for the reflection from a rough surface in electrical conduction. It derives a specularity parameter $p(\vec{k})$ which depends on the momentum, given by

$$p(\vec{k}) = e^{-4l_r^2|k|^2\cos^2\Theta}\,, \tag{4.11}$$

where l_r is the rms height of the rough interface, and Θ_B is th angle between the incident electron and the interface surface normal.

Reflection BC is a widely studied topic in the context of the kinetic theory of gases modelled by Boltzmann Equations. However, in the context of

kinetic models for electron transport in semiconductors, there is less extensive previous work related to the study of the effect of reflection boundary conditions such as diffusive, specular, or mixed reflection. A non-exhaustive list of references where reflection BC are studied for Boltzmann equations in the context of kinetic theory of gases would include the works of Cercignani [53] and Sone [52], where the specular, diffusive, and mixed reflection BC are formulated for the Boltzmann Eq. for gases. V. D. Borman, S. Yu. Krylov, A. V. Chayanov [59] study the nonequilibrium phenomena at a gas-solid interface. The recent paper of Brull, Charrier, Mieussens [60] studies the gas-surface interaction at a nano-scale and the boundary conditions for the associated Boltzmann equation. The recent work of Struchtrup [61] studies as well the Maxwell boundary condition and velocity dependent accommodation coefficients in the context of gases mentioned. It considers the convex combination of specular reflection, isotropic scattering, and diffusive reflection, incorporating velocity dependent coefficients into a Maxwell-type reflection kernel. It develops a modification of Maxwell's BC, extending the Maxwell model by allowing it to incorporate velocity dependent accomodation coefficients into the microscopic description and satisfying conditions of reciprocity and unitary probability normalization.

Regarding reflectivity in the context of Boltzmann models of electron transport, Fuchs [56] proposed a boundary condition for the probability density function of free electrons incident in the material surface, which is a convex combination of specular & diffuse reflection with a constant specularity pa-

rameter p. Greene ([57], [58]) studied conditions for the Fuchs BC in which the specularity parameter $p(\vec{k})$ is dependant on the angle of the momentum $\vec{k}$, deriving a boundary condition for electron distributions at crystal surfaces valid for metal, semimetal, & semiconductor surfaces, and showing that Fuchs reflectivity parameter differs from the kinetic specularity parameter in physical significance and in magnitude. It considers the unperturbed electron states of a crystal with an ideal perfectly specular surface as standing wave states, and the diffusive reflection killing partially the incoming wave function. Soffer [55] studies a statistical model for the electrical conduction, and derives under certain assumptions, such as a rough surface random model with a Gaussian probability of height above or below a horizontal plane, analytical formulas for a momentum dependant specularity parameter $p(\vec{k}) = \exp(-4l_r^2|k|^2\cos^2\Theta)$ associated to this physical phenomena, abovementioned in (4.11). As mentioned before, l_r is the rms height of rough interface, and Θ_B is th angle between the incident electron and the interface surface normal.

The reference book of Markowich, Ringhofer, & Schmeiser [17] for semiconductor equations discusses the mathematical definition of boundaries according to the physical phenomena, and defines accordingly the kind of BC to be imposed at those boundaries: Dirichlet, Neumann, Inflow and Outflow boundaries. A work of particular importance for us is the one by Cercignani, Gamba, and Levermore [54]. They study high field approximations to a Boltzmann-Poisson system and boundary conditions in a semiconductor. The BP system for electrons in a semiconductor in the case of high fields

and small devices is considered. Boundary conditions are proposed at the kinetic level that yield charge neutrality at ohmic contacts, which are Dirichlet boundaries, and at insulating Neumann boundaries. Both BC, either the one yielding charge neutrality at Dirichlet boundaries, or the one rendering zero flux of electrons at the boundary, assume that the pdf is proportional to a ground state associated to an asymptotic expansion of a dimensionless Boltzmann-Poisson system. Then they study closures of moment equations and BC for both the pdf and for the moment closures. Jüngel mentions in his semiconductors book [2] the different kinds of reflection BC common on the kinetic theory of gases, specular, diffusive, and mixed reflection but no further study of diffusive and mixed reflection BC in the context of semiconductors is pursued.

We intend to present in this work a mathematical, numerical, and computational study of the effect of diffusive, specular, and mixed reflection BC in Boltzmann-Poisson models of electron transport in semiconductors, solved by means of Discontinuous Galerkin FEM solvers. We study the mathematical formulation of these reflection BC in the context of BP models for semiconductors, and derive equivalent numerical formulations of the diffusive and mixed reflection BC with non-constant $p(\vec{k})$, such that an equivalent numerical zero flux condition is satisfied pointwise at the insulating Neumann boundaries at the numerical level. We present numerical simulations for a 2D silicon diode and a 2D double gated MOSFET, comparing the effects of specular, diffusive, and mixed reflection boundary conditions in the physical observable quantities

obtained from the simulations.

4.2 BP system with $\vec{k}$ coordinate transformation assuming a Kane Energy Band

The Kane Energy Band Model is a dispersion relation between the conduction energy band ε (measured from a local minimum) and the norm of the electron wave vector $|k|$, given by the analytical function (α is a constant parameter, m^* is the electron reduced mass for Si, and $\hbar$ is Planck's constant)

$$\varepsilon(1+\alpha\varepsilon) = \frac{\hbar^2|k|^2}{2m^*} \quad . \tag{4.12}$$

For our preliminary numerical studies we will use a Boltzmann-Poisson model as in [34] , in which the conduction energy band is assumed to be given by a Kane model. We use the following dimensionalized variables, with the related characteristic parameters

$$t = \mathrm{t}/t_*, (x,y) = \vec{x}/\ell_*, \ell_* = 10^{-6}m, t_* = 10^{-12}s, V_* = 1\mathrm{V}\,.$$

A transformed Boltzmann transport equation is used as in [34] as well, where the coordinates used to describe $\vec{k}$ are: μ, the cosine of the polar angle, the azimuthal angle φ, and the dimensionless Kane Energy $w = \varepsilon/K_BT$, which is assumed as the conduction energy band. K_B is Boltzmann's constant, T is the wall temperature, which we will assume to be equal to the lattice temperature T_L, so $T_W = T = T_L$, and $\alpha_K = \alpha K_B T$. So

$$\vec{k}(w,\mu,\varphi) = \frac{\sqrt{2m^*k_BT_L}}{\hbar}\sqrt{w(1+\alpha_K w)}\left(\mu, \sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi\right). \tag{4.13}$$

A new unknown function Φ is used in the transformed Boltzmann Eq. [34] , which is proportional to the Jacobian of the transformation and to the density of states (up to a constant factor)

$$\Phi(t, x, y, w, \mu, \varphi) = s(w) f(\mathrm{t}, \vec{x}, \vec{k}) \,,$$

where

$$s(w) = \sqrt{w(1 + \alpha_K w)}(1 + 2\alpha_K w) \,. \tag{4.14}$$

The transformed Boltzmann transport equation for Φ used in [34] is

$$\frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial x}(g_1 \Phi) + \frac{\partial}{\partial y}(g_2 \Phi) + \frac{\partial}{\partial w}(g_3 \Phi) + \frac{\partial}{\partial \mu}(g_4 \Phi) + \frac{\partial}{\partial \varphi}(g_5 \Phi) = C(\Phi). \tag{4.15}$$

The vector (g_1, g_2) represent the 2D cartesian components of the electron velocity $\frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon(\vec{k})$, in the coordinate system (w, μ, φ). The triplet (g_3, g_4, g_5) represent the transport in the phase space of the new momentum coordinates (w, μ, φ) due to the self consistent electric field

$$\vec{E}(t, x, y) = (E_x(t, x, y), E_y(t, x, y), 0) \,,$$

with

$$
\begin{aligned}
g_1(\cdot) &= c_x \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w}\mu\,, \\
g_2(\cdot) &= c_x \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w}\sqrt{1-\mu^2}\cos\varphi\,, \\
g_3(\cdot) &= -c_k \frac{2\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w}\left[\mu\, E_x(t,x,y)+\sqrt{1-\mu^2}\cos\varphi\, E_y(t,x,y)\right], \\
&= -c_k \frac{2\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w}\,\hat{e}_w\cdot\vec{E}(t,x,y)\,, \\
g_4(\cdot) &= -c_k \frac{\sqrt{1-\mu^2}}{\sqrt{w(1+\alpha_K w)}}\left[\sqrt{1-\mu^2}\, E_x(t,x,y)-\mu\cos\varphi\, E_y(t,x,y)\right], \\
&= -c_k \frac{\sqrt{1-\mu^2}}{\sqrt{w(1+\alpha_K w)}}\,\hat{e}_\mu\cdot\vec{E}(t,x,y)\,, \\
g_5(\cdot) &= -c_k \frac{-\sin\varphi}{\sqrt{w(1+\alpha_K w)}\sqrt{1-\mu^2}}\, E_y(t,x,y) \\
&= -c_k \frac{1}{\sqrt{w(1+\alpha_K w)}\sqrt{1-\mu^2}}\,\hat{e}_\varphi\cdot\ \vec{E}(t,x,y)\,,
\end{aligned}
$$

$$
c_x = \frac{t_*}{\ell_*}\sqrt{\frac{2\,k_B T_L}{m^*}} \text{ and } \quad c_k = \frac{t_* q E_*}{\sqrt{2m^* k_B T_L}}\,,
$$

and $\hat{e}_w$, $\hat{e}_\mu$, $\hat{e}_\varphi$ the orthonormal vector basis in our momentum coordinate space.

The right hand side of (4.15) is the collision operator (having applied the Dirac Delta's due to electron-phonon scattering, which depend on the energy differences between transitions)

$$
\begin{aligned}
C(\Phi)(t,x,y,w,\mu,\varphi) &= s(w)\left\{c_0\int_0^\pi d\varphi'\int_{-1}^1 d\mu'\,\Phi(t,x,y,w,\mu',\varphi')\right. \\
&\left.+\int_0^\pi d\varphi'\int_{-1}^1 d\mu'\,[c_+\Phi(t,x,y,w+\gamma,\mu',\varphi')+c_-\Phi(t,x,y,w-\gamma,\mu',\varphi')]\right\} \\
&-\Phi(t,x,y,w,\mu,\varphi)\,2\pi\,[c_0 s(w)+c_+ s(w-\gamma)+c_- s(w+\gamma)]\,,
\end{aligned}
$$

with the dimensionless parameters

$$(c_0, c_+, c_-) = \frac{2m^*\, t_*}{\hbar^3}\sqrt{2\, m^*\, k_B T_L}\,(K_0, (n_q+1)K, n_q K)\,, \quad \gamma = \frac{\hbar\omega_p}{k_B T_L}\,.$$

The electron density is

$$n(t_* t, \ell_* x, \ell_* y) = \int_{\mathbb{R}^3} f(t_* t, \ell_* x, \ell_* y, \mathbf{k})\, d\mathbf{k} = \left(\frac{\sqrt{2\, m^* k_B T_L}}{\hbar}\right)^3 \rho(t, x, y)\,,$$

where

$$\rho(t, x, y) = \int_0^{+\infty} dw \int_{-1}^{1} d\mu \int_0^{\pi} d\varphi\; \Phi(t, x, y, w, \mu, \varphi)\,. \tag{4.16}$$

Hence, the dimensionless Poisson equation is

$$\frac{\partial}{\partial x}\left(\epsilon_r \frac{\partial \Psi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\epsilon_r \frac{\partial \Psi}{\partial y}\right) = c_p\left[\rho(t, x, y) - \mathcal{N}_D(x, y)\right]\,, \tag{4.17}$$

with

$$\mathcal{N}_D(x, y) = \left(\frac{\sqrt{2\, m^* k_B T_L}}{\hbar}\right)^{-3} N_D(\ell_* x, \ell_* y) \;\text{ and }\; c_p = \left(\frac{\sqrt{2\, m^* k_B T_L}}{\hbar}\right)^3 \frac{\ell_*^2 q}{\epsilon_0}\,.$$

4.3 Discontinuous Galerkin Method for Transformed Boltzmann - Poisson System and Implementation of Boundary Conditions

The domain of the devices to be considered can be represented by means of a rectangular grid in both position and momentum space. This rectangular grid, bidimensional in position space and tridimensional in momentum space, is defined as

$$\Omega_{ijkmn} = \underbrace{\left[x_{i-\frac{1}{2}},\, x_{i+\frac{1}{2}}\right] \times \left[y_{j-\frac{1}{2}},\, y_{j+\frac{1}{2}}\right]}_{X_{ij}} \times \underbrace{\left[w_{k-\frac{1}{2}},\, w_{k+\frac{1}{2}}\right] \times \left[\mu_{m-\frac{1}{2}},\, \mu_{m+\frac{1}{2}}\right] \times \left[\varphi_{n-\frac{1}{2}},\, \varphi_{n+\frac{1}{2}}\right]}_{K_{kmn}},$$

where $i = 1, \ldots N_x$, $j = 1, \ldots N_y$, $k = 1, \ldots N_w$, $m = 1, \ldots N_\mu$, $n = 1, \ldots N_\varphi$,

$$x_{i\pm\frac{1}{2}} = x_i \pm \frac{\Delta x_i}{2}\,, \quad y_{j\pm\frac{1}{2}} = y_j \pm \frac{\Delta y_j}{2}\,,$$
$$w_{k\pm\frac{1}{2}} = w_k \pm \frac{\Delta w_k}{2}\,, \quad \mu_{m\pm\frac{1}{2}} = \mu_m \pm \frac{\Delta \mu_m}{2}\,, \quad \varphi_{n\pm\frac{1}{2}} = \varphi_n \pm \frac{\Delta \varphi_n}{2}.$$

The finite dimensional space used to approximate the functions is the space of piecewise continuous polynomials which are piecewise linear in (x, y) and piecewise constant in (w, μ, φ)

$$V_h = \{v : v|_{\Omega_{ijkmn}} \in Q^{1,0}(\Omega_{ijkmn}) = P^1(X_{ij}) \otimes P^0(K_{kmn})\}, \tag{4.18}$$

with the set $Q^{1,0}(\Omega_{ijkmn})$ of tensor product polynomials, linear over the element $X_{ij} = \left[x_{i-\frac{1}{2}},\, x_{i+\frac{1}{2}}\right] \times \left[y_{j-\frac{1}{2}},\, y_{j+\frac{1}{2}}\right]$ and constant over the element $K_{kmn} = \left[w_{k-\frac{1}{2}},\, w_{k+\frac{1}{2}}\right] \times \left[\mu_{m-\frac{1}{2}},\, \mu_{m+\frac{1}{2}}\right] \times \left[\varphi_{n-\frac{1}{2}},\, \varphi_{n+\frac{1}{2}}\right]$.

The function Φ_h will denote the piecewise polynomial approximation of Φ over elements Ω_I,

$$\Phi_h \;=\; \sum_I \chi_I(x, y, w, \mu, \varphi) \left[T_I(t) + X_I(t)\,\frac{(x - x_i)}{\Delta x_i/2} + Y_I(t)\,\frac{(y - y_j)}{\Delta y_j/2}\right], \quad I = (i, j, k, m, n).$$

Under this approximation, the density on the cell $[x_{i-\frac{1}{2}},\, x_{i+\frac{1}{2}}] \times [y_{j-\frac{1}{2}},\, y_{j+\frac{1}{2}}]$ is

$$\begin{aligned}
\rho_h(t, x, y) \;&=\; \sum_{k=1}^{N_w}\sum_{m=1}^{N_\mu}\sum_{n=1}^{N_\varphi}\left[T_{ijkmn} + X_{ijkmn}\frac{(x - x_i)}{\Delta x_i/2} + Y_{ijkmn}\frac{(y - y_j)}{\Delta y_j/2}\right]\Delta w_k \Delta\mu_m \Delta\varphi_n \\
&=\; \sum_{k=1}^{N_w}\sum_{m=1}^{N_\mu}\sum_{n=1}^{N_\varphi} T_{ijkmn}\Delta w_k \Delta\mu_m \Delta\varphi_n \\
&+\; \left(\sum_{k=1}^{N_w}\sum_{m=1}^{N_\mu}\sum_{n=1}^{N_\varphi} X_{ijkmn}\Delta w_k \Delta\mu_m \Delta\varphi_n\right)\frac{(x - x_i)}{\Delta x_i/2} \\
&+\; \left(\sum_{k=1}^{N_w}\sum_{m=1}^{N_\mu}\sum_{n=1}^{N_\varphi} Y_{ijkmn}\Delta w_k \Delta\mu_m \Delta\varphi_n\right)\frac{(y - y_j)}{\Delta y_j/2}\,.
\end{aligned}$$

4.3.1 DG Formulation for Transformed Boltzmann Eq.

The Discontinuous Galerkin formulation for the Boltzmann equation (4.15) is as follows. Find $\Phi_h \in V_h$, s.t.

$$\int_{\Omega_{ijkmn}} (\Phi_h)_t \, v_h \, d\Omega - \int_{\Omega_{ijkmn}} g_1 \Phi_h \, (v_h)_x \, d\Omega - \int_{\Omega_{ijkmn}} g_2 \Phi_h \, (v_h)_y \, d\Omega \tag{4.19}$$
$$+ F_x^+ - F_x^- + F_y^+ - F_y^- + F_w^+ - F_w^- + F_\mu^+ - F_\mu^- + F_\varphi^+ - F_\varphi^- = \int_{\Omega_{ijkmn}} C(\Phi_h) \, v_h \, d\Omega.$$

for any test function $v_h \in V_h$. In (4.19), the boundary integrals are given by

$$F_x^{\pm} = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{w_{k-\frac{1}{2}}}^{w_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} \widehat{g_1 \Phi} \, v_h^{\mp}(x_{i\pm\frac{1}{2}}, y, w, \mu, \varphi) dy \, dw \, d\mu \, d\varphi,$$

$$F_y^{\pm} = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{w_{k-\frac{1}{2}}}^{w_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} \widehat{g_2 \Phi} \, v_h^{\mp}(x, y_{j\pm\frac{1}{2}}, w, \mu, \varphi) dx \, dw \, d\mu \, d\varphi,$$

$$F_w^{\pm} = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} \widehat{g_3 \Phi} \, v_h^{\mp}(x, y, w_{k\pm\frac{1}{2}}, \mu, \varphi) dx \, dy \, d\mu \, d\varphi,$$

$$F_\mu^{\pm} = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{w_{k-\frac{1}{2}}}^{w_{k+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} \widehat{g_4 \Phi} \, v_h^{\mp}(x, y, w, \mu_{m\pm\frac{1}{2}}, \varphi) dx \, dy \, dw \, d\varphi,$$

$$F_\varphi^{\pm} = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{w_{k-\frac{1}{2}}}^{w_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \widehat{g_5 \Phi} \, v_h^{\mp}(x, y, w, \mu, \varphi_{n\pm\frac{1}{2}}) dx \, dy \, dw \, d\mu,$$

where the upwind numerical fluxes $\widehat{g_s \Phi}$, $s = 1, ..., 5$ are defined as

$$
\begin{aligned}
\widehat{g_1\Phi}|_{x_{i\pm1/2}} &= \left(\frac{g_1+|g_1|}{2}\right)\Phi_h|^-_{x_{i\pm1/2}} + \left(\frac{g_1-|g_1|}{2}\right)\Phi_h|^+_{x_{i\pm1/2}}\,,\\
\widehat{g_2\Phi}|_{y_{j\pm1/2}} &= \left(\frac{g_2+|g_2|}{2}\right)\Phi_h|^-_{y_{j\pm1/2}} + \left(\frac{g_2-|g_2|}{2}\right)\Phi_h|^+_{y_{j\pm1/2}}\,,\\
\widehat{g_3\Phi}|_{w_{k\pm1/2}} &= \left(\frac{g_3+|g_3|}{2}\right)\Phi_h|^-_{w_{k\pm1/2}} + \left(\frac{g_3-|g_3|}{2}\right)\Phi_h|^+_{w_{k\pm1/2}}\,,\\
\widehat{g_4\Phi}|_{\mu_{m\pm1/2}} &= \left(\frac{g_4+|g_4|}{2}\right)\Phi_h|^-_{\mu_{m\pm1/2}} + \left(\frac{g_4-|g_4|}{2}\right)\Phi_h|^+_{\mu_{m\pm1/2}}\,,\\
\widehat{g_5\Phi}|_{\varphi_{n\pm1/2}} &= \left(\frac{g_5+|g_5|}{2}\right)\Phi_h|^-_{\varphi_{n\pm1/2}} + \left(\frac{g_5-|g_5|}{2}\right)\Phi_h|^+_{\varphi_{n\pm1/2}}\,. \qquad (4.20)
\end{aligned}
$$

4.3.2 Poisson Equation - Local Discontinuous Galerkin (LDG) Method

The Poisson equation (4.17) is solved by the LDG method as in [34] . By means of this scheme we find a solution $\Psi_h, q_h, s_h \in W_h^1$, where $(q,s) = (\partial_x\Psi,\, \partial_y\Psi)$ and $W_h^1 = \{v : v|_{X_{ij}} \in P^1(X_{ij})\}$, $P^1(X_{ij})$ the set of linear polynomials on X_{ij}. It involves rewriting the equation into the following form,

$$
\begin{cases}
q = \dfrac{\partial\Psi}{\partial x}, \qquad s = \dfrac{\partial\Psi}{\partial y}\\
\dfrac{\partial}{\partial x}\left(\epsilon_r q\right) + \dfrac{\partial}{\partial y}\left(\epsilon_r s\right) = R(t,x,y)\,,
\end{cases} \qquad (4.21)
$$

where $R(t,x,y) = c_p\left[\rho(t,x,y) - \mathcal{N}_D(x,y)\right]$ is a known function that can be computed at each time step once Φ is solved from (4.19), and the coefficient ϵ_r depends on x, y. The Poisson system is only on the (x,y) domain. Hence, we use the grid $I_{ij} = \left[x_{i-\frac{1}{2}},\, x_{i+\frac{1}{2}}\right] \times \left[y_{j-\frac{1}{2}},\, y_{j+\frac{1}{2}}\right]$, with $i = 1,\ldots,N_x$, $j = 1,\ldots,N_y+M_y$, where $j = N_y+1,\ldots,N_y+M_y$ denotes the oxide-silicon region, and the grid in $j = 1,\ldots,N_y$ is consistent with the five-dimensional

rectangular grid for the Boltzmann equation in the silicon region. The approximation space is defined as

$$W_h^\ell = \{v : v|_{I_{ij}} \in P^\ell(I_{ij})\}. \tag{4.22}$$

Here $P^\ell(I_{ij})$ denotes the set of all polynomials of degree at most ℓ on I_{ij}. The LDG scheme for (4.21) is: to find $q_h, s_h, \Psi_h \in V_h^\ell$, such that

$$\begin{aligned}
&\int_{I_{i,j}} q_h v_h dxdy + \int_{I_{i,j}} \Psi_h (v_h)_x dxdy - \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \hat{\Psi}_h v_h^-(x_{i+\frac{1}{2}}, y)dy + \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \hat{\Psi}_h v_h^+(x_{i-\frac{1}{2}}, y)dy = 0,\\
&\int_{I_{i,j}} s_h w_h dxdy + \int_{I_{i,j}} \Psi_h (w_h)_y dxdy - \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \tilde{\Psi}_h w_h^-(x, y_{j+\frac{1}{2}})dx + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \tilde{\Psi}_h w_h^+(x, y_{j-\frac{1}{2}})dx = 0,\\
&\quad - \int_{I_{i,j}} \epsilon_r q_h (p_h)_x dxdy + \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \widehat{\epsilon_r q}_h p_h^-(x_{i+\frac{1}{2}}, y)dy - \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \widehat{\epsilon_r q}_h p_h^+(x_{i-\frac{1}{2}}, y)dy\\
&\quad - \int_{I_{i,j}} \epsilon_r s_h (p_h)_y dxdy + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \widetilde{\epsilon_r s}_h p_h^-(x, y_{j+\frac{1}{2}})dx - \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \widetilde{\epsilon_r s}_h p_h^+(x, y_{j-\frac{1}{2}})dx\\
&\quad = \int_{I_{i,j}} R(t,x,y) p_h dxdy\,,
\end{aligned} \tag{4.23}$$

hold true for any $v_h, w_h, p_h \in W_h^\ell$. In the above formulation, we choose the flux as follows, in the x-direction, we use $\hat{\Psi}_h = \Psi_h^-$, $\widehat{\epsilon_r q}_h = \epsilon_r q_h^+ - [\Psi_h]$. In the y-direction, we use $\tilde{\Psi}_h = \Psi_h^-$, $\widetilde{\epsilon_r s}_h = \epsilon_r s_h^+ - [\Psi_h]$. On some part of the domain boundary, the above flux needs to be changed to accommodate various boundary conditions. For example, in the case of a double gate MOSFET device, for the boundary condition of the Poisson equation, $\Psi = 0.52354$ at source, $\Psi = 1.5235$ at drain and $\Psi = 1.06$ at gate. For the rest of the boundary regions, we have homogeneous Neumann boundary conditions, i.e., $\frac{\partial \Psi}{\partial n} = 0$. The relative dielectric constant in the oxide-silicon region is $\epsilon_r = 3.9$, in the silicon

region is $\epsilon_r = 11.7$. Near the drain then, we are given Dirichlet boundary condition, so we need to flip the flux in $x-$direction: let $\hat{\Psi}_h(x_{i+\frac{1}{2}}, y) = \Psi_h^+(x_{i+\frac{1}{2}}, y)$ and $\widehat{\epsilon_r q}_h(x_{i+\frac{1}{2}}, y) = \epsilon_r q_h^-(x_{i+\frac{1}{2}}, y) - [\Psi_h](x_{i+\frac{1}{2}}, y)$, if the point $(x_{i+\frac{1}{2}}, y)$ is at the drain. For the gate, we need to flip the flux in $y-$direction: let $\tilde{\Psi}_h(x, y_{j+\frac{1}{2}}) = \Psi_h^+(x, y_{j+\frac{1}{2}})$ and $\widetilde{\epsilon_r s}_h(x, y_{j+\frac{1}{2}}) = \epsilon_r s_h^-(x, y_{j+\frac{1}{2}}) - [\Psi_h](x, y_{j+\frac{1}{2}})$, if the point $(x, y_{j+\frac{1}{2}})$ is at the gate. For the bottom, we need to use the Neumann condition, and flip the flux in y-direction, i.e., $\tilde{\Psi}_h = \Psi_h^+$, $\widetilde{\epsilon_r s}_h = \epsilon_r s_h^-$. This scheme described above will enforce the continuity of Ψ and $\epsilon_r \frac{\partial \Psi}{\partial n}$ across the interface of silicon and oxide-silicon interface. The solution of (4.23) gives us approximations to both the potential Ψ_h and the electric field $(E_x)_h = -c_v q_h$, $(E_y)_h = -c_v s_h$.

4.3.3 RK-DG Algorithm for BP, from t^n to t^{n+1}

The following RK-DG algorithm for BP is a dynamic extension of the Gummel iteration map. To evolve from time t^n to time t^{n+1}:

1. Compute the electron density $\rho_h(x, y, t)$.

2. Solve Poisson Eq. for the given $\rho_h(x, y, t)$ by Local DG, obtaining the potential Ψ_h and the electric field $\mathbf{E}_h = -(q_h, s_h)$. Compute then the respective transport terms g_s, $s = 1, ..., 5$.

3. Solve by DG the advection and collision part of the Boltzmann Equation. A Method of Lines (an ODE system) for the time dependent coefficients of Φ_h (degrees of freedom) is obtained.

4. Evolve ODE system by Runge-Kutta from t^n to t^{n+1}. (If partial time step necessary, repeat Step 1 to 3 as needed).

4.4 Boundary Conditions Implementation for 2D-$\vec{x}$, 3D-$\vec{k}$ devices at x, w, μ, φ Boundaries

We will consider in this work 2D devices in position space, which need a 3D momentum description for kinetic equations modeling semiconductors. For example, a common device of interest is a 2D double gate MOSFET. A schematic plot of it is given in Figure 4.1. The shadowed region denotes the oxide-silicon region, whereas the rest is the silicon region. Potential bias are applied at the source, drain, and gates. The problem is symmetric about the x-axis.

Another possible 2D problem is the case of a bi-dimensional bulk silicon diode, for which the doping is constant all over the physical domain, and which would have just an applied potential (bias) between the source $x = 0$ and the drain $x = L_x$ (no gates), with insulating reflecting boundaries at $y = 0$ and $y = L_y$.

We consider in the following sections the different kinds of boundary conditions for 2D devices and their numerical implementation, either at $\vec{x}$-boundaries or at $\vec{w}$-boundaries.

4.4.1 Poisson Eq. Boundary Condition

The BC for Poisson Eq. are imposed over the (x, y)-domain.

For example, for the case of a 2D Double gated MOSFET, Dirichlet

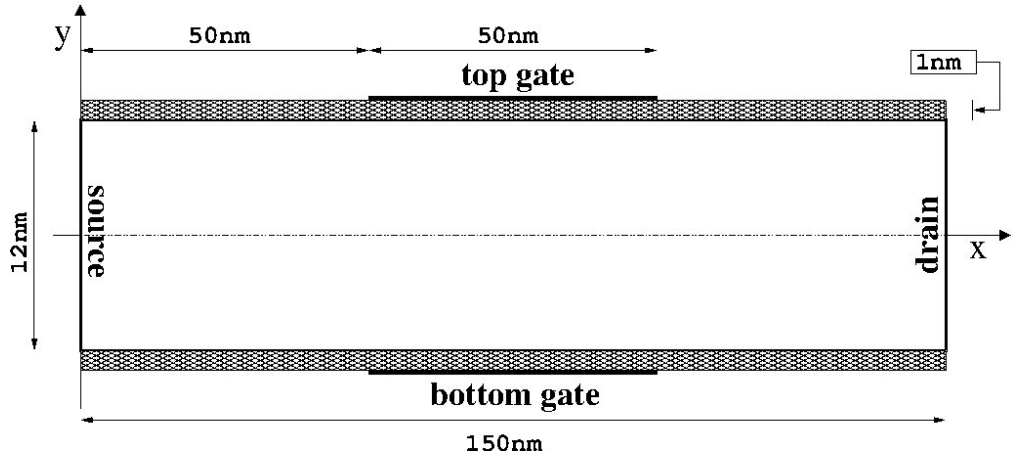


Figure 4.1: Schematic representation of a 2D double gate MOSFET device

BC would be imposed to the potential Ψ, as we have three different applied potentials biases, $\Psi = 0.5235$ Volts at the source $x = 0$, $\Psi = 1.5235$ Volts at the drain $x = L_x$, $\Psi = 1.06$ Volts at the gates. Homogeneous Neumann BC would be imposed for the rest of the boundaries, that is, $\partial_{\hat{n}}\Psi = 0$.

For the case of a 2D bulk silicon diode, we impose Dirichlet BC for the difference of potential Ψ between source and drain, $\Psi = 0.5235$ Volts at the source $x = 0$, $\Psi = 1.5235$ Volts at the drain $x = L_x$. For the boundaries $y = 0, L_y$ we impose Homogeneous Neumann BC too, that is, $\partial_y \Psi|_{y_0} = 0, \quad y_0 = 0, L_y$.

4.4.2 Charge Neutrality BC

As in [34], at the source and drain contacts, we implement the charge neutrality boundary condition (4.1). Ghost cells for $i = 0$ and $i = N_x + 1$

at the respective boundaries are used, implementing this BC numerically as below:

$$\Phi(i=0) = \Phi(i=1)\frac{N_D(i=1)}{\rho(i=1)},$$

and

$$\Phi(i=N_x+1) = \Phi(i=N_x)\frac{N_D(i=N_x)}{\rho(i=N_x)}.$$

4.4.3 Cut - Off BC

In the (w, μ, φ)-space, we only need to apply a cut-off Boundary Condition. At $w = w_{\max}$, Φ_h is made machine zero,

$$\Phi_h(x, y, w, \mu, \varphi, t)|_{w=w_{\max}} = 0. \tag{4.24}$$

No other boundary condition is necessary for $\vec{w}$-boundaries, since analytically we have that

- at $w = 0$, $g_3 = 0$,
- at $\mu = \pm 1$, $g_4 = 0$,
- at $\varphi = 0, \pi$, $g_5 = 0$,

so, at such regions, the numerical flux always vanishes.

4.5 Reflection BC on BP

Reflection Boundary Conditions can be expressed in the form

$$f(\vec{x}, \vec{k}, t)|_{\Gamma_{N^-}} = F_R(f|_{\Gamma_{N^+}}) \tag{4.25}$$

such that the following pointwise zero flux condition is satisfied at reflecting boundaries

$$
\begin{aligned}
0 &= \eta(\vec{x}) \cdot J(\vec{x},t) = \eta(\vec{x}) \cdot \int_{\Omega_{\vec{k}}} \vec{v}(\vec{k})\, f(\vec{x},\vec{k},t)\, d\vec{k}\,, \qquad (4.26)\\
0 &= \int_{\eta(\vec{x})\cdot\vec{v}(\vec{k})>0} \eta(\vec{x}) \cdot \vec{v}(\vec{k})\, f(\vec{x},\vec{k},t)|_{\Gamma_{N^+}}\, d\vec{k} \,+\, \int_{\eta(\vec{x})\cdot\vec{v}(\vec{k})<0} \eta(\vec{x}) \cdot \vec{v}(\vec{k})\, f(\vec{x},\vec{k},t)|_{\Gamma_{N^-}}\, d\vec{k}\,,\\
0 &= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_{\Gamma_{N^+}}\, d\vec{k} \,+\, \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, F_R(f|_{\Gamma_{N^+}})\, d\vec{k}\,,
\end{aligned}
$$

as in Cercignani, Gamba, and Levermore, [54] where the given BC at Neumann boundary regions at the kinetic level is such that the particle flow vanishes.

For simplicity we write $\vec{v} = \vec{v}(\vec{k}) = \nabla_{\vec{k}}\varepsilon(\vec{k})/\hbar$. We will study three kinds of reflective boundary conditions: specular, diffusive, and mixed reflection. The last one is a convex combination of the previous two, but the convexity parameter can be either constant or momentum dependant, $p(\vec{k})$. We go over the mathematics and numerics related to these conditions below.

4.5.1 Specular Reflection

It is clear that, at the analytical level, the specular reflection BC (4.6) satisfies the zero flux condition pointwise at reflecting boundaries, since

$$
\int_{\eta\cdot\vec{v}>0} |\eta(\vec{x})\cdot\vec{v}(\vec{k})|\; f(\vec{x},\vec{k},t)\Big|_{\Gamma_{N^+}}\, d\vec{k} - \int_{-\eta\cdot\vec{v}<0} |\eta(\vec{x})\cdot\vec{v}(\vec{k})|\; f(\vec{x},\vec{k}',t)\Big|_{\Gamma_{N^+}}\, d\vec{k} = 0. \qquad (4.27)
$$

Specular reflection BC in our transformed Boltzmann Eq. for the new coordinate system is mathematically formulated in our problem as

$$
\Phi|_-(x,y,w,\mu,\varphi,t) = \Phi|_+(x,y,w,\mu,\pi-\varphi,t), \quad (x,y,w,\mu,\varphi)\in\Gamma_N^-. \qquad (4.28)
$$

To impose numerically specular reflection BC at $y = 0,\, L_y$ in the DG method, we follow the procedure of [34]. We relate the inflow values of the pdf, associated to the outer ghost cells, to the outflow values of the pdf, which are associated to the interior cells adjacent to the boundary, as given below

$$\Phi_h|_-(x, y_{1/2}, w, \mu, \varphi, t) = \Phi_h|_+(x, y_{1/2}, w, \mu, \pi - \varphi, t), \quad y_{1/2} = 0, \tag{4.29}$$
$$\Phi_h|_-(x, y_{N_y+\frac{1}{2}}, w, \mu, \varphi, t) = \Phi_h|_+(x, y_{N_y+\frac{1}{2}}, w, \mu, \pi - \varphi, t), \quad y_{N_y+\frac{1}{2}} = L_y.$$

In the case of the boundary $y_{1/2} = 0$, assuming $\Delta y_0 = \Delta y_1$, $\Delta\varphi_{n'} = \Delta\varphi_n$, with $n' = N_\varphi - n + 1$, if $(x, y_{1/2} - y, w, \mu, \varphi) \in \Omega_{i0kmn}$ then $(x, y_{1/2} + y, w, \mu, \pi - \varphi) \in \Omega_{i1kmn'}$. The values of $\Phi_h|^{\pm}_{y_{1/2}}$ at the related inner and outer boundary cells Ω_{i0kmn} $(j = 0)$ and $\Omega_{i1kmn'}$ $(j = 1)$ must be equal at the boundary $y_{1/2} = 0$. Indeed

$$\begin{aligned}
&\Phi_h|^-_{\Omega_{i0kmn}}(x, y_{1/2}, w, \mu, \varphi, t) = \Phi_h|^+_{\Omega_{i1kmn'}}(x, y_{1/2}, w, \mu, \pi - \varphi, t) \implies \\
&T_{i0kmn} + X_{i0kmn}\frac{(x - x_i)}{\Delta x_i/2} + Y_{i0kmn}\frac{(y_{1/2} - y_0)}{\Delta y_0/2} = \\
&T_{i1kmn'} + X_{i1kmn'}\frac{(x - x_i)}{\Delta x_i/2} + Y_{i1kmn'}\frac{(y_{1/2} - y_1)}{\Delta y_1/2}\,.
\end{aligned}$$

Therefore, from the equality above we find the relation between the coefficients of Φ_h at inner and outer adjacent boundary cells, given by

$$T_{i0kmn} = T_{i1kmn'},\; X_{i0kmn} = X_{i1kmn'},\; Y_{i0kmn} = -Y_{i1kmn'}\,. \tag{4.30}$$

Following an analogous procedure for the boundary $y_{N_y+1/2}$, we have

$$\Phi_h|^-_{\Omega_{i,N_y+1,kmn}}(x, y_{N_y+\frac{1}{2}}, w, \mu, \varphi, t) = \Phi_h|^+_{\Omega_{i,N_y,kmn'}}(x, y_{N_y+\frac{1}{2}}, w, \mu, \pi - \varphi, t)\,,$$

then

$$T_{i,N_y+1,kmn} + X_{i,N_y+1,kmn}\frac{(x-x_i)}{\Delta x_i/2} + Y_{i,N_y+1,kmn}\frac{(y_{N_y+\frac{1}{2}} - y_{N_y+1})}{\Delta y_{N_y+1}/2} =$$
$$T_{i,N_y,kmn'} + X_{i,N_y,kmn'}\frac{(x-x_i)}{\Delta x_i/2} + Y_{i,N_y,kmn'}\frac{(y_{N_y+\frac{1}{2}} - y_{N_y})}{\Delta y_{N_y}/2}\,, \qquad (4.31)$$

hence

$$T_{i,N_y+1,kmn} = T_{i,N_y,kmn'}, \quad X_{i,N_y+1,kmn} = X_{i,N_y,kmn'}, \quad Y_{i,N_y+1,kmn} = -Y_{i,N_y,kmn'}\,.$$

4.5.2 Diffusive Reflection

The diffusive reflection BC can be formulated in the following way

$$f(\vec{x},\vec{k},t)|_- = F_D(f|_+) = C\,\sigma\left\{f|_+\right\}(\vec{x},t)\,e^{-\varepsilon(\vec{k})/K_BT_L}\,, \quad (\vec{x},\vec{k}) \in \Gamma_N^-\,, \quad (4.32)$$

where $\sigma\left\{f|_+\right\}(\vec{x},t) = \sigma(\vec{x},t)$ and $C = C\{\eta(\vec{x})\}$ are the function and parameter such that the zero flux condition is satisfied at each of the points of the Neumann Boundary

$$\begin{aligned} 0 &= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_{\Gamma_{N^+}}\, d\vec{k} + \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\,\left[C\sigma(\vec{x},t)e^{-\varepsilon(\vec{k})/K_BT_L}\right]\, d\vec{k}\,, \\ 0 &= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_{\Gamma_{N^+}}\, d\vec{k} - \sigma(\vec{x},t)\cdot C\int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, e^{-\varepsilon(\vec{k})/K_BT_L}\, d\vec{k}\,. \end{aligned}$$

It follows then that

$$\sigma\left\{f|_+\right\}(\vec{x},t) = \int_{\vec{v}(\vec{k})\cdot\eta>0} \vec{v}\cdot\eta\, f|_{\Gamma_{N^+}}(\vec{x},\vec{k},t)\, d\vec{k}\,, \qquad (4.33)$$

$$C\left\{\eta(\vec{x})\right\} = \left(\int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, e^{-\varepsilon(\vec{k})/K_BT_L}\, d\vec{k}\right)^{-1}\,, \qquad (4.34)$$

$$f(\vec{x},\vec{k},t)|_- = \frac{e^{-\varepsilon(\vec{k})/K_BT_L}\int_{\vec{v}(\vec{k})\cdot\eta>0}\vec{v}\cdot\eta\, f|_{\Gamma_{N^+}}(\vec{x},\vec{k},t)\,d\vec{k}}{\int_{\vec{v}\cdot\eta<0}|\vec{v}\cdot\eta|\, e^{-\varepsilon(\vec{k})/K_BT_L}\,d\vec{k}}\,. \tag{4.35}$$

The diffusive reflection BC, formulated in terms of the unknown function Φ of the transformed Boltzmann Equation 4.15, is expressed as

$$\Phi|_-(x,y,w,\mu,\varphi,t) = F_D(\Phi|_+) = C\,\sigma\left\{\Phi|_+\right\}(x,y,t)\,e^{-w}s(w)\,, \tag{4.36}$$

$$\sigma(x,y,t) = \int_{(g_1,g_2)\cdot\eta>0}\eta\cdot(g_1,g_2)(w,\mu,\varphi)\,\Phi|_+\,dwd\mu d\varphi\,, \tag{4.37}$$

$$C(\eta) = \left(\int_{(g_1,g_2)\cdot\eta<0}|(g_1,g_2)\cdot\eta|\,e^{-w}s(w)\,dwd\mu d\varphi\right)^{-1}. \tag{4.38}$$

We have, over the portion of the boundary considered, that $\eta=(0,-1,0)$ for $y=0$ and $\eta=(0,1,0)$ for $y=L_y$. Therefore

$$\Phi|_-(x,y_b,w,t) = \frac{e^{-w}s(w)\int_{-g_2>0}|g_2|\,\Phi|_+\,dwd\mu d\varphi}{\int_{-g_2<0}|g_2|\,e^{-w}s(w)\,dwd\mu d\varphi}\,,\quad y_b=0\,, \tag{4.39}$$

$$\Phi|_-(x,y_b,w,t) = \frac{e^{-w}s(w)\int_{+g_2>0}|g_2|\,\Phi|_+\,dwd\mu d\varphi}{\int_{+g_2<0}|g_2|\,e^{-w}s(w)\,dwd\mu d\varphi}\,,\quad y_b=L_y\,. \tag{4.40}$$

4.5.2.1 Numerical Formulation of Diffusive BC for DG

For the DG numerical method, we have to project the boundary conditions to be imposed in the space V_h. Our goal is to have at the numerical level an equivalent pointwise zero flux condition at the reflection boundary regions.

We formulate then the diffusive BC for the DG method in the following way

$$\begin{aligned}\Phi_h|_-(x,y_b,w,\mu,\varphi,t) &= \Pi_h\left\{F_D(\Phi_h|_+)\right\}\\ &= \Pi_h\left\{C\,\sigma_h\left\{\Phi_h|_+\right\}(x,y_b,t)\,e^{-w}s(w)\right\},\quad y_b=0,L_y.\end{aligned}$$

where $\sigma_h \in V_h$ is a function in our piecewise polynomial space for (x, y) and C is a parameter such that the zero flux condition is satisfied numerically

$$\begin{aligned} 0 &= \int_{\vec{g}\cdot\eta>0} \vec{g}\cdot\eta\,\Phi_h|_+ d\vec{w} + \int_{\vec{g}\cdot\eta<0} \vec{g}\cdot\eta\,\Phi_h|_- d\vec{w} \\ &= \int_{\vec{g}\cdot\eta>0} \vec{g}\cdot\eta\,\Phi_h|_+ d\vec{w} + \int_{\vec{g}\cdot\eta<0} \vec{g}\cdot\eta\,\Pi_h\left\{F_D(\Phi_h|_+)\right\} d\vec{w} \qquad (4.41) \\ &= \int_{\vec{g}\cdot\eta>0} \vec{g}\cdot\eta\,\Phi_h|_+ d\vec{w} + \int_{\vec{g}\cdot\eta<0} \vec{g}\cdot\eta\,\Pi_h\left\{C\,\sigma_h\left\{\Phi_h|_+\right\}(x, y_b, t)\, e^{-w} s(w)\right\} d\vec{w}\,. \end{aligned}$$

In the space V_h of piecewise continuous polynomials which are tensor products of polynomials of degree p in $\vec{x}$ and of degree q in $\vec{w}$, the following holds

$$\begin{aligned} &\Pi_h\left\{f_1(\vec{x}) f_2(\vec{w})\right\} = \Pi_h\left\{f_1(\vec{x})\right\}\,\Pi_h\left\{f_2(\vec{w})\right\}\,, \qquad (4.42) \\ &V_h = \{v : v|_{\Omega_{ijkmn}} \in Q^{p,q}(\Omega_{ijkmn}) = P^p(X_{ij}) \otimes P^q(K_{kmn})\}. \end{aligned}$$

Therefore, for our particular case we have that

$$\Pi_h\left\{C\,\sigma_h(x, y_b, t)\, e^{-w} s(w)\right\} = C\,\sigma_h(x, y_b, t)\,\Pi_h\left\{e^{-w} s(w)\right\}\,, \qquad (4.43)$$

so for the numerical zero flux condition pointwise we have that

$$\begin{aligned} 0 &= \int_{\vec{g}\cdot\eta>0} \vec{g}\cdot\eta\,\Phi_h|_+ d\vec{w} + \int_{\vec{g}\cdot\eta<0} \vec{g}\cdot\eta\, C\,\sigma_h\left\{\Phi_h|_+\right\}(x, y_b, t)\,\Pi_h\left\{e^{-w} s(w)\right\} d\vec{w} \\ 0 &= \int_{\vec{g}\cdot\eta>0} \vec{g}\cdot\eta\,\Phi_h|_+ d\vec{w} - \sigma_h\left\{\Phi_h|_+\right\}(x, y_b, t)\, C \int_{\vec{g}\cdot\eta<0} |\vec{g}\cdot\eta|\,\Pi_h\left\{e^{-w} s(w)\right\} d\vec{w}\,. \end{aligned}$$

We observe then that we can obtain a numerical equivalent of the pointwise zero flux condition if we define

$$\begin{aligned} &\sigma_h\left\{\Phi_h|_+\right\}(x, y_b, t) = \int_{\pm g_2=\vec{g}\cdot\eta>0} \vec{g}\cdot\eta\,\Phi_h|_+ d\vec{w} = \sigma\left\{\Phi_h|_+\right\}(x, y_b, t)\,, \quad y_b = 0,\, L_y\,. \\ &C\left\{\eta\right\} = C\left\{\pm\hat{y}\right\} = \left(\int_{\pm g_2=\vec{g}\cdot\eta<0} |\vec{g}\cdot\eta|\,\Pi_h\left\{e^{-w} s(w)\right\} d\vec{w}\right)^{-1}, \quad \eta = \pm\hat{y} \quad . \end{aligned}$$

In our particular case, in which we have chosen our function space as piecewise linear in (x, y) and piecewise constant in (w, μ, φ), the projection of the Maxwellian is a piecewise constant approximation representing its average value over each momentum cell , that is

$$\Pi_h \left\{ e^{-w} s(w) \right\} = \sum_{k,m,n} \chi_{kmn} \frac{\int_{kmn} e^{-w} s(w)\, dw\, d\mu\, d\varphi}{\Delta w_k \Delta \mu_m \Delta \varphi_n} = \sum_{k,m,n} \chi_{kmn} \frac{\int_{w_{k-}}^{w_{k+}} e^{-w} s(w)\, dw}{\Delta w_k}\,. \tag{4.44}$$

Therefore, for the particular space we have chosen, we have that

$$\begin{aligned}
&\sigma_h \left\{ \Phi_h|_+ \right\} (x, y_b, t) = \int_{\pm g_2 > 0} \pm g_2\, \Phi_h|_+ d\vec{w} = \sigma \left\{ \Phi_h|_+ \right\} (x, y_b, t)\,, \qquad (4.45)\\
&\quad y_b = 0 = y_{1/2} \quad (\eta = -\hat{y})\,, \quad \text{or} \quad y_b = L_y = y_{N_y+1/2} \quad (\eta = +\hat{y})\,,\\
&C^{-1} = \sum_{k,m,n}^{\pm g_2 < 0} \frac{1}{\Delta w_k} \int_{w_{k-1/2}}^{w_{k+1/2}} e^{-w} s(w)\, dw \int_{k,m,n} |g_2|\, dw\, d\mu\, d\varphi, \quad \eta = \pm \hat{y}\,,\\
&\Phi_h|_-(x, y_b, w, \mu, \varphi, t) = C\, \sigma_h \left\{ \Phi_h|_+ \right\} (x, y_b, t)\, \Pi_h \left\{ e^{-w} s(w) \right\}, \quad y_b = 0, L_y,\\
&\Phi_h|_-(x, y_b, w, \mu, \varphi, t) = \frac{\int_{\pm g_2 > 0} |g_2|\, \Phi_h|_+ d\vec{w} \times \sum_{k,m,n}^{\pm g_2 < 0} \chi_{k,m,n} \int_k e^{-w} s(w)\, dw/\Delta w_k}{\sum_{k,m,n}^{\pm g_2 < 0} \int_{kmn} |g_2|\, dw\, d\mu\, d\varphi \int_k e^{-w} s(w)\, dw/\Delta w_k}\,.
\end{aligned}$$

We notice that the polynomial approximation σ_h is equal to the analytical function σ operating on the polynomial approximation $\Phi_h|_+$. However, the constant C needed in order to achieve the zero flux condition numerically is not equal to the value of this parameter in the analytical solution. In this case C is an approximation of the analytical value using a piecewise constant approximation of the Maxwellian (its average over cells).

The approximate operator $\sigma_h \left\{ \Phi_h|_+ \right\} (x, y, t)$ gives a piecewise linear polynomial dependant on (x, y) with time dependent coefficients. We have

that

$$\Phi_h|_+ \in V_h \implies \sigma_h\left\{\Phi_h|_+\right\}(x,y,t) = \int_{\pm\cos\varphi>0} |g_2|\,\Phi_h|_+\, dwd\mu d\varphi \in V_h$$

where $\Phi_h|_+$ is such that, at the boundary $y = y_b$ of the cell Ω_{ijkmn}, is given by

$$\Phi_h|_+(t,x,y,w,\mu,\varphi) = T_{ijkmn}(t) + X_{ijkmn}(t)\,\frac{2(x-x_i)}{\Delta x_i} + Y_{ijkmn}(t)\,\frac{2(y-y_j)}{\Delta y_j}\,.$$

We define $I = ijkmn$, so in $\Omega_I = X_{ij}\times K_{kmn}$. Then,

$$\sigma_h(x,y,t) = \sigma_I^0(t) + \sigma_I^x(t)\frac{(x-x_i)}{\Delta x_i/2} + \sigma_I^y(t)\frac{(y-y_j)}{\Delta y_j/2}\,. \tag{4.46}$$

We summarize the main results of these calculations for σ_h and $\Phi_h|_-$, by showing just the ones related to $y = L_y$ (the case $y = 0$ is analogous). At the boundary $y = L_y$, the inner cells associated to outflow have $j = N_y$, adjacent to the boundary, whereas the ghost cells related to inflow have the index $j = N_y + 1$. We compute the integral σ_h as follows

$$\begin{aligned}\sigma_h\left\{\Phi_h|_+\right\}(x,y,t) &= \int_{\cos\varphi\geq 0} \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w}\sqrt{1-\mu^2}\cos\varphi\ \Phi_h|_+\, dwd\mu d\varphi \\ &= \sum_{k,m,n}^{n\leq N_p/2}\int_{K_{kmn}} \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w}\sqrt{1-\mu^2}\cos\varphi\,\Phi_h|_+\, dwd\mu d\varphi\,.\end{aligned}$$

Therefore, we have, with $I = (i,j,k,m,n),\ j = N_y$ below, that

$$\sigma_I^0 = \sum_{k,m,n}^{n\leq N_{\varphi/2}} T_{iN_ykmn}\int_{w_{k-1/2}}^{w_{k+1/2}} \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w}dw\int_{\mu_{m-1/2}}^{\mu_{m+1/2}}\sqrt{1-\mu^2}d\mu\int_{\varphi_{n-1/2}}^{\varphi_{n+1/2}}\cos\varphi d\varphi\,,$$

$$\sigma_I^x = \sum_{k,m,n}^{n\leq N_{\varphi/2}} X_{iN_ykmn}\int_{w_{k-1/2}}^{w_{k+1/2}} \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w}dw\int_{\mu_{m-1/2}}^{\mu_{m+1/2}}\sqrt{1-\mu^2}d\mu\int_{\varphi_{n-1/2}}^{\varphi_{n+1/2}}\cos\varphi d\varphi\,,$$

$$\sigma_I^y = \sum_{k,m,n}^{n\leq N_{\varphi}/2} Y_{iN_ykmn} \int_{w_{k-1/2}}^{w_{k+1/2}} \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \sqrt{1-\mu^2} d\mu \int_{\varphi_{n-1/2}}^{\varphi_{n+1/2}} \cos\varphi d\varphi \,. \tag{4.47}$$

Once the coefficients of σ_h have been computed, we use them to obtain the polynomial approximation $\Phi_h|_-$, with $j = N_y + 1$, from (4.45)

$$\Phi_h|_{y=L_y}^- = \sum_i \sum_{k,m,n}^{n\geq N_{\varphi}/2} \chi_{iN_y}\chi_{kmn} C \left[\sigma_I^0 + \sigma_I^x \frac{(x-x_i)}{\Delta x_i/2} + \sigma_I^y(+1)\right] \frac{\int_k e^{-w} s(w)\, dw}{\Delta w_k} \quad . \tag{4.48}$$

We have at the same time, by definition, that

$$\Phi_h|_{y=L_y}^- = \sum_{i,k,m,n}^{n\geq N_{\varphi}/2} \chi_{i,N_y+1,kmn} \left[T_{i,N_y+1,k,m,n} + X_{i,N_y+1,k,m,n} \frac{(x-x_i)}{\Delta x_i/2} + Y_{i,N_y+1,k,m,n}(-1)\right].$$

Therefore, the coefficients for $\Phi_h|_{y=L_y}^-$ are

$$T_{i,N_y+1,kmn}(t) = C\sigma^0_{iN_ykmn}(t) \frac{\int_k e^{-w} s(w) dw}{\Delta w_k} \,, \tag{4.49}$$

$$X_{i,N_y+1,kmn}(t) = C\sigma^x_{iN_ykmn}(t) \frac{\int_k e^{-w} s(w) dw}{\Delta w_k} \,, \tag{4.50}$$

$$Y_{i,N_y+1,kmn}(t) = (-1)C\sigma^y_{iN_ykmn}(t) \frac{\int_k e^{-w} s(w) dw}{\Delta w_k} \,, \tag{4.51}$$

keeping in mind that our parameter C is given by the formula below

$$C^{-1} = \sum_{k,m,n}^{n\geq N_p/2} \frac{\int_k e^{-w} s(w) dw}{\Delta w_k} \int_k \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int_m \sqrt{1-\mu^2} d\mu \int_n \cos\varphi d\varphi \,. \tag{4.52}$$

4.5.3 Mixed Reflection

The mixed reflection condition is a convex combination of the specular and diffusive reflections:

$$f(\vec{x},\vec{k},t)|_- = pf|_+(\vec{x},\vec{k}',t) \,+\, (1-p)C\sigma\left\{f|_+\right\}(\vec{x},t)e^{-\varepsilon(\vec{k})/K_BT}\,, \quad (\vec{x},\vec{k})\in\Gamma_N^-\,,$$

p is the Specularity Parameter, $0 \le p \le 1$. p can be either constant or $p = p(\vec{k})$, a function of the wave vector momentum.

For p constant, it can be shown easily that the previous formulas obtained for the specular and diffusive BC, in particular the previous formulas for $\sigma\, C(x)$, works also in this case to obtain a zero flux condition at the Neumann boundaries:

$$\begin{aligned}
\eta\cdot J &= \int_{\vec{v}\cdot\eta>0}\vec{v}\cdot\eta\, f|_+\, d\vec{k} \,+\, \int_{\vec{v}\cdot\eta<0}\vec{v}\cdot\eta\,\left[pf(\vec{x},\vec{k}',t)|_+ + (1-p)Ce^{-\varepsilon(\vec{k})/K_BT_L}\sigma(\vec{x},t)\right]\, d\vec{k}\\
&= \int_{\vec{v}\cdot\eta>0}\vec{v}\cdot\eta\, f|_+\, d\vec{k} \,+\, p\int_{\vec{v}\cdot\eta<0}\vec{v}\cdot\eta\, f(\vec{x},\vec{k}',t)|_+\, d\vec{k} + (1-p)\,\sigma C\int_{\vec{v}\cdot\eta<0}\vec{v}\cdot\eta\, e^{\frac{-\varepsilon(\vec{k})}{K_BT_L}}\, d\vec{k}\\
&= \sigma(\vec{x},t) \,-\, p\sigma(\vec{x},t) + (1-p)\,\sigma(\vec{x},t)\,(-1) = 0\,.
\end{aligned}$$

However, for $p(\vec{k})$ a function of the crystal momentum the same choice of $\sigma(\vec{x},t)$ and $C(x)$ as in the diffusive case does not necessarily guarantee that the zero flux condition will be satisfied at Neumann boundaries. Therefore, a new condition for C in order to satisfy this condition must be derived. We derive it below.

The general mixed reflection BC can be formulated as

$$f(\vec{x},\vec{k},t)|_- = p(\vec{k})f|_+(\vec{x},\vec{k}',t) + (1-p(\vec{k}))\,C'\sigma'\left\{f|_+\right\}(\vec{x},t)\,e^{-\varepsilon(\vec{k})/K_BT}\,, \quad (\vec{x},\vec{k})\in\Gamma_N^-$$

where $\sigma'\{f|_+\}(\vec{x},t)$ and C' are the function and parameter such that the pointwise zero flux condition is satisfied at the Neumann boundaries

$$\begin{aligned} 0 &= \eta(\vec{x})\cdot J(\vec{x},t) \\ &= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k} + \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta \left[p(\vec{k}) f(\vec{x},\vec{k}',t)|_+ + (1-p(\vec{k}))C' e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}} \sigma'(\vec{x},t)\right] d\vec{k}\,. \end{aligned}$$

Since

$$0 = \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k} + \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, p(\vec{k})\, f(\vec{x},\vec{k}',t)|_+\, d\vec{k} - \sigma'(\vec{x},t)\, C' \int_{\vec{v}\cdot\eta<0} (1-p(\vec{k}))|\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon}{K_B T_L}}\, d\vec{k}\,,$$

we conclude then that

$$\sigma'\{f|_+\}(\vec{x},t) = \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k} - \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, p(\vec{k})\, f(\vec{x},\vec{k}',t)|_+\, d\vec{k}\,, \quad (4.53)$$

$$C'\{\eta(\vec{x})\} = \left(\int_{\vec{v}\cdot\eta<0} (1-p(\vec{k}))|\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon}{K_B T_L}}\, d\vec{k}\right)^{-1}. \quad (4.54)$$

The general mixed reflection BC then has the specific form

$$\begin{aligned} f(\vec{x},\vec{k},t)|_- &= p(\vec{k})\, f|_+(\vec{x},\vec{k}',t) \\ &+ (1-p(\vec{k}))\, e^{-\frac{\varepsilon(\vec{k})}{K_B T}} \frac{\left(\int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k} - \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, p(\vec{k})\, f(\vec{x},\vec{k}',t)|_+\, d\vec{k}\right)}{\int_{\vec{v}\cdot\eta<0}(1-p(\vec{k}))|\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}}\, d\vec{k}}\,, \end{aligned}$$

with $\quad (\vec{x},\vec{k}) \in \Gamma_N^-\,, \quad (\vec{x},\vec{k}') \in \Gamma_N^+$ s.t. $\vec{v}(\vec{k}') = \vec{v}(\vec{k}) - 2(\vec{v}(\vec{k})\cdot\eta)\eta\,.$

Notice that the product $C'\sigma'(\vec{x},t)$ has the form

$$C'\sigma'(\vec{x},t) = \frac{\left(\int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k} \;-\; \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, p(\vec{k})\, f(\vec{x},\vec{k}',t)|_+\, d\vec{k}\right)}{\int_{\vec{v}\cdot\eta<0}(1-p(\vec{k}))|\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}}\, d\vec{k}} \qquad (4.55)$$

which for the case of p constant, it reduces to the original function $\sigma(\vec{x},t)$ and parameter $C\,\{\eta(\vec{x})\}$.

$$\begin{aligned}
\text{If} \quad p &= \text{ct}, \\
C'\sigma'(\vec{x},t) &= \frac{\left(\int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k} \;-\; p\int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, f(\vec{x},\vec{k}',t)|_+\, d\vec{k}\right)}{\int_{\vec{v}\cdot\eta<0}(1-p)|\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}}\, d\vec{k}} \\
&= \frac{(1-p)\int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k}}{(1-p)\int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}}\, d\vec{k}} \\
&= \frac{\int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k}}{\int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}}\, d\vec{k}} \\
&= C\,\sigma\,(\vec{x},t)\,.
\end{aligned}$$

However, for the non-constant case $p(\vec{k})$ the new function and parameter $\sigma'(\vec{x},t)$, $C'(\eta)$ need to be used instead, as the previous $\sigma(\vec{x},t)$, $C(\eta)$ will not satisfy the zero flux condition in general for $p(\vec{k})$

$$0 = \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k} + \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, p(\vec{k})\, f(\vec{x},\vec{k}',t)|_+\, d\vec{k} - \sigma'\, C' \int_{\vec{v}\cdot\eta<0} (1-p(\vec{k}))|\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon}{K_B T_L}}\, d\vec{k},$$

$$\begin{aligned}
C'\sigma' &= \frac{\int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k} \;+\; \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, p(\vec{k})\, f(\vec{x},\vec{k}',t)|_+\, d\vec{k}}{\int_{\vec{v}\cdot\eta<0}(1-p(\vec{k}))|\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon}{K_B T_L}}\, d\vec{k}} \\
&\neq \frac{\int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, f|_+\, d\vec{k}}{\int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, e^{\frac{-\varepsilon(\vec{k})}{K_B T_L}}\, d\vec{k}} = C\sigma(\vec{x},t) \quad \text{in general for } p(\vec{k}).
\end{aligned}$$

A more general possible case of mixed reflection BC would have a specularity parameter $p(\vec{x},\vec{k},t)$ dependent on position, momentum, and time. The related reflective BC would then be

$$f|_-(\vec{x},\vec{k},t) \quad = \quad p(\vec{x},\vec{k},t)f|_+(\vec{x},\vec{k}',t) + \Big(1-p(\vec{x},\vec{k},t)\Big)\, C^*(\vec{x},t)\sigma^*(\vec{x},t)M(\vec{x},\vec{k})$$
$$(\vec{x},\vec{k}) \in \Gamma_{N^-}, \quad \text{and} \quad (\vec{x},\vec{k}') \in \Gamma_{N^+}\,, \tag{4.56}$$

where $M(\vec{x},\vec{k})$ is the equilibrium probability distribution (not necessarily a Maxwellian) according to which the electrons diffusively reflect on the physical boundary. $\sigma^*(\vec{x},t)$ and $C^*(\vec{x},t)$ are the functions such that the zero flux condition is satisfied pointwise at insulating boundaries

$$\begin{aligned}
0 \;&=\; \eta(\vec{x})\cdot\int_{\Omega_{\vec{k}}}\vec{v}(\vec{k})f d\vec{k} = \int_{\vec{v}\cdot\eta>0}\eta(\vec{x})\cdot\vec{v}(\vec{k})f|_+ d\vec{k} \;+\; \int_{\vec{v}\cdot\eta<0}\eta(\vec{x})\cdot\vec{v}(\vec{k})f|_- d\vec{k} \\
&=\; \int_{\vec{v}\cdot\eta>0}\eta\cdot\vec{v}f|_+ d\vec{k} \\
&+\; \int_{\vec{v}\cdot\eta<0}\eta\cdot\vec{v}\left[p(\vec{x},\vec{k},t)f|_+(\vec{x},\vec{k}',t) + \Big(1-p(\vec{x},\vec{k},t)\Big)\, C^*(\vec{x},t)\sigma^*(\vec{x},t)M(\vec{x},\vec{k})\right] d\vec{k} \\
&=\; \int_{\vec{v}\cdot\eta>0}\eta\cdot\vec{v}f|_+ d\vec{k} \;+\; \int_{\vec{v}\cdot\eta<0}\eta\cdot\vec{v}\,p(\vec{x},\vec{k},t)f|_+(\vec{x},\vec{k}',t) d\vec{k} \\
&-\; \sigma^*(\vec{x},t)\, C^*(\vec{x},t)\int_{\vec{v}\cdot\eta<0}|\eta\cdot\vec{v}|\,\Big(1-p(\vec{x},\vec{k},t)\Big)\, M(\vec{x},\vec{k}) d\vec{k}\,.
\end{aligned}$$

Therefore we conclude for this reflection case that

$$\sigma^*\left\{f|_+\right\}(\vec{x},t) = \int_{\vec{v}\cdot\eta>0}|\eta\cdot\vec{v}|f|_+ d\vec{k} \;-\; \int_{\vec{v}\cdot\eta<0}|\eta\cdot\vec{v}|\,p(\vec{x},\vec{k},t)f|_+(\vec{x},\vec{k}',t) d\vec{k}\,, \tag{4.57}$$

$$C^*(\vec{x},t) = \left(\int_{\vec{v}\cdot\eta<0}|\eta\cdot\vec{v}|\,\Big(1-p(\vec{x},\vec{k},t)\Big)\, M(\vec{x},\vec{k}) d\vec{k}\right)^{-1}, \tag{4.58}$$

and then the full BC formula for the $p(\vec{x},\vec{k},t)$ reflection case is

$$f|_-(\vec{x},\vec{k},t) = p(\vec{x},\vec{k},t)f|_+(\vec{x},\vec{k}',t) \quad + \\ \Big(1-p(\vec{x},\vec{k},t)\Big)\, M(\vec{x},\vec{k}) \frac{\Big[\int_{\vec{v}\cdot\eta>0} |\eta\cdot\vec{v}| f|_+ d\vec{k} \;-\; \int_{\vec{v}\cdot\eta<0} |\eta\cdot\vec{v}|\, p(\vec{x},\vec{k},t) f|_+(\vec{x},\vec{k}',t) d\vec{k}\Big]}{\int_{\vec{v}\cdot\eta<0} |\eta\cdot\vec{v}| \Big(1-p(\vec{x},\vec{k},t)\Big)\, M(\vec{x},\vec{k}) d\vec{k}}\,.$$

Remark: $p(\vec{x},\vec{k},t)$ can be any iid random variable in $(\vec{x},\vec{k},t)$.

4.5.3.1 Numerical Implementation

The numerical implementation of the general mixed reflection with specularity parameter $p(\vec{k})$ is done in such a way that a numerical equivalent of the pointwise zero flux condition is achieved.

The general mixed reflection boundary condition in our DG numerical scheme is

$$\begin{aligned} \Phi_h|_- &= \Pi_h \left\{ F_M \left(\Phi_h|_+ \right) \right\} \qquad (4.59) \\ &= \Pi_h \left\{ p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t) + (1-p(\vec{w}))C'\sigma'_h \left\{ \Phi_h|_+ \right\}(\vec{x},t)\, e^{-w} s(w) \right\}. \end{aligned}$$

We will be using the notation

$$\vec{w} = (w,\mu,\varphi), \quad d\vec{w} = dw\, d\mu\, d\varphi\,, \quad \vec{w}' = (w,\mu,\pi-\varphi). \qquad (4.60)$$

The specific form of C' and σ' will be deduced from the numerical analogous of the mixed reflection boundary condition. We want to satisfy

numerically the zero flux condition

$$
\begin{aligned}
0 &= \eta(\vec{x}) \cdot \int_{\Omega_{\vec{w}}} \vec{v}(\vec{w})\, \Phi_h d\vec{w} \qquad (4.61)\\
&= \int_{\vec{v}\cdot\eta>0} \vec{v}(\vec{w}) \cdot \eta\, \Phi_h|_+ d\vec{w} + \int_{\vec{v}\cdot\eta<0} \vec{v}(\vec{w}) \cdot \eta\, \Phi_h|_- d\vec{w}\\
&= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, \Phi_h|_+ d\vec{w}\\
&+ \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, \Pi_h \left\{ p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t) + (1-p(\vec{w}))C'\sigma_h'(\vec{x},t)e^{-w}s(w) \right\} d\vec{w}\\
&= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\, \Phi_h|_+ d\vec{w} - \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\, \Pi_h \left\{ p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t) \right\} d\vec{w}\\
&+ \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, \Pi_h \left\{ (1-p(\vec{w}))C'\sigma_h'(\vec{x},t)e^{-w}s(w) \right\} d\vec{w}. \qquad (4.62)
\end{aligned}
$$

In the space V_h of piecewise continuous polynomials which are tensor products of polynomials of degree p in $\vec{x}$ and of degree q in $\vec{w}$, it holds that

$$
\begin{aligned}
&\Pi_h \left\{ f_1(\vec{x}) f_2(\vec{w}) \right\} = \Pi_h \left\{ f_1(\vec{x}) \right\} \Pi_h \left\{ f_2(\vec{w}) \right\}, \qquad (4.63)\\
&V_h = \{ v : v|_{\Omega_{ijkmn}} \in Q^{p,q}(\Omega_{ijkmn}) = P^p(X_{ij}) \otimes P^q(K_{kmn}) \}.
\end{aligned}
$$

Therefore, we have for our particular case that

$$
\Pi_h \left\{ (1-p(\vec{w}))C'\sigma_h'(\vec{x},t)e^{-w}s(w) \right\} = C'\sigma_h'(\vec{x},t) \left[\sum_{k,m,n} \chi_{kmn} \frac{\int_{K_{kmn}} (1-p(\vec{w}))e^{-w}s(w)d\vec{w}}{\int_{K_{kmn}} d\vec{w}} \right].
$$

Using this, our numerical pointwise zero flux condition is

$$
\begin{aligned}
0 &= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\,\Phi_h|_+ d\vec{w} - \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\,\Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\} d\vec{w} \\
&+ \int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\, C'\sigma_h'(\vec{x},t)\left[\sum_{k,m,n}\chi_{kmn}\frac{\int_{K_{kmn}}(1-p(\vec{w}))e^{-w}s(w)d\vec{w}}{\int_{K_{kmn}}d\vec{w}}\right] d\vec{w} \\
&= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\,\Phi_h|_+ d\vec{w} - \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\,\Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\} d\vec{w} \\
&+ C'\sigma_h'(\vec{x},t)\int_{\vec{v}\cdot\eta<0} \vec{v}\cdot\eta\left[\sum_{k,m,n}\chi_{kmn}\frac{\int_{K_{kmn}}(1-p(\vec{w}))e^{-w}s(w)d\vec{w}}{\int_{K_{kmn}}d\vec{w}}\right] d\vec{w} \\
&= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\,\Phi_h|_+ d\vec{w} - \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\,\Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\} d\vec{w} \\
&- C'\sigma_h'(\vec{x},t)\sum_{k,m,n}\chi_{kmn}\int_{\vec{v}\cdot\eta<0}|\vec{v}\cdot\eta|\,d\vec{w}\,\frac{\int_{K_{kmn}}(1-p(\vec{w}))e^{-w}s(w)d\vec{w}}{\int_{K_{kmn}}d\vec{w}} \\
&= \int_{\vec{v}\cdot\eta>0} \vec{v}\cdot\eta\,\Phi_h|_+ d\vec{w} - \int_{\vec{v}\cdot\eta<0} |\vec{v}\cdot\eta|\,\Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\} d\vec{w} \\
&- \sigma_h'(\vec{x},t)\,C'\sum_{k,m,n,\,\vec{v}\cdot\eta<0}\int_{K_{kmn}}|\vec{v}\cdot\eta|\,d\vec{w}\,\frac{\int_{K_{kmn}}(1-p(\vec{w}))e^{-w}s(w)d\vec{w}}{\int_{K_{kmn}}d\vec{w}}\,.
\end{aligned}
$$

We conclude then that we can achieve a numerical equivalent of the pointwise zero flux condition by defining

$$
\sigma_h'\left\{\Phi_h|_+\right\}(\vec{x},t) = \int_{\vec{v}\cdot\eta>0}\vec{v}\cdot\eta\,\Phi_h|_+ d\vec{w} - \int_{\vec{v}\cdot\eta<0}|\vec{v}\cdot\eta|\,\Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\} d\vec{w}, \tag{4.64}
$$

$$
\left(C'\{\eta\}\right)^{-1} = \sum_{k,m,n,\,\vec{v}\cdot\eta<0}\int_{K_{kmn}}|\vec{v}\cdot\eta|\,d\vec{w}\,\frac{\int_{K_{kmn}}(1-p(\vec{w}))e^{-w}s(w)d\vec{w}}{\Delta w_k\Delta\mu_m\Delta\varphi_n}. \tag{4.65}
$$

Therefore, the inflow BC in our DG numerical method is given by the

expression

$$\begin{aligned}\Phi_h|_- &= \Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\}\\ &+ \Pi_h\left\{(1-p(\vec{w}))C'\left(\int_{\vec{v}\cdot\eta>0}\vec{v}\cdot\eta\,\Phi_h|_+ d\vec{w}\right.\right.\\ &- \left.\left.\int_{\vec{v}\cdot\eta<0}|\vec{v}\cdot\eta|\,\Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\}d\vec{w}\right)e^{-w}s(w)\right\}.\end{aligned}$$

The particular form of the coefficients defining the piecewise polynomial approximation $\Phi_h|_-$ for the general mixed reflection BC is presented below for the boundary $y = L_y$, since the calculations for the case of the boundary $y = 0$ are analogous.

For the boundary $y_{N_y+1/2} = L_y\,, \quad \eta\cdot\vec{v} \propto +\hat{y}\cdot\vec{g} = g_2 \propto \cos\varphi\,$, which defines the sign of g_2. Outflow cells have the index $j = N_y\,$. They are cells inside the domain adjacent to the boundary. Inflow cells have the index $j = N_y + 1$. They are ghost cells adjacent to the boundary. We have in our case that

$$\begin{aligned}\sigma'_h &= \int_{\cos\varphi>0} g_2\,\Phi_h|_+ d\vec{w} - \int_{\cos\varphi<0}|g_2|\,\Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\}d\vec{w}\\ &= \sum_{k,m,n}^{n\le N_\varphi/2}\int_{K_{kmn}} g_2\,\Phi_h|_+ d\vec{w} - \sum_{k,m,n}^{n>N_\varphi/2}\int_{K_{kmn}}|g_2|\,\Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\}d\vec{w}\,.\end{aligned}$$

If $I = (i, N_y + 1, k, m, n)$ (inflow), $I' = (i, N_y, k, m, n')$, $n' = N'_\varphi - n + 1$ (outflow), the projection integrand is given by

$$\Pi_h\left\{p(\vec{w})\Phi_h|_+(\vec{x},\vec{w}',t)\right\} = \sum_I^{n>N_\varphi/2}\chi_I\,\frac{\int_{kmn}p(\vec{w})d\vec{w}}{\int_{kmn}d\vec{w}}\left[T_{I'} + X_{I'}\frac{(x-x_i)}{\Delta x_i/2} + Y_{I'}(+1)\right].$$

The coefficients of σ'_h are given below. We have now that $I = (i, N_y, k, m, n)$, $I' = (i, N_y, k, m, n')$, $\quad n' = N'_\varphi - n + 1$, so from the previous two formulas then

$$
\begin{aligned}
\sigma'^{0}_{i,N_y} &= \sum_{k,m,n}^{n\le N_p/2} T_I(t) \int_k \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int_m \sqrt{1-\mu^2} d\mu \int_n \cos\varphi d\varphi \qquad (4.66)\\
&- \sum_{k,m,n}^{n>N_p/2} T_{I'}(t) \int_k \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int_m \sqrt{1-\mu^2} d\mu \int_n |\cos\varphi| d\varphi \, \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}},\\
\sigma'^{x}_{i,N_y} &= \sum_{k,m,n}^{n\le N_p/2} X_I(t) \int_k \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int_m \sqrt{1-\mu^2} d\mu \int_n \cos\varphi d\varphi\\
&- \sum_{k,m,n}^{n>N_p/2} X_{I'}(t) \int_k \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int_m \sqrt{1-\mu^2} d\mu \int_n |\cos\varphi| d\varphi \, \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}},\\
\sigma'^{y}_{i,N_y} &= \sum_{k,m,n}^{n\le N_p/2} Y_I(t) \int_k \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int_m \sqrt{1-\mu^2} d\mu \int_n \cos\varphi d\varphi\\
&- \sum_{k,m,n}^{n>N_p/2} Y_{I'}(t) \int_k \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} dw \int_m \sqrt{1-\mu^2} d\mu \int_n |\cos\varphi| d\varphi \, \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}}.
\end{aligned}
$$

Since on one hand we have

$$
\begin{aligned}
\Phi_h|^-_{L_y} &= \Pi_h \left\{ p(\vec{w}) \Phi_h|_+ (\vec{x}, \vec{w}', t) \right\} + \Pi_h \left\{ (1 - p(\vec{w})) C' \sigma'_h \left\{ \Phi_h|_+ \right\} (\vec{x}, t) \, e^{-w} s(w) \right\}\\
&= \sum_{i,k,m,n}^{n>N_\varphi/2} \chi_{i,N_y+1,k,m,n} \, \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} \left[T_{i,N_y,k,m,n'} + X_{i,N_y,k,m,n'} \frac{(x - x_i)}{\Delta x_i/2} + Y_{i,N_y,k,m,n'} \right]\\
&+ \sum_{i,k,m,n}^{n>N_\varphi/2} \chi_{i,N_y+1,k,m,n} \, \frac{\int_{kmn} (1 - p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{kmn} d\vec{w}} \times\\
&\times \; C' \left[\sigma'^{0}_{i,N_y} + \sigma'^{x}_{i,N_y} \frac{(x - x_i)}{\Delta x_i/2} + \sigma'^{y}_{i,N_y} (+1) \right],
\end{aligned}
$$

and on the other hand

$$\Phi_h|^-_{y_{N_y+1/2}} = \sum_{i,k,m,n}^{n>N_\varphi/2} \chi_{i,N_y+1,k,m,n} \left[T_{i,N_y+1,k,m,n} + X_{i,N_y+1,k,m,n} \frac{(x-x_i)}{\Delta x_i/2} + Y_{i,N_y+1,k,m,n}(-1) \right],$$

we conclude that the coefficients for $\Phi_h|_-$ are

$$\begin{aligned}
T_{i,N_y+1,k,m,n} &= T_{I'} \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} + C' \sigma'^0_{i,N_y} \frac{\int_{kmn} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{kmn} d\vec{w}}, \\
X_{i,N_y+1,k,m,n} &= X_{I'} \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} + C' \sigma'^x_{i,N_y} \frac{\int_{kmn} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{kmn} d\vec{w}}, \\
Y_{i,N_y+1,k,m,n} &= -\left(Y_{I'} \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} + C' \sigma'^y_{i,N_y} \frac{\int_{kmn} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{kmn} d\vec{w}} \right), \\
I' &= (i, N_y, k, m, n'), \quad I = (i, N_y, k, m, n)\,. \qquad (4.67)
\end{aligned}$$

4.6 Numerical Results

4.6.1 2D bulk silicon

We present results of numerical simulations for the case of n 2D bulk silicon diode with an applied bias between the boundaries $x = 0,\ L_x$, and reflection BC at the boundaries $y = 0,\ L_y$ (Figs. 4.2). The required dimensionality in momentum space is a 3D $\vec{k}(w, \mu, \varphi)$. The specifics of our simulations are:

Initial Condition: $\Phi(w)|_{t=0} = \Pi_h \{N e^{-w} s(w)\}$. Final Time: 1.0ps

Boundary Conditions (BC):

$\vec{k}$-space: Cut-off - at $w = w_{max}$, Φ is machine zero.

Only needed BC in (w, μ, φ): transport normal to the boundary analitically zero at 'singular points' boundaries:

At $w = 0,\ g_3 = 0$. At $\mu = \pm 1,\ g_4 = 0$. At $\varphi = 0, \pi,\ g_5 = 0$.

$\vec{x}$-space: Charge Neutrality at boundaries $x = 0$, $x = 0.15\mu m$.

Bias - Potential: $V|_{x=0} = 0.5235$ V, $V|_{x=0.15\mu m} = 1.5235$ V.

Neumann BC for Potential at $y = 0$, $L_y = 12nm$: $\partial_y V|_{y=0,\,L_y} = 0$.

Reflection BC at $y = 0, y = 12nm$: Specular, Diffusive, Mixed Reflection with constant specularity $p = 0.5$, and Mixed Reflection using a momentum dependent specularity $p(\vec{k}) = \exp(-4\eta^2|k|^2 \sin^2\varphi)$, the nondimensional roughness rms height coefficient being $\eta = 0.5$.

We observe an influence of the Diffusive and Mixed Reflection in macroscopic observables. It is particularly noticeable in the kinetic moments. For example, the charge density slightly increases with diffusivity close to the reflecting boundaries, and, due to mass conservation, alters the density profile over the domain. Momentum & mean velocity increase with diffusive reflection over the domain, while the energy is decreased by diffusive reflection over the domain. There is a negligible difference in the electric field x component below its orders of magnitude for the different reflection cases.

4.6.2 2D double gated MOSFET

We present as well the results of numerical simulations for the case of a 2D double gated MOSFET device (Figs. 4.3). On one hand, the BC for the Poisson Eq. for this device would be the Dirichlet BC $\Psi = 0.5235$ Volts at the source $x = 0$, $\Psi = 1.5235$ Volts at the drain $x = L_x$, and $\Psi = 1.06$ Volts at the gates. On the other hand, Homogeneous Neumann BC $\partial_{\hat{n}}\Psi = 0$ are imposed at the rest of the boundaries. Specular reflection is applied at the boundary

$y = 0$ because the solution is symmetric with respect to $y = 0$ for our 2D double gate MOSFET (Fig. 4.1). On the other hand, at the boundary $y = L_y$ we apply specular, diffusive, and mixed reflection BC, both with constant $p = 0.5$, and with a momentum dependent $p(\vec{k}) = \exp(-4\eta^2|k|^2 \sin^2 \varphi)$ with roughness coefficient $\eta = 0.5$. We use again the initial condition: $\Phi(w)|_{t=0} = \Pi_h \{N_D(x, y)e^{-w}s(w)\}$, running the simulations up to the physical time of 1.0ps. We use again as well a cut-off BC in the boundary of the momentum domain, so Φ is machine zero at $w = w_{max}$, and we apply charge neutrality BC at $x = 0$, $x = 0.15\mu m$.

We observe a quantitative difference in the kinetic moments and other observables between the different cases of reflective BC, with the physical quantities being of the same order of magnitude. The electron density increases close to the gates with diffusive reflection, and close to the center of the device, given by the boundary $y = 0$, the density profile is greater for specular reflection. The energy moment clearly decreases with diffusive reflection over the physical domain. The momentum x-component for specular reflection is less than for the other reflective cases. There is a difference in the profile of the electric field x-component between the specular reflection and the other cases that include diffusivity, increasing it with diffusive reflection close to the drain. The electric field y-component increases with diffusive reflection close to the boundary $y = 0$ representing the center of the device. The electric potential is greater for the cases including diffusive reflection than for the perfectly specular case.

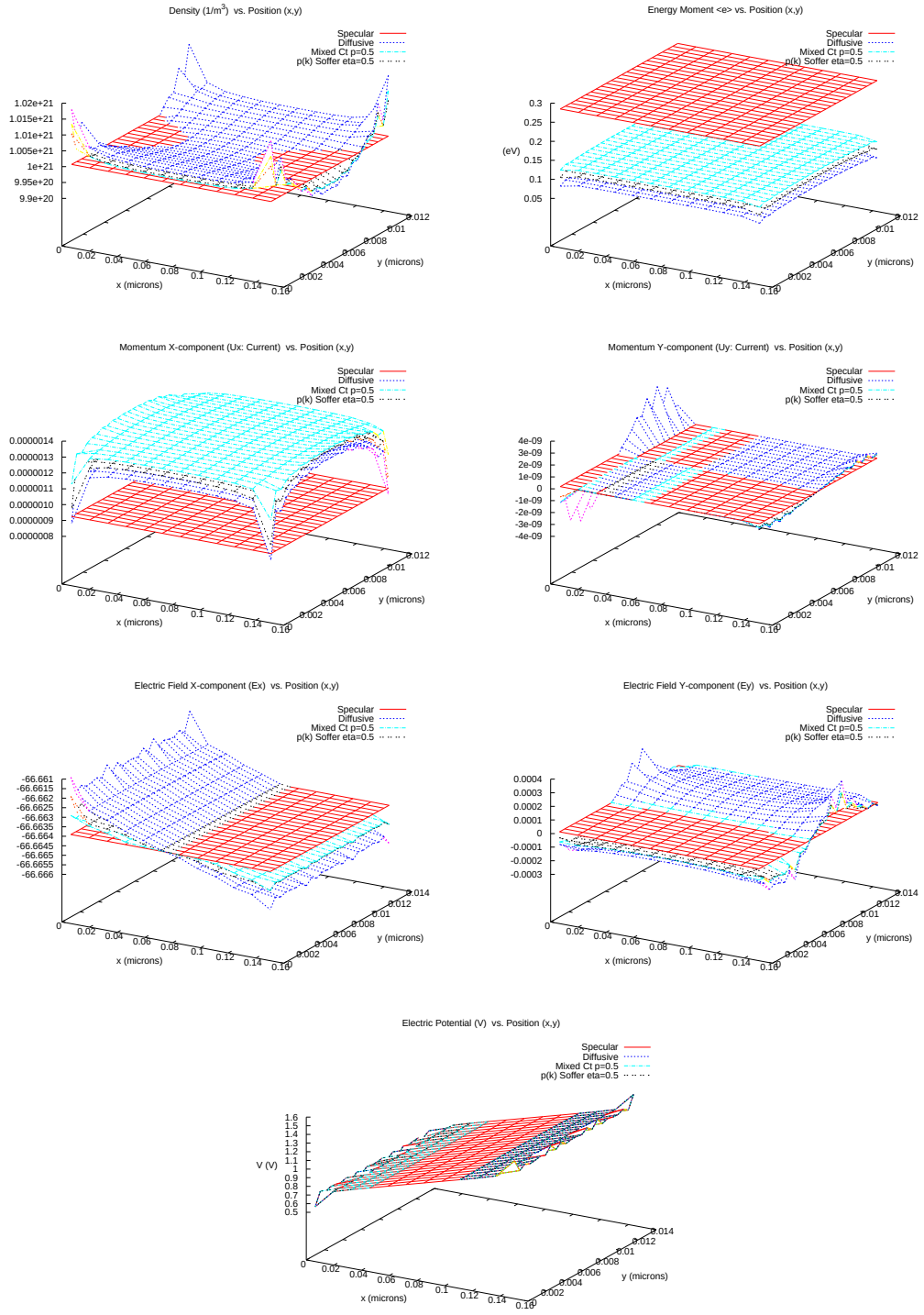


Figure 4.2: Density ρ (m^{-3}), 132 Mean energy $e(eV)$, Momentum $U_x, U_y\,(10^{28}\frac{cm^{-2}}{s})$, Electric Field Components E_x and E_y, and Potential $V(Volts)$ vs Position (x, y) in (μm) plot for Specular, Diffusive, Mixed $p = 0.5$ & Mixed $p(\vec{k}) = \exp(-4\eta^2|k|^2\sin^2\varphi)$, $\eta = 0.5$ Reflection for 2D bulk silicon.

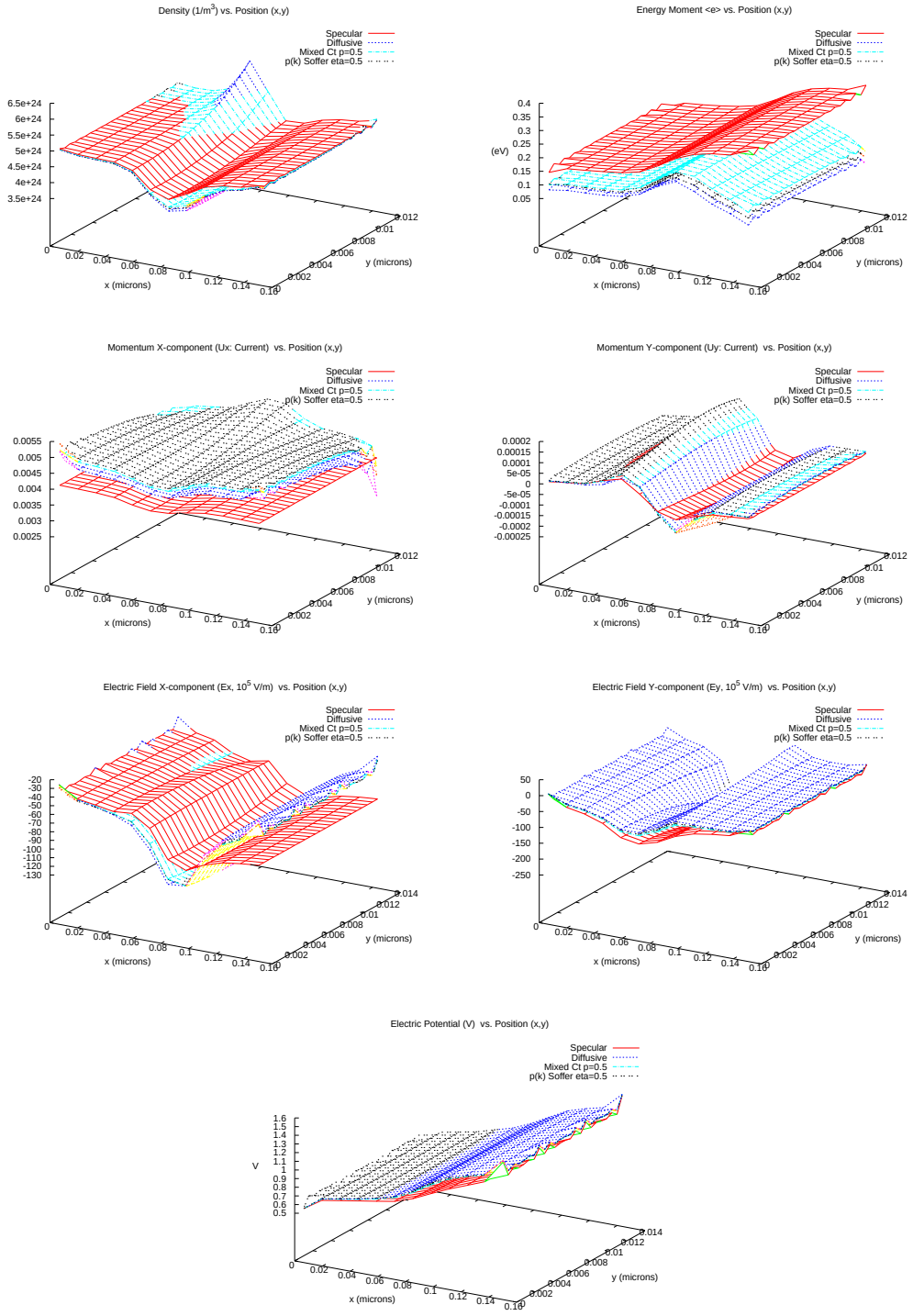


Figure 4.3: Density ρ (m^{-3}), 133 Mean energy $e(eV)$, Momentum $U_x, U_y\,(10^{28}\frac{cm^{-2}}{s})$, Electric Field Components E_x and E_y, and Potential $V(Volts)$ vs Position (x, y) in (μm) plot for Specular, Diffusive, Mixed $p = 0.5$ & Mixed $p(\vec{k}) = \exp(-4\eta^2|k|^2\sin^2\varphi)$, $\eta = 0.5$ Reflection for a 2D double gated MOSFET.

Chapter 5

Positivity preserving DG schemes for a Boltzmann - Poisson model of electrons in semiconductors in curvilinear momentum coordinates

5.1 Introduction: Boltzmann Equation with Momentum in Curvilinear Coordinates

We can write the Boltzmann - Poisson model for electron transport in semiconductors for a more general set of collision operators as the system in the $(\vec{x}, \vec{p})$ position-momentum phase space for electrons

$$\partial_t f + \partial_{\vec{x}} f \cdot \partial_{\vec{p}} \varepsilon + \partial_{\vec{p}} f \cdot q \partial_x V = Q(f) = \int_{\Omega_{\vec{p}}} S(\vec{p}' \to \vec{p}) f' d\vec{p}' - f \int_{\Omega_{\vec{p}}} S(\vec{p} \to \vec{p}') d\vec{p}' \,, \tag{5.1}$$

$$-\partial_{\vec{x}} \cdot (\epsilon \partial_{\vec{x}} V)(\vec{x}, t) = q \left[N(\vec{x}) - \int_{\Omega_{\vec{p}}} f(\vec{x}, \vec{p}, t) d\vec{p} \right], \quad \vec{E}(\vec{x}, t) = -\partial_{\vec{x}} V(\vec{x}, t) \,. \tag{5.2}$$

The momentum variable is $\vec{p} = \hbar \vec{k}$, $\vec{k}$ is the crystal momentum wave vector, $\varepsilon(\vec{p})$ is the conduction energy band for electrons in the semiconductor, $f(\vec{x}, \vec{p}, t)$ is the probability density function (pdf) in the phase space for electrons in the conduction band, $\vec{v}(\vec{p}) = \partial_{\vec{p}} \varepsilon(\vec{p})$ is the quantum mechanical electron group velocity, q is the positive electric charge, $V(\vec{x}, t)$ is the electric potential (we assume that the only force over the electrons is the self-consistent electric

field, and that it is given by the negative gradient of the electric potential), ϵ is the permittivity for the material, $N(\vec{x})$ is the fixed doping background in the semiconductor material, and $S(\vec{p}' \to \vec{p})$ is the scattering kernel that defines the gain and loss operators, whose difference give the collision integral $Q(f)$.

For many collision mechanisms in semiconductors, the scattering kernel $S(\vec{p}' \to \vec{p})$ depends on the difference $\varepsilon(\vec{p}) - \varepsilon(\vec{p}')$, as in collision operators of the form $\delta(\varepsilon(\vec{p}) - \varepsilon(\vec{p}') + l\hbar w_p)$ for electron - phonon collisions. This form is related to energy conservation equations such as Planck's law, in which the jump in energy from one state to another is balanced with the energy of a phonon. The mathematical consequence of this is that we can obtain much simpler expressions for the integration of the collision operator if we express the momentum in curvilinear coordinates that involve the energy $\varepsilon(\vec{p})$ as one of the variables [21], [24], [26], [34] . The other two momentum coordinates could be either an orthogonal system in the level set of energies, orthogonal to the energy gradient itself, or angular coordinates which are known to be orthogonal to the energy in the limit of low energies close to a local conduction band minimum, such as (μ, φ).

This gives both physical and mathematical motivations to pose the Boltzmann Equation for semiconductors in curvilinear coordinates for the momentum $\vec{k}(k_1, k_2, k_3)$, to later on choose the particular case of curvilinear coordinates such as $(\varepsilon, \mu, \varphi)$. We will assume in the rest of this chapter that our system of curvilinear coordinates for the momentum is orthogonal, as in the case $(\varepsilon, \mu, \varphi)$ in which $\varepsilon(|\vec{p}|)$ is a monotone increasing function, so this set of

coordinates is equivalent to the representation in spherical coordinates for the momentum.

The Boltzmann Equation for semiconductors (or more general forms of linear collisional plasma models) written in orthogonal curvilinear coordinates $\vec{p}(p_1, p_2, p_3)$ for the momentum $\vec{p} = (p_x, p_y, p_z)$ is

$$\partial_t(Jf)+\partial_{\vec{x}}\cdot(Jf\vec{v})+q\left[\partial_{p_1}\left(\frac{Jf\partial_{\vec{x}}V\cdot\hat{e}_{p_1}}{h_1}\right)+\partial_{p_2}\left(\frac{Jf\partial_{\vec{x}}V\cdot\hat{e}_{p_2}}{h_2}\right)+\partial_{p_3}\left(\frac{Jf\partial_{\vec{x}}V\cdot\hat{e}_{p_3}}{h_3}\right)\right]$$
$$= C(f) = JQ(f) = J\int_{\Omega_{\vec{p}}} S(\vec{p}'\to\vec{p})J'f'\,dp_1'\,dp_2'\,dp_3' - Jf\int_{\Omega_{\vec{p}}} S(\vec{p}\to\vec{p}')J'\,dp_1'\,dp_2'\,dp_3',$$

with $h_j = \left|\frac{\partial\vec{p}}{\partial p_j}\right|$, $j = 1, 2, 3$, $h_1h_2h_3 = J = \frac{\partial\vec{p}}{\partial(p_1,p_2,p_3)}$ the jacobian of the transformation, $J' = \frac{\partial\vec{p}'}{\partial(p_1',p_2',p_3')}$, and $\hat{e}_j$ the unitary vectors associated to each curvilinear coordinate p_j at the point (p_1, p_2, p_3).

We notice that we have expressed the Boltzmann Eq. in divergence form with respect to the momentum curvilinear coordinates. We can write it even more compactly in the form

$$\partial_t(Jf) + \partial_{\vec{x}}\cdot(Jf\vec{v}(\vec{p})) + \sum_{j=1}^{3}\partial_{p_j}\left(Jf\frac{q\partial_{\vec{x}}V(\vec{x},t)\cdot\hat{e}_{p_j}}{h_j}\right) = C(f). \qquad (5.3)$$

If $J \geq 0$, we can interpret $Jf(\vec{x}, p_1, p_2, p_3, t)$ as a probability density function in the phase space $(\vec{x}, p_1, p_2, p_3)$

This Boltzmann Eq. is a more general form for orthogonal curvilinear coordinates, from which our previous spherical coordinate systems from Chapter 3 and Chapter 4 can be derived. For the one in Chapter 3, the orthogonal curvilinear system is (r, μ, φ), with $r \propto k^2$. The one in Chapter 4 is (w, μ, φ), with $w \propto \varepsilon$. assuming a Kane band energy ε.

5.2 1Dx-2Dp Diode Symmetric Problem

As we have mentioned, for the case of a 1D silicon diode, the main collision mechanisms are electron-phonon scatterings

$$S(\vec{p}' \to \vec{p}) = \sum_{j=-1}^{+1} c_j \delta(\varepsilon(\vec{p}') - \varepsilon(\vec{p}) + j\hbar\omega), \quad c_1 = (n_{ph}+1)K,\ c_{-1} = n_{ph}K,$$

with ω the phonon frequency, assumed constant, and $n_{ph} = n_{ph}(\omega)$ the phonon density. K, c_0 are constants.

If we assume that the energy band just depends on the momentum norm, $\varepsilon(p)$, $\quad p = |\vec{p}|$, and that the initial condition for the pdf has azimuthal symmetry, $f|_{t=0} = f_0(x,p,\mu)$, $\partial_\varphi f = 0$, $\vec{p} = p(\mu, \sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi)$, then the dimensionality of the problem is reduced to 3D+time, 1D in x, 2D in (p,μ), and the BP system for $f(x,p,\mu,t)$, $V(x,t)$ is written in spherical coordinates $\vec{p}(p,\mu,\varphi)$ for the momentum as

$$\partial_t f + \partial_x(f\partial_p\varepsilon\mu) + \left[\frac{\partial_p(p^2 f\mu)}{p^2} + \frac{\partial_\mu(f(1-\mu^2))}{p}\right] q\partial_x V(x,t) = Q(f)\,, \quad (5.4)$$

$$-\partial_x^2 V = \frac{q}{\epsilon}\left[N(x) - 2\pi\int_{-1}^{+1}\int_0^{p_{max}} f p^2 dp d\mu,\right], \quad V(0)=0,\ V(L)=V_0.$$

We have assumed that the permittivity ϵ is constant. The Poisson BVP above can be easily solved and an analytic integral solution is easily obtained for $V(x,t)$ and $E(x,t) = -\partial_x V(x,t)$, which later can be projected in the adequate space for the numerical method. For this problem we only need to concern about the Boltzmann Equation, since given the electron density we know the solution for the potential and electric field.

The collision operator, in this case, has the form

$$Q(f) = 2\pi \left[\sum_{j=-1}^{+1} c_j \int_{-1}^{+1} d\mu' \; f(x, p(\varepsilon'), \mu') \, p^2(\varepsilon') \frac{dp'}{d\varepsilon'}\bigg|_{\varepsilon'=\varepsilon(p)+j\hbar\omega} \chi(\varepsilon(p) + j\hbar\omega) \right.$$
$$\left. - \, f(x, p, \mu, t) \sum_{j=-1}^{+1} c_j \, 2 \, p^2(\varepsilon') \frac{dp'}{d\varepsilon'}\bigg|_{\varepsilon'=\varepsilon(p)-j\hbar\omega} \chi(\varepsilon(p) - j\hbar\omega) \right] ,$$

where $\chi(\varepsilon)$ is 1 if $\varepsilon \in [0, \varepsilon_{max}]$ and 0 if $\varepsilon \notin [0, \varepsilon_{max}]$, with $\varepsilon_{max} = \varepsilon(p_{max})$. The domain of the BP problem is $x \in [0, L]$, $p \in [0, p_{max}]$, $\mu \in [-1, +1]$, $t > 0$. Moreover, since $\varepsilon(p)$, then $\partial_{\vec{p}}\varepsilon = \frac{d\varepsilon}{dp}\hat{p}$. We assume that $\frac{d\varepsilon}{dp} > 0$ is well behaved enough such that $p(\varepsilon)$ is a monotonic function for which $\frac{dp}{d\varepsilon} = (\frac{d\varepsilon}{dp})^{-1}$ exists.

The collision frequency is

$$\nu(\varepsilon(p)) = \sum_{j=-1}^{+1} c_j \, 4\pi \, \chi(\varepsilon(p) - j\hbar\omega) \; p^2(\varepsilon') \frac{dp'}{d\varepsilon'}\bigg|_{\varepsilon'=\varepsilon(p)-j\hbar\omega} = \sum_{j=-1}^{+1} c_j n(\varepsilon(p) - j\hbar\omega) \, , \tag{5.5}$$

where

$$n(\varepsilon(p) - j\hbar\omega) = \int_{\Omega_{\vec{p}}} \delta(\varepsilon(\vec{p}') - \varepsilon(\vec{p}) + j\hbar\omega) \, d\vec{p}' \tag{5.6}$$

is the density of states with energy $\varepsilon(p) - j\hbar\omega$.

5.3 DG for Boltzmann-Poisson 1Dx-2Dp Problem

5.3.1 Weak Form of the Transformed Boltzmann Eq.

Since for $f(x, p, \mu)$, $g(x, p, \mu)$ we have that

$$\int_{\Omega_x} \int_{\Omega_{\vec{p}}} f g \, d\vec{p} dx = 2\pi \int_{\Omega_x} \int_{\Omega_{(p,\mu)}} f g \, p^2 \, dp d\mu dx \, , \tag{5.7}$$

we define the inner product of two functions f and g in the (x, p, μ) space as

$$(f, g)_{X \times K} = \int_X \int_K f g \, p^2 \, dp d\mu dx \, , \tag{5.8}$$

where $X \subset [0, L]$ and $K \subset [0, p_{max}] \times [-1, +1]$.

The Boltzmann Equation for our problem is written in weak form as

$$(\partial_t f, g)_\Omega + (\partial_x(f \partial_p \varepsilon\mu),\, g)_\Omega + \left(\left[\frac{\partial_p(p^2 f\mu)}{p^2} + \frac{\partial_\mu(f(1-\mu^2))}{p} \right] q\partial_x V(x,t), g \right)_\Omega = (Q(f), g)_\Omega \,,$$

where $\Omega = X \times K$. More specifically, we have that ($\partial_t g = 0$)

$$\begin{aligned} & \partial_t \int_\Omega f\, g\, p^2\, dpd\mu dx \, + \int_\Omega \partial_x(f \partial_p \varepsilon\mu)\, g\, p^2 dpd\mu dx \\ + & \int_\Omega \partial_p(p^2 f\mu) q\partial_x V(x,t) g\, dpd\mu dx + \int_\Omega \partial_\mu(f(1-\mu^2)) q\partial_x V(x,t) g\, p\, dpd\mu dx \\ = & \int_\Omega Q(f)\, g\, p^2 dpd\mu dx \,. \end{aligned}$$

5.3.2 DG-FEM Formulation for the Transformed Boltzmann Eq. in the (x, p, μ) domain

We will use the following mesh in the domain

$$\Omega_{ikm} = X_i \times K_{k,m} = [x_{i^-}, x_{i^+}] \times [p_{k^-}, p_{k^+}] \times [\mu_{m^-}, \mu_{m^+}] \,, \tag{5.9}$$

where

$$x_{i^\pm} = x_{i\pm 1/2}, \quad p_{k^\pm} = p_{k\pm 1/2}, \quad \mu_{m^\pm} = \mu_{m\pm 1/2} \,. \tag{5.10}$$

We define the notation for the internal product in our problem, using the above mentioned mesh, as

$$\int_{ikm} f g\, p^2 dpd\mu\, dx = (f, g)_{\Omega_{ikm}} \,. \tag{5.11}$$

The semi-discrete DG Formulation for our Transformed Boltzmann Equation in curvilinear coordinates is to find $f_h \in V_h^k$ such that $\forall\, g_h \in V_h^k$

and $\forall\, \Omega_{ikm}$,

$$
\begin{aligned}
&\partial_t \int_{ikm} f_h\, g_h\, p^2 dp d\mu dx \\
-\int_{ikm} \partial_p \varepsilon(p)\, f_h\, \mu\, \partial_x g_h\, p^2 dp d\mu dx \quad &\pm \quad \int_{km} \partial_p \varepsilon\, \widehat{f_h \mu}|_{x_{i\pm}}\, g_h|^{\mp}_{x_{i\pm}}\, p^2 dp d\mu \\
-\int_{ikm} p^2 (-qE)(x,t) f_h \mu\, \partial_p g_h\, d\mu dx \quad &\pm \quad \int_{im} p^2_{k\pm}\, (-q\widehat{E f_h \mu})|_{p_{k\pm}} g_h|^{\mp}_{p_{k\pm}}\, d\mu dx \\
-\int_{ikm} (1-\mu^2) f_h (-qE)(x,t)\, \partial_\mu g_h\, p\, dp d\mu dx \quad &\pm \quad \int_{ik} (1-\mu^2_{m\pm})(-q\widehat{E f_h})|_{\mu_{m\pm}}\, g_h|^{\mp}_{\mu_{m\pm}}\, p\, dp dx \\
&= \quad \int_{ikm} Q(f_h) g_h\, p^2 dp d\mu dx\,.
\end{aligned}
$$

The Numerical Flux used is the Upwind Rule. Therefore we have that

$$
\begin{aligned}
\widehat{f_h \mu}|_{x_{i\pm}} &= \left(\frac{\mu + |\mu|}{2}\right) f_h|^-_{x_{i\pm}} + \left(\frac{\mu - |\mu|}{2}\right) f_h|^+_{x_{i\pm}}\,, \\
-\widehat{qE\mu f_h}|_{p_{k\pm}} &= \left(\frac{-qE\mu + |qE\mu|}{2}\right) f_h|^-_{p_{k\pm}} + \left(\frac{-qE\mu - |qE\mu|}{2}\right) f_h|^+_{p_{k\pm}}\,, \\
-\widehat{qE f_h}|_{\mu_{m\pm}} &= \left(\frac{-qE + |qE|}{2}\right) f_h|^-_{\mu_{m\pm}} + \left(\frac{-qE - |qE|}{2}\right) f_h|^+_{\mu_{m\pm}}\,.
\end{aligned}
$$

Using the notation in the paper of Eindeve, Hauck, Xing, Mezzacappa [65], the semi-discrete DG formulation is written as follows. Find $f_h \in V_h^k$ such that $\forall\, g_h \in V_h^k$ and $\forall\, \Omega_{ikm}$

$$
\begin{aligned}
&\partial_t \int_{\Omega_{ikm}} f_h\, g_h\, p^2 dp d\mu dx \\
-\int_{\Omega_{ikm}} H^{(x)}\, f_h\, \partial_x g_h\, p^2 dp d\mu dx \quad &\pm \quad \int_{\tilde{\Omega}^{(x)}_{km}} \widehat{H^{(x)} f_h}|_{x_{i\pm}}\, g_h|^{\mp}_{x_{i\pm}}\, p^2 dp d\mu \\
-\int_{\Omega_{ikm}} p^2\, H^{(p)} f_h\, \partial_p g_h\, d\mu dx \quad &\pm \quad p^2_{k\pm} \int_{\tilde{\Omega}^{(p)}_{im}} \widehat{H^{(p)} f_h}|_{p_{k\pm}}\, g_h|^{\mp}_{p_{k\pm}}\, d\mu dx \\
-\int_{\Omega_{ikm}} (1-\mu^2) H^{(\mu)} f_h\, \partial_\mu g_h\, p\, dp d\mu dx \quad &\pm \quad (1-\mu^2_{m\pm}) \int_{\tilde{\Omega}^{(\mu)}_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m\pm}}\, g_h|^{\mp}_{\mu_{m\pm}}\, p\, dp dx \\
&= \quad \int_{\Omega_{ikm}} Q(f_h) g_h\, p^2 dp d\mu dx\,,
\end{aligned}
$$

where we have defined the terms ($\partial_p \varepsilon(p) > 0$)

$$
\begin{aligned}
H^{(x)}(p,\mu) &= \mu\,\partial_p\varepsilon(p)\,, \quad \widehat{H^{(x)}f}|_{x_{i\pm}} = \partial_p\varepsilon\widehat{f_h\mu}|_{x_{i\pm}}\,,\\
H^{(p)}(t,x,\mu) &= -qE(x,t)\mu\,, \quad \widehat{H^{(p)}f}|_{p_{k\pm}} = -q\widehat{Ef_h\mu}|_{p_{k\pm}}\,,\\
H^{(\mu)}(x,t) &= -qE(x,t)\,, \quad \widehat{H^{(\mu)}f}|_{\mu_{m\pm}} = -q\widehat{Ef_h}|_{\mu_{m\pm}}\,,
\end{aligned}
$$

$$
\begin{aligned}
\tilde{\Omega}^{(x)}_{km} &= [r_{k-}, r_{k+}] \times [\mu_{m-}, \mu_{m+}] = \partial_x \Omega_{km}\,,\\
\tilde{\Omega}^{(p)}_{im} &= [x_{i-}, x_{i+}] \times [\mu_{m-}, \mu_{m+}] = \partial_p \Omega_{im}\,,\\
\tilde{\Omega}^{(\mu)}_{ik} &= [x_{i-}, x_{i+}] \times [r_{k-}, r_{k+}] = \partial_\mu \Omega_{ik}\,.
\end{aligned}
$$

The weak form of the collisional operator in the DG scheme is, specifically,

$$
\begin{aligned}
&\int_{\Omega_{ikm}} Q(f_h)\, g_h\, p^2\, dpd\mu dx \;=\; \int_{\Omega_{ikm}} \left[G(f_h) - \nu(\varepsilon(p)) f_h\right]\, g_h\, p^2\, dpd\mu dx \;= \qquad (5.12)\\
&2\pi \int_{\Omega_{ikm}} \left(\sum_{j=-1}^{+1} c_j\, \chi(\varepsilon(p) + j\hbar\omega) \int_{-1}^{+1} d\mu' \left[f_h(x, p(\varepsilon'), \mu')\, p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \right] \Big|_{\varepsilon(p)+j\hbar\omega} \right) g_h\, p^2\, dpd\mu dx\\
&-4\pi \int_{\Omega_{ikm}} f_h(x,p,\mu,t) \left(\sum_{j=-1}^{+1} c_j\, \chi(\varepsilon(p) - j\hbar\omega) \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \right] \Big|_{\varepsilon'=\varepsilon(p)-j\hbar\omega} \right) g_h\, p^2\, dpd\mu dx\,.
\end{aligned}
$$

The cell average of f_h in Ω_{ikm} is

$$
\bar{f}_{ikm} = \frac{\int_{\Omega_{ikm}} f_h\, p^2\, dpd\mu dx}{\int_{\Omega_{ikm}} p^2\, dpd\mu dx} = \frac{\int_{\Omega_{ikm}} f_h\, dV}{V_{ikm}}, \qquad (5.13)
$$

where for our spherical curvilinear coordinates we have

$$
V_{ikm} = \int_{\Omega_{ikm}} dV\,,\; dV = \tau \prod_{d=1}^{3} z_d, \quad (z_1, z_2, z_3) = \mathbf{z} = (x, p, \mu), \quad \tau = \sqrt{\gamma\lambda},\; \gamma = 1,\; \lambda = p^2\,. \qquad (5.14)
$$

The time evolution of the cell average in the DG scheme is given by

$$
\begin{aligned}
&\partial_t \bar{f}_{ikm} = \\
- \;& \frac{1}{V_{ikm}} \left[\int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i+}} \, p^2 dp d\mu - \int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i-}} \, p^2 dp d\mu \right. \\
+ \;& p_{k+}^2 \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k+}} \, d\mu dx - p_{k-}^2 \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k-}} \, d\mu dx \\
+ \;& \left. (1-\mu_{m+}^2) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m+}} \, p \, dp dx - (1-\mu_{m-}^2) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m-}} \, p \, dp dx \right] \\
+ \;& \left[2\pi \int_{\Omega_{ikm}} \left(\sum_{j=-1}^{+1} c_j \int_{-1}^{+1} d\mu' \left[f_h(x, p(\varepsilon'), \mu') \, p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon(p)+j\hbar\omega} \right) p^2 \, dp d\mu dx \right. \\
& \left. -4\pi \int_{\Omega_{ikm}} f_h(x,p,\mu,t) \left(\sum_{j=-1}^{+1} c_j \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon'=\varepsilon(p)-j\hbar\omega} \right) p^2 \, dp d\mu dx \right] \frac{1}{V_{ikm}} \, .
\end{aligned}
$$

Regarding the time discretization, we will apply a TVD RK-DG scheme. These schemes are convex combinations of Euler methods. We consider therefore the time evolution of the cell average in the DG scheme using Forward Euler: $\partial_t \bar{f}_{ikm} \approx (\bar{f}_{ikm}^{n+1} - \bar{f}_{ikm}^{n})/\Delta t^n$

$$
\begin{aligned}
\bar{f}^{n+1}_{ikm} &= \bar{f}^{n}_{ikm} \\
&- \frac{\Delta t^n}{V_{ikm}} \left[\int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i+}} \, p^2 dp d\mu - \int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i-}} \, p^2 dp d\mu \right. \\
&+ p^2_{k^+} \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k+}} \, d\mu dx - p^2_{k^-} \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k-}} \, d\mu dx \\
&+ \left. (1-\mu^2_{m+}) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m+}} \, p \, dp dx - (1-\mu^2_{m-}) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m-}} \, p \, dp dx \right] \\
&+ \left[2\pi \int_{\Omega_{ikm}} \left(\sum_{j=-1}^{+1} c_j \int_{-1}^{+1} d\mu' \left[\chi(\varepsilon') f_h(x, p(\varepsilon'), \mu') \, p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \right] \Big|_{\varepsilon' = \varepsilon(p) + j\hbar\omega} \right) p^2 \, dp d\mu dx \right. \\
&\quad \left. -4\pi \int_{\Omega_{ikm}} f_h(x,p,\mu,t) \left(\sum_{j=-1}^{+1} c_j \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon' = \varepsilon(p) - j\hbar\omega} \right) p^2 \, dp d\mu dx \right] \frac{\Delta t^n}{V_{ikm}} \,,
\end{aligned}
$$

or, more briefly,

$$
\bar{f}^{n+1}_{ikm} = \bar{f}^{n}_{ikm} + \Gamma_T + \Gamma_C \,, \tag{5.15}
$$

where the transport and collision terms for the cell average time evolution are defined as

$$
\begin{aligned}
\Gamma_T &= -\frac{\Delta t^n}{V_{ikm}} \left[\int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i+}} \, p^2 dp d\mu - \int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i-}} \, p^2 dp d\mu \right. \\
&\quad + p^2_{k^+} \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k+}} \, d\mu dx - p^2_{k^-} \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k-}} \, d\mu dx \\
&\quad + \left. (1-\mu^2_{m+}) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m+}} \, p \, dp dx - (1-\mu^2_{m-}) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m-}} \, p \, dp dx \right] ,
\end{aligned}
$$

$$
\begin{aligned}
\Gamma_C &= \left[2\pi \int_{\Omega_{ikm}} \left(\sum_{j=-1}^{+1} c_j \int_{-1}^{+1} d\mu' \; f_h(x, p(\varepsilon'), \mu') \, p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \Big|_{\varepsilon(p) + j\hbar\omega} \right) p^2 \, dp d\mu dx \right. \\
&\quad \left. -4\pi \int_{\Omega_{ikm}} f_h(x,p,\mu,t) \left(\sum_{j=-1}^{+1} c_j \; p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \Big|_{\varepsilon' = \varepsilon(p) - j\hbar\omega} \right) p^2 \, dp d\mu dx \right] \frac{\Delta t^n}{V_{ikm}} \,.
\end{aligned}
$$

5.3.3 Positivity Preservation in DG Scheme for BP

We use the strategy of Zhang & Shu in [63], [64], for conservation laws, Eindeve, Hauck, Xing, Mezzacappa [65] for conservative phase space advection in curvilinear coordinates, and Cheng, Gamba, Proft for Vlasov-Boltzmann with a linear non-degenerate collisional forms [36] to preserve the positivity of our probability density function in our DG scheme treating the collision term as a source, this being possible as our collisional form is mass preserving. We will use a convex combination parameter $\alpha \in [0,1]$ such that

$$\bar{f}_{ikm}^{n+1} = \alpha \underbrace{\left(\bar{f}_{ikm}^{n} + \frac{\Gamma_T}{\alpha} \right)}_{I} + (1-\alpha) \underbrace{\left(\bar{f}_{ikm}^{n} + \frac{\Gamma_C}{1-\alpha} \right)}_{II}, \tag{5.16}$$

and we will find conditions such that I and II are positive, to guarantee the positivity of the cell average of our numerical probability density function for the next time step. The positivity of the numerical solution to the pdf in the whole domain can be guaranteed just by applying the limiters in [63], [64] that preserve the cell average but modify the slope of the piecewise linear solutions in order to make the function non - negative.

Regarding I, the conditions for its positivity are derived below.

$$\begin{aligned} I \;=\; & \bar{f}_{ikm}^{n} + \frac{\Gamma_T}{\alpha} \;=\; \frac{\int_{\Omega_{ikm}} f_h \, p^2 \, dpd\mu dx}{V_{ikm}} \\ & - \frac{\Delta t^n}{\alpha V_{ikm}} \left[\int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i+}} \, p^2 dpd\mu - \int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i-}} \, p^2 dpd\mu \right. \\ & + p_{k+}^2 \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k+}} \, d\mu dx - p_{k-}^2 \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k-}} \, d\mu dx \\ & \left. + (1-\mu_{m+}^2) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m+}} \, p \, dpdx - (1-\mu_{m-}^2) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m-}} \, p \, dpdx \right] . \end{aligned}$$

We will split the cell average using 3 convex parameters $s_l \geq 0$, $l = 1, 2, 3$, s.t. $s_1 + s_2 + s_3 = 1$. We have then

$$
\begin{aligned}
I = \frac{1}{V_{ikm}} \Bigg[& (s_1 + s_2 + s_3) \int_{\Omega_{ikm}} f_h \, p^2 \, dp d\mu dx \\
& - \frac{\Delta t^n}{\alpha} \Bigg(\int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i+}} \, p^2 dp d\mu - \int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i-}} \, p^2 dp d\mu \\
& + p_{k^+}^2 \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k+}} \, d\mu dx - p_{k^-}^2 \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k-}} \, d\mu dx \\
& + \, (1 - \mu_{m+}^2) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m+}} \, p \, dp dx - (1 - \mu_{m-}^2) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m-}} \, p \, dp dx \Bigg) \Bigg]
\end{aligned}
$$

$$
\begin{aligned}
= \frac{1}{V_{ikm}} \Bigg[& s_1 \int_{x_{i-}}^{x_{i+}} \int_{\partial_x \Omega_{km}} f_h \, p^2 \, dp d\mu dx \\
& + s_2 \int_{p_{k-}}^{p_{k+}} \int_{\partial_p \Omega_{im}} f_h \, p^2 \, dp d\mu dx + s_3 \int_{\mu_{m-}}^{\mu_{m+}} \int_{\partial_\mu \Omega_{ik}} f_h \, p^2 \, dp d\mu dx \\
& - \frac{\Delta t^n}{\alpha} \Bigg(\int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i+}} \, p^2 dp d\mu - \int_{\partial_x \Omega_{km}} \widehat{H^{(x)} f_h}|_{x_{i-}} \, p^2 dp d\mu \Bigg) \\
& - \frac{\Delta t^n}{\alpha} \Bigg(p_{k^+}^2 \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k+}} \, d\mu dx - p_{k^-}^2 \int_{\partial_p \Omega_{im}} \widehat{H^{(p)} f_h}|_{p_{k-}} \, d\mu dx \Bigg) \\
& - \frac{\Delta t^n}{\alpha} \Bigg((1 - \mu_{m+}^2) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m+}} \, p \, dp dx - (1 - \mu_{m-}^2) \int_{\partial_\mu \Omega_{ik}} \widehat{H^{(\mu)} f_h}|_{\mu_{m-}} \, p \, dp dx \Bigg) \Bigg] \\
= \frac{1}{V_{ikm}} \Bigg[& \int_{\partial_x \Omega_{km}} \left\{ s_1 \int_{x_{i-}}^{x_{i+}} f_h \, p^2 \, dx - \frac{\Delta t^n}{\alpha} \left(\widehat{H^{(x)} f_h}|_{x_{i+}} \, p^2 - \widehat{H^{(x)} f_h}|_{x_{i-}} \, p^2 \right) \right\} dp \, d\mu \\
& + \int_{\partial_p \Omega_{im}} \left\{ s_2 \int_{p_{k-}}^{p_{k+}} f_h \, p^2 \, dp - \frac{\Delta t^n}{\alpha} \left(p_{k^+}^2 \widehat{H^{(p)} f_h}|_{p_{k+}} - p_{k^-}^2 \widehat{H^{(p)} f_h}|_{p_{k-}} \right) \right\} d\mu \, dx \\
& + \int_{\partial_\mu \Omega_{ik}} \left\{ s_3 \int_{\mu_{m-}}^{\mu_{m+}} f_h \, p^2 \, d\mu - \frac{\Delta t^n}{\alpha} p \left[(1 - \mu_{m+}^2) \widehat{H^{(\mu)} f_h}|_{\mu_{m+}} - (1 - \mu_{m-}^2) \widehat{H^{(\mu)} f_h}|_{\mu_{m-}} \right] \right\} dp dx \Bigg]
\end{aligned}
$$

All the functions to be integrated are polynomials inside a given interval, rectangle or element. Therefore, we can integrate them exactly using a quadrature rule of enough degree, which could be either the usual Gaussian quadrature or the Gauss-Lobatto, which involves the end-points of the interval. We use Gauss-Lobatto quadratures for the integrals of $f_h\, p^2$ over intervals, so that the values at the endpoints can balance the flux terms of boundary integrals, obtaining then CFL conditions.

$$
\begin{aligned}
I = \frac{1}{V_{ikm}} \Bigg[& \int_{\partial_x \Omega_{km}} \left\{ s_1 \sum_{\hat{q}=1}^{N} \hat{w}_{\hat{q}} f_h|_{x_{\hat{q}}}\, p^2\, \Delta x_i - \frac{\Delta t^n}{\alpha} \left(\widehat{H^{(x)} f_h}|_{x_{i+}}\, p^2 - \widehat{H^{(x)} f_h}|_{x_{i-}}\, p^2 \right) \right\} dp\, d\mu \\
& + \int_{\partial_p \Omega_{im}} \left\{ s_2 \sum_{\hat{r}=1}^{N} \hat{w}_{\hat{r}} f_h|_{p_{\hat{r}}}\, p_{\hat{r}}^2\, \Delta p_k - \frac{\Delta t^n}{\alpha} \left(p_{k^+}^2 \widehat{H^{(p)} f_h}|_{p_{k+}} - p_{k^-}^2 \widehat{H^{(p)} f_h}|_{p_{k-}} \right) \right\} d\mu\, dx \\
& + \int_{\partial_\mu \Omega_{ik}} \left\{ s_3 \sum_{\hat{s}=1}^{N} \hat{w}_{\hat{s}} f_h|_{\mu_{\hat{s}}}\, p^2\, \Delta \mu_m - \frac{\Delta t^n}{\alpha} \left[p(1-\mu_{m\pm}^2) \widehat{H^{(\mu)} f_h}|_{\mu_{m\pm}} \right] \right\} dp dx \Bigg] \\
= & \left[\int_{\partial_x \Omega_{km}} \left\{ s_1 \Delta x_i \left(\hat{w}_1 f_h|_{x_{i-}}^{+} + \hat{w}_N f_h|_{x_{i+}}^{-} + \sum_{\hat{q}=2}^{N-1} \hat{w}_{\hat{q}} f_h|_{x_{\hat{q}}} \right) - \frac{\Delta t^n}{\alpha} \left(\widehat{H^{(x)} f_h}|_{x_{i-}}^{x_{i+}} \right) \right\} p^2 dp d\mu \right. \\
& + \int_{\partial_p \Omega_{im}} \left\{ s_2 \left(\hat{w}_1 f_h|_{p_{k-}}^{+}\, p_{k-}^2 + \hat{w}_N f_h|_{p_{k+}}^{-}\, p_{k+}^2 + \sum_{\hat{r}=2}^{N-1} \hat{w}_{\hat{r}} f_h|_{p_{\hat{r}}}\, p_{\hat{r}}^2 \right) \Delta p_k \right. \\
& \qquad \left. - \frac{\Delta t^n}{\alpha} \left(p_{k^+}^2 \widehat{H^{(p)} f_h}|_{p_{k+}} - p_{k^-}^2 \widehat{H^{(p)} f_h}|_{p_{k-}} \right) \right\} d\mu\, dx \\
& + \int_{\partial_\mu \Omega_{ik}} \left\{ s_3 \left(\hat{w}_1 f_h|_{\mu_{m-}}^{+} + \hat{w}_N f_h|_{\mu_{m+}}^{-} + \sum_{\hat{s}=2}^{N-1} \hat{w}_{\hat{s}} f_h|_{\mu_{\hat{s}}} \right) p^2\, \Delta \mu_m \right. \\
& \qquad \left. \left. - \frac{\Delta t^n}{\alpha} \left[(1-\mu_{m+}^2) \widehat{H^{(\mu)} f_h}|_{\mu_{m+}} \; - \; (1-\mu_{m-}^2) \widehat{H^{(\mu)} f_h}|_{\mu_{m-}} \right] p \right\} dp dx \right] \frac{1}{V_{ikm}} \\
= & \left[\int_{\partial_x \Omega_{km}} s_1 \Delta x_i \left\{ \sum_{\hat{q}=2}^{N-1} \hat{w}_{\hat{q}} f_h|_{x_{\hat{q}}} + \left(\hat{w}_1 f_h|_{x_{i-}}^{+} + \hat{w}_N f_h|_{x_{i+}}^{-} \right) \right. \right. \\
& \left. \left. - \frac{\Delta t^n}{\alpha s_1 \Delta x_i} \left(\widehat{H^{(x)} f_h}|_{x_{i+}} - \widehat{H^{(x)} f_h}|_{x_{i-}} \right) \right\} p^2 dp d\mu \right. \\
& + \int_{\partial_p \Omega_{im}} s_2 \Delta p_k \left\{ \left(\hat{w}_1 f_h|_{p_{k-}}^{+}\, p_{k-}^2 + \hat{w}_N f_h|_{p_{k+}}^{-}\, p_{k+}^2 \right) + \sum_{\hat{r}=2}^{N-1} \hat{w}_{\hat{r}} f_h|_{p_{\hat{r}}}\, p_{\hat{r}}^2 \right. \\
& \qquad \left. - \frac{\Delta t^n}{\alpha s_2 \Delta p_k} \left(p_{k^+}^2 \widehat{H^{(p)} f_h}|_{p_{k+}} - p_{k^-}^2 \widehat{H^{(p)} f_h}|_{p_{k-}} \right) \right\} d\mu\, dx \\
& + \int_{\partial_\mu \Omega_{ik}} s_3\, p^2\, \Delta \mu_m \left\{ \left(\hat{w}_1 f_h|_{\mu_{m-}}^{+} + \hat{w}_N f_h|_{\mu_{m+}}^{-} \right) + \sum_{\hat{s}=2}^{N-1} \hat{w}_{\hat{s}} f_h|_{\mu_{\hat{s}}} \right. \\
& \qquad \left. \left. - \frac{\Delta t^n}{\alpha s_3 p\, \Delta \mu_m} \left[(1-\mu_{m+}^2) \widehat{H^{(\mu)} f_h}|_{\mu_{m+}} \; - \; (1-\mu_{m-}^2) \widehat{H^{(\mu)} f_h}|_{\mu_{m-}} \right] \right\} dp dx \right] \frac{1}{V_{ikm}}\,.
\end{aligned}
$$

We reorganize the terms involving the endpoints, which are in parenthesis. So

$$
\begin{aligned}
I &= \frac{1}{V_{ikm}}\left[\int_{\partial_x\Omega_{km}} s_1\Delta x_i\left\{\left(\hat{w}_1 f_h|^+_{x_{i-}} + \frac{\Delta t^n}{\alpha s_1\Delta x_i}\widehat{H^{(x)}f_h}|_{x_{i-}}\right) + \left(\hat{w}_N f_h|^-_{x_{i+}} - \frac{\Delta t^n}{\alpha s_1\Delta x_i}\widehat{H^{(x)}f_h}|_{x_{i+}}\right)\right.\right.\\
&+ \left.\sum_{\hat{q}=2}^{N-1}\hat{w}_{\hat{q}} f_h|_{x_{\hat{q}}}\right\} p^2 dp d\mu + \int_{\partial_p\Omega_{im}} s_2\Delta p_k\left\{\sum_{\hat{r}=2}^{N-1}\hat{w}_{\hat{r}} f_h|_{p_{\hat{r}}}\, p^2_{\hat{r}} + \right.\\
&+ \left. p^2_{k-}\left(\hat{w}_1 f_h|^+_{p_{k-}} + \frac{\Delta t^n}{\alpha s_2\Delta p_k}\widehat{H^{(p)}f_h}|_{p_{k-}}\right) + p^2_{k+}\left(\hat{w}_N f_h|^-_{p_{k+}} - \frac{\Delta t^n}{\alpha s_2\Delta p_k}\widehat{H^{(p)}f_h}|_{p_{k+}}\right)\right\} d\mu\, dx\\
&+ \int_{\partial_\mu\Omega_{ik}} dx\, dp\, p^2\, s_3\,\Delta\mu_m\left\{\sum_{\hat{s}=2}^{N-1}\hat{w}_{\hat{s}} f_h|_{\mu_{\hat{s}}} + \right.\\
&+ \left.\left.\left(\hat{w}_1 f_h|^+_{\mu_{m-}} + \frac{\Delta t^n(1-\mu^2_{m-})}{\alpha s_3 p\,\Delta\mu_m}\widehat{H^{(\mu)}f_h}|_{\mu_{m-}}\right) + \left(\hat{w}_N f_h|^-_{\mu_{m+}} - \frac{\Delta t^n(1-\mu^2_{m+})}{\alpha s_3 p\,\Delta\mu_m}\widehat{H^{(\mu)}f_h}|_{\mu_{m+}}\right)\right\}\right].
\end{aligned}
$$

To guarantee the positivity of I, assuming that the terms $f_h|_{x_{\hat{q}}},\ f_h|_{p_{\hat{r}}},\ f_h|_{\mu_{\hat{s}}}$ are positive at time t^n, we only need that the terms in parenthesis related to interval endpoints are positive. Since $\hat{w}_1 = \hat{w}_N$ for Gauss-Lobatto Quadrature, we want the non-negativity of the terms

$$
\begin{aligned}
0 &\le \left(\hat{w}_N f_h|^{\mp}_{x_{i\pm}} \mp \frac{\Delta t^n}{\alpha s_1\Delta x_i}\widehat{H^{(x)}f_h}|_{x_{i\pm}}\right),\\
0 &\le \left(\hat{w}_N f_h|^{\mp}_{p_{k\pm}} \mp \frac{\Delta t^n}{\alpha s_2\Delta p_k}\widehat{H^{(p)}f_h}|_{p_{k\pm}}\right), \qquad (5.17)\\
0 &\le \left(\hat{w}_N f_h|^{\mp}_{\mu_{m\pm}} \mp \frac{\Delta t^n(1-\mu^2_{m\pm})}{\alpha s_3 p\,\Delta\mu_m}\widehat{H^{(\mu)}f_h}|_{\mu_{m\pm}}\right).
\end{aligned}
$$

We remember that we have used the following notation for the numerical flux terms, given by the upwind rule,

$$
\begin{aligned}
\widehat{H^{(x)}f}|_{x_{i\pm}} &= \partial_p\varepsilon\widehat{f_h\mu}|_{x_{i\pm}} = \partial_p\varepsilon\left[\left(\frac{\mu+|\mu|}{2}\right)f_h|^-_{x_{i\pm}} + \left(\frac{\mu-|\mu|}{2}\right)f_h|^+_{x_{i\pm}}\right],\\
\widehat{H^{(p)}f}|_{p_{k\pm}} &= -q\widehat{Ef_h\mu}|_{p_{k\pm}} = q\left[\left(\frac{|E\mu|-E\mu}{2}\right)f_h|^-_{p_{k\pm}} - \left(\frac{|E\mu|+E\mu}{2}\right)f_h|^+_{p_{k\pm}}\right],\\
\widehat{H^{(\mu)}f}|_{\mu_{m\pm}} &= -q\widehat{Ef_h}|_{\mu_{m\pm}} = q\left[\left(\frac{-E+|E|}{2}\right)f_h|^-_{\mu_{m\pm}} + \left(\frac{-E-|E|}{2}\right)f_h|^+_{\mu_{m\pm}}\right].
\end{aligned}
$$

We have assumed that the positivity of the pdf evaluated at Gauss-Lobatto points, which include endpoints, so we know $f_h|^{\mp}_{x_{i\pm}}$, $f_h|^{\mp}_{p_{k\pm}}$, $f_h|^{\mp}_{\mu_{m\pm}}$ are positive. The worst case scenario for positivity is having negative flux terms. In that case,

$$\begin{aligned}
0 &\leq \hat{w}_N f_h|^{\mp}_{x_{i\pm}} - \frac{\Delta t^n}{\alpha s_1 \Delta x_i}\partial_p \varepsilon\,|\mu| f_h|^{\mp}_{x_{i\pm}} = f_h|^{\mp}_{x_{i\pm}} \left(\hat{w}_N - \frac{\Delta t^n}{\alpha s_1 \Delta x_i}\partial_p \varepsilon\,|\mu|\right), \\
0 &\leq \hat{w}_N f_h|^{\mp}_{p_{k\pm}} - \frac{\Delta t^n}{\alpha s_2 \Delta p_k} q|E(x,t)\mu| f_h|^{\mp}_{p_{k\pm}} = f_h|^{\mp}_{p_{k\pm}} \left(\hat{w}_N - \frac{\Delta t^n}{\alpha s_2 \Delta p_k} q|E(x,t)\mu|\right), \\
0 &\leq \hat{w}_N f_h|^{\mp}_{\mu_{m\pm}} - \frac{\Delta t^n (1-\mu^2_{m\pm})}{\alpha s_3 p\,\Delta \mu_m} q|E(x,t)| f_h|^{\mp}_{\mu_{m\pm}} = f_h|^{\mp}_{\mu_{m\pm}} \left(\hat{w}_N - \frac{\Delta t^n (1-\mu^2_{m\pm})}{\alpha s_3 p\,\Delta \mu_m} q|E(x,t)|\right).
\end{aligned}$$

We need then for the worst case scenario that

$$\begin{aligned}
\hat{w}_N &\geq \frac{\Delta t^n}{\alpha s_1 \Delta x_i}\partial_p \varepsilon\,|\mu|, \\
\hat{w}_N &\geq \frac{\Delta t^n}{\alpha s_2 \Delta p_k} q|E(x,t)\mu|, \\
\hat{w}_N &\geq \frac{\Delta t^n (1-\mu^2_{m\pm})}{\alpha s_3 p\,\Delta \mu_m} q|E(x,t)|,
\end{aligned}$$

or equivalently,

$$\begin{aligned}
\hat{w}_N \frac{\alpha s_1 \Delta x_i}{\partial_p \varepsilon\,|\mu|} &\geq \Delta t^n, \\
\hat{w}_N \frac{\alpha s_2 \Delta p_k}{q|E(x,t)\mu|} &\geq \Delta t^n, \\
\hat{w}_N \frac{\alpha s_3\,\Delta \mu_m\, p}{q|E(x,t)|(1-\mu^2_{m\pm})} &\geq \Delta t^n.
\end{aligned}$$

Therefore, the CFL conditions necessary to satisfy the positivity of the trans-

port term I are

$$\begin{aligned}
\frac{\alpha s_1 \hat{w}_N \Delta x_i}{\max_{\hat{r}} \partial_p \varepsilon(p_{\hat{r}}) \cdot \max_{\pm} |\mu_{m\pm}|} &\geq \Delta t^n \,, \\
\frac{\alpha s_2 \hat{w}_N \Delta p_k}{q \max_{\hat{q}} |E(x_{\hat{q}}, t)| \cdot \max_{\pm} |\mu_{m\pm}|} &\geq \Delta t^n \,, \\
\frac{\alpha s_3 \hat{w}_N \Delta \mu_m \cdot p_{k-}}{q \max_{\hat{q}} |E(x_{\hat{q}}, t)| \cdot \max_{\pm} (1 - \mu_{m\pm}^2)} &\geq \Delta t^n \,.
\end{aligned}$$

Regarding II, there are several ways to guarantee its positivity. One possible way to guarantee its positive is given below, by separating the gain and the loss part, combining the cell average with the loss term and deriving a CFL condition related to the collision frequency, and imposing a positivity condition on the points where the gain term is evaluated, which differs for inelastic scatterings from the previous Gauss-Lobatto points because of the addition or subtraction of the phonon energy $\hbar\omega$. We would need an additional set of points in which to impose positivity in order to guarantee positivity of II as a whole.

$$
\begin{aligned}
&II = \bar{f}^n_{ikm} + \frac{\Gamma_C}{1-\alpha} = \\
&\bar{f}^n_{ikm} + \left[2\pi \int_{\Omega_{ikm}} \left(\sum_{j=-1}^{+1} c_j \int_{-1}^{+1} d\mu' \left[f_h(x, p(\varepsilon'), \mu')\, p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon(p)+j\hbar\omega} \right) p^2\, dpd\mu dx \right. \\
&\left. - \int_{\Omega_{ikm}} f_h(x,p,\mu,t) \left(4\pi \sum_{j=-1}^{+1} c_j \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon(p)-j\hbar\omega} \right) p^2\, dpd\mu dx \right] \frac{\Delta t^n}{V_{ikm}(1-\alpha)} = \\
&\left[\frac{2\pi\Delta t^n}{(1-\alpha)} \int_{\Omega_{ikm}} \left(\sum_{j=-1}^{+1} c_j \int_{-1}^{+1} d\mu' \left[f_h(x, p(\varepsilon'), \mu')\, p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon(p)+j\hbar\omega} \right) p^2\, dpd\mu dx + \right. \\
&\left. \int_{\Omega_{ikm}} f_h dV - \frac{4\pi\Delta t^n}{(1-\alpha)} \int_{\Omega_{ikm}} f_h \left(\sum_{j=-1}^{+1} c_j \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon(p)-j\hbar\omega} \right) p^2\, dpd\mu dx \right] \frac{1}{V_{ikm}} = \\
&\left[\frac{2\pi\Delta t^n}{(1-\alpha)} \sum_{j=-1}^{+1} c_j \int_{\Omega_{ikm}} \int_{-1}^{+1} d\mu' \left[f_h(x, p(\varepsilon'), \mu')\, p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon(p)+j\hbar\omega} p^2\, dpd\mu dx + \right. \\
&\left. \int_{\Omega_{ikm}} f_h(x,p,\mu,t) \left(1 - \frac{4\pi\Delta t^n}{(1-\alpha)} \sum_{j=-1}^{+1} c_j \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon(p)-j\hbar\omega} \right) p^2\, dpd\mu dx \right] \frac{1}{V_{ikm}} = \\
&\left[\frac{2\pi\Delta t^n}{(1-\alpha)} \sum_{j=-1}^{+1} c_j |\Omega_{ikm}| \sum_{s,r,q} w_{s,r,q} f_h(x_s, p'(\varepsilon(p_r) + j\hbar\omega), \mu'_q) \left[p'^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon(p_r)+j\hbar\omega} p_r^2 \right. \\
&\left. + \int_{\Omega_{ikm}} f_h(x,p,\mu,t) \left(1 - \frac{4\pi\Delta t^n}{(1-\alpha)} \sum_{j=-1}^{+1} c_j \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon(p)-j\hbar\omega} \right) p^2\, dpd\mu dx \right] \frac{1}{V_{ikm}} ,
\end{aligned}
$$

where the notation for the measure of the elements is

$$
|\Omega_{ikm}| = \Delta x_i \Delta p_k \Delta \mu_m \,. \tag{5.18}
$$

Given that the collision frequency

$$
\nu(p) = 4\pi \sum_{j=-1}^{+1} c_j\, \chi(\varepsilon(p) - j\hbar\omega) \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \right] \Big|_{\varepsilon' = \varepsilon(p) - j\hbar\omega} > 0 \tag{5.19}
$$

is positive, as it is made of positive and non negative terms, we combine the cell average with the loss term in order to derive the following CFL condition related to the collision frequency. If

$$1 - \frac{4\pi\Delta t^n}{(1-\alpha)} \sum_{j=-1}^{+1} c_j \, \chi(\varepsilon(p) - j\hbar\omega) \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \right] \Big|_{\varepsilon' = \varepsilon(p) - j\hbar\omega} > 0 \,,$$

then

$$\Delta t^n < \frac{(1-\alpha)}{4\pi} \left(\max_{p_k} \sum_{j=-1}^{+1} c_j \, \left[\chi(\varepsilon') p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \right] \Big|_{\varepsilon(p_k) - j\hbar\omega} \right)^{-1} = \frac{(1-\alpha)}{\max_{p_k} \nu(p_k)} \,,$$

where the maximum is taken over the Gaussian Quadrature Points p_k.

To completely guarantee the positivity of II, we must impose a positivity condition on the set of points where the gain term is evaluated, which differs for inelastic scatterings from the previous Gauss-Lobatto points because of the addition or subtraction of the phonon energy $\hbar\omega$. That is, we want

$$\sum_{s,r,q} w_{s,r,q} f_h(x_s, p'(\varepsilon(p_r) + j\hbar\omega), \mu'_q) \, \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon' = \varepsilon(p_r) + j\hbar\omega} p_r^2 \geq 0.$$

So, in order to get the positivity of this term, we need that in the additional set of points $(x_s, p'(\varepsilon(p_r) + j\hbar\omega), \mu'_q)$ it is satisfied that

$$f_h(x_s, p'(\varepsilon(p_r) + j\hbar\omega), \mu'_q) \geq 0 \,.$$

Another possible way to guarantee positivity for II is by considering the collision term as a whole. The difference between the gain minus the loss integrals will give us a smaller source term overall, and therefore a more

relaxed CFL condition for Δt^n. We have that

$$II = \bar{f}^n_{ikm} + \frac{\Gamma_C}{1-\alpha} = \frac{\int_{\Omega_{ikm}} f_h dV}{V_{ikm}} + \frac{\Delta t^n \int_{\Omega_{ikm}} Q(f_h) dV}{(1-\alpha) V_{ikm}} = \frac{1}{V_{ikm}} \left[\int_{\Omega_{ikm}} f_h dV + \frac{\Delta t^n}{(1-\alpha)} \times \right.$$
$$\left. \int_{\Omega_{ikm}} \left(2\pi \sum_{j=-1}^{+1} c_j \int_{-1}^{1} d\mu' \; f_h(x, p(\varepsilon'), \mu') p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \Big|_{\varepsilon(p)+j\hbar\omega} - f_h \nu(p) \right) p^2 dp d\mu dx \right].$$

We will treat then the cell average of the collision term as a whole by taking the difference of the gain minus the loss terms and considering this difference as a source term, and we will apply the same techniques for positivity preserving DG schemes for transport equations with source terms.

$$\begin{aligned}
II &= \frac{1}{V_{ikm}} \left[\int_{\Omega_{ikm}} f_h \, p^2 \, dp d\mu dx + \frac{\Delta t^n}{(1-\alpha)} \int_{\Omega_{ikm}} Q(f_h) \, p^2 \, dp d\mu dx \right], \\
Q(f_h) &= 2\pi \sum_{j=-1}^{+1} c_j \int_{-1}^{+1} d\mu' \; f_h(x, p(\varepsilon'), \mu') \, p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \Big|_{\varepsilon' = \varepsilon(p)+j\hbar\omega} - f_h \nu(p), \\
\nu(p) &= 4\pi \sum_{j=-1}^{+1} c_j \left[p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \chi(\varepsilon') \right] \Big|_{\varepsilon' = \varepsilon(p)-j\hbar\omega} = \nu(\varepsilon(p)). \qquad (5.20)
\end{aligned}$$

We want II to be positive. If the collision operator part was negative, we choose the time step Δt^n such that II is positive on total. We will get this way our CFL condition in order to guarantee the positivity of II. We want

$$\begin{aligned}
II &= \frac{1}{V_{ikm}} \int_{\Omega_{ikm}} \left[f_h(x, p, \mu, t) + \frac{\Delta t^n}{(1-\alpha)} Q(f_h)(x, p, \mu, t) \right] p^2 \, dp d\mu dx \geq 0, \\
II &= \frac{|\Omega_{ikm}|}{V_{ikm}} \sum_{q,r,s} w_q w_r w_s \left[f_h(x_q, p_r, \mu_s, t) + \frac{\Delta t^n}{(1-\alpha)} Q(f_h)(x_q, p_r, \mu_s, t) \right] p_r^2 \geq 0.
\end{aligned}$$

If $0 > Q(f_h)$ for any of the points (x_q, p_r, μ_s) at time t^n, then choose Δt^n s.t.

$$\begin{aligned} 0 &\leq f_h(x_q, p_r, \mu_s, t) + \frac{\Delta t^n}{(1-\alpha)} Q(f_h)(x_q, p_r, \mu_s, t)\,, \\ 0 &\leq f_h(x_q, p_r, \mu_s, t) - \frac{\Delta t^n}{(1-\alpha)} |Q(f_h)|(x_q, p_r, \mu_s, t)\,, \\ \Delta t^n &\leq \frac{(1-\alpha) f_h(x_q, p_r, \mu_s, t)}{|Q(f_h)|(x_q, p_r, \mu_s, t)}\,. \end{aligned}$$

Our CFL condition in this case would be then

$$\Delta t^n \leq (1-\alpha) \min_{Q(f_h)(x_q, p_r, \mu_s, t^n) < 0} \left\{ \frac{f_h(x_q, p_r, \mu_s, t^n)}{|Q(f_h)|(x_q, p_r, \mu_s, t^n)} \right\}. \quad (5.21)$$

The minimum for the CFL condition is taken over the subset of Gaussian Quadrature points (x_q, p_r, μ_s) inside the cell Ω_{ikm} (whichever the chosen quadrature rule was) over which $Q(f_h)(x_q, p_r, \mu_s, t^n) < 0$. This subset of points might be different for each time t^n then.

We have figured out the respective CFL conditions for the transport and collision parts. Finally, we only need to choose the optimal parameter α that gives us the most relaxed CFL condition for Δt^n such that positivity is preserved for the cell average at the next time, $\bar{f}_{ikm}^{n+1}$. The positivity of the whole numerical solution to the pdf, not just its cell average, can be guaranteed by applying the limiters in [63], [64], which preserve the cell average but modify the slope of the piecewise linear solutions in order to make the function non - negative in case it was negative before.

5.4 Stability of the scheme under an entropy norm

We can prove the stability of the scheme under the entropy norm related to the interior product

$$\int f_h \, g_h e^H \, p^2 dp d\mu dx \, , \tag{5.22}$$

inspired in the strategy of Cheng, Gamba, Proft [36]. This estimates are possible due to the dissipative property of the linear collisional operator applied to the curvilinear representation of the momentum, with the entropy norm related to the function $e^{H(x,p,t)} = \exp\left(\varepsilon(p) - qV(x,t)\right)$. Assuming periodic boundary conditions in all directions for simplicity of the stability proof, we look for $f_h \in V_h^k$ such that, $\forall\, g_h \in V_h^k$ and $\forall\, \Omega_{ikm}$,

$$\begin{aligned}
&\int_{ikm} \partial_t f_h \, g_h e^H \, p^2 dp d\mu dx \qquad\qquad (5.23)\\
-\int_{ikm} \partial_p \varepsilon(p) \, f_h \, \mu \, \partial_x (g_h e^H) \, p^2 dp d\mu dx \quad &\pm \quad \int_{km} \partial_p \varepsilon \, \widehat{f_h \mu}|_{x_{i\pm}} \, g_h e^H|_{x_{i\pm}}^{\mp} \, p^2 dp d\mu \\
-\int_{ikm} p^2(-qE)(x,t) f_h \mu \, \partial_p (g_h e^H) \, d\mu dx \quad &\pm \quad \int_{im} p_{k\pm}^2 \, (-q\widehat{E f_h \mu})|_{p_{k\pm}} g_h e^H|_{p_{k\pm}}^{\mp} \, d\mu dx \\
+\int_{ikm} (1-\mu^2) f_h q E(x,t) \partial_\mu (g_h e^H) p \, dp d\mu dx \quad &\mp \quad \int_{ik} (1-\mu_{m\pm}^2) q\widehat{E f_h}|_{\mu_{m\pm}} g_h e^H|_{\mu_{m\pm}}^{\mp} p dp dx \\
&= \quad \int_{ikm} Q(f_h) g_h e^H \, p^2 dp d\mu dx \, ,
\end{aligned}$$

where we are including as a factor the inverse of a Maxwellian along the characteristic flow generated by the Hamiltonian transport field $(\partial_p \varepsilon(p), q\partial_x V(x,t))$

$$e^{H(x,p,t)} = \exp(\varepsilon(p) - qV(x,t)) = \left(e^{qV(x,t)} e^{-\varepsilon(p)}\right)^{-1} \, , \tag{5.24}$$

which is an exponential of the Hamiltonian energy, assuming the energy is measured in $K_B T$ units.

We include this modified inverse Maxwellian factor because we can use the entropy inequalities related to the collision operator derived on the introduction. That is, we know from (2.39) the following dissipative property

$$\int_{\Omega_{\vec{p}}} Q(f) g d\vec{p} = -\frac{1}{2} \int_{\Omega_{\vec{p}}} S(\vec{p}' \to \vec{p}) e^{-\varepsilon(p')} \left(\frac{f'}{e^{-\varepsilon(p')}} - \frac{f}{e^{-\varepsilon(p)}} \right) (g' - g) d\vec{p}' d\vec{p}, \tag{5.25}$$

which can be also expressed as (multiplying and dividing by $e^{-qV(x,t)}$)

$$\int_{\Omega_{\vec{p}}} Q(f) g d\vec{p} = -\frac{1}{2} \int_{\Omega_{\vec{p}}} S(\vec{p}' \to \vec{p}) e^{-H'} \left(\frac{f'}{e^{-H'}} - \frac{f}{e^{-H}} \right) (g' - g) d\vec{p}' d\vec{p}. \tag{5.26}$$

Therefore, if we choose a monotone increasing function $g(f/e^{-H})$, namely $g = f/e^{-H} = fe^{H}$, we have an equivalent dissipative property but now with the exponential of the full Hamiltonian,

$$\int_{\Omega_{\vec{p}}} Q(f) \frac{f}{e^{-H}} d\vec{p} = -\frac{1}{2} \int_{\Omega_{\vec{p}}} S(\vec{p}' \to \vec{p}) e^{-H'} \left(\frac{f'}{e^{-H'}} - \frac{f}{e^{-H}} \right)^2 d\vec{p}' d\vec{p} \leq 0\,. \tag{5.27}$$

So we have found the following dissipative entropy inequality

$$\int_{\Omega_{\vec{p}}} Q(f) f e^{H} p^2 dp d\mu d\varphi = \int_{\Omega_{\vec{p}}} Q(f) \frac{f}{e^{-H}} d\vec{p} \leq 0\,. \tag{5.28}$$

As a consequence of this dissipative entropy inequality we obtain the following stability theorem of the scheme under an entropy norm.

Theorem 5.4.1. (Stability under the entropy norm $\int f_h\, g_h e^{H}\, p^2 dp d\mu dx$): *Consider the semi-discrete solution f_h to the DG formulation in (5.23) for the BP system in momentum curvilinear coordinates. We have then*

$$0 \geq \int_{\Omega} f_h \partial_t f_h\, e^{H(x,p,t)}\, p^2\, dp d\mu dx = \frac{1}{2} \int_{\Omega} \partial_t f_h^2 e^{H(x,p,t)}\, p^2\, dp d\mu dx\,. \tag{5.29}$$

Proof. Choosing $g_h = f_h$ in (5.23), and considering the union of all the cells Ω_{ikm}, which gives us the whole domain $\Omega = \Omega_x \times \Omega_{p,\mu}$ for integration, we have

$$\begin{aligned}
0 \geq \int_\Omega Q(f_h) f_h e^H \, p^2 dp d\mu dx &= \int_\Omega \partial_t f_h \, f_h e^H \, p^2 dp d\mu dx \\
- \int_\Omega \partial_p \varepsilon(p) \, f_h \, \mu \, \partial_x (f_h e^H) \, p^2 dp d\mu dx &+ \int_{\partial_x \Omega} \partial_p \varepsilon \, \widehat{f_h \mu} \, f_h e^H \, p^2 dp d\mu \\
- \int_\Omega p^2 (-qE) f_h \mu \, \partial_p (f_h e^H) \, d\mu dx &+ \int_{\partial_p \Omega} p^2 \, (-q \widehat{E f_h \mu}) f_h e^H \, d\mu dx \\
- \int_\Omega (1-\mu^2) f_h (-qE) \, \partial_\mu (f_h e^H) \, p \, dp d\mu dx &+ \int_{\partial_\mu \Omega} (1-\mu^2)(-q \widehat{E f_h}) \, f_h e^H \, p \, dp dx \, .
\end{aligned}$$

We can express this in the more compact form

$$0 \geq \int_\Omega \partial_t f_h \, f_h e^H \, p^2 \, dp d\mu dx - \int_\Omega f_h \beta \cdot \partial (f_h e^H) \, dp d\mu dx + \int_{\partial\Omega} \widehat{f_h} \beta \cdot \hat{n} \, f_h e^H \, d\sigma \, , \tag{5.30}$$

defining the transport vector β with the properties

$$\begin{aligned}
\beta &= \left(p^2 \mu \partial_p \varepsilon(p), -qE \, p^2 \mu, -qEp(1-\mu^2) \right) \, , \qquad (5.31) \\
\partial \beta &= \partial_{(x,p,\mu)} \beta = (0, -2pqE\mu, 2\mu qE) \, , \quad \partial \cdot \beta = -2pqE\mu + 2pqE\mu = 0, \\
\beta \cdot \partial H &= \left(p^2 \mu \partial_p \varepsilon(p), -qE \, p^2 \mu, -qEp(1-\mu^2) \right) \cdot (qE, \partial_p \varepsilon, 0) = 0, \quad \partial_\mu \varepsilon = 0 \, .
\end{aligned}$$

We integrate by parts again the transport integrals, obtaining

$$\begin{aligned}
\int_\Omega f_h \beta \cdot \partial (f_h e^H) \, dp d\mu dx &= - \int_\Omega \partial \cdot (f_h \beta) f_h e^H \, dp d\mu dx + \int_{\partial\Omega} f_h \beta \cdot \hat{n} f_h e^H \, d\sigma \\
&= - \int_\Omega (\beta \cdot \partial f_h) f_h e^H \, dp d\mu dx + \int_{\partial\Omega} f_h \beta \cdot \hat{n} f_h e^H \, d\sigma \, ,
\end{aligned}$$

but since

$$\beta \cdot \partial (f_h e^H) = \beta \cdot e^H \partial f_h + \beta \cdot f_h e^H \partial H = e^H \beta \cdot \partial f_h \, , \tag{5.32}$$

then we have

$$\int_\Omega f_h \beta \cdot \partial (f_h e^H)\, dp d\mu dx \;=\; \int_\Omega (\beta \cdot \partial f_h) f_h e^H\, dp d\mu dx \;=\; \frac{1}{2}\int_{\partial\Omega} f_h \beta \cdot \hat{n} f_h e^H\, d\sigma\,. \tag{5.33}$$

We can express our entropy inequality then as

$$0 \geq \int_\Omega \partial_t f_h\, f_h e^H\, p^2\, dp d\mu dx - \frac{1}{2}\int_{\partial\Omega} f_h \beta\cdot\hat{n} f_h e^H\, d\sigma + \int_{\partial\Omega} \widehat{f_h}\beta\cdot\hat{n}\, f_h e^H\, d\sigma\,, \tag{5.34}$$

remembering that we are integrating over the whole domain by considering the union of all the cells defining our mesh. We distinguish between the boundaries of cells for which $\beta\cdot\hat{n}\geq 0$ and the ones for which $\beta\cdot\hat{n}\leq 0$, defining uniquely the boundaries. Remembering that the upwind flux rule is such that $\hat{f}_h = f_h^-$, we have that the value of the solution inside the cells close to boundaries for which $\beta\cdot\hat{n}\geq 0$ is f_h^-, and for boundaries $\beta\cdot\hat{n}\leq 0$ the value of the solution inside the cell close to that boundary is f_h^+. We have then that

$$\begin{aligned}
0 \;&\geq\; \int_\Omega \partial_t f_h\, f_h e^H\, p^2\, dp d\mu dx - \frac{1}{2}\int_{\partial\Omega} f_h \beta\cdot\hat{n} f_h e^H\, d\sigma \;+ \int_{\partial\Omega} f_h^- \beta\cdot\hat{n}\, f_h e^H\, d\sigma \\
0 \;&\geq\; \int_\Omega \partial_t f_h\, f_h e^H\, p^2\, dp d\mu dx - \frac{1}{2}\int_{\beta\cdot\hat{n}\geq 0} f_h^- |\beta\cdot\hat{n}| f_h^- e^H\, d\sigma \;+ \int_{\beta\cdot\hat{n}\geq 0} f_h^- |\beta\cdot\hat{n}|\, f_h^- e^H\, d\sigma \\
&+\; \frac{1}{2}\int_{\beta\cdot\hat{n}\leq 0} f_h^+ |\beta\cdot\hat{n}| f_h^+ e^H\, d\sigma \;- \int_{\beta\cdot\hat{n}\leq 0} f_h^- |\beta\cdot\hat{n}|\, f_h^+ e^H\, d\sigma\,,
\end{aligned}$$

and using a notation e_h for the boundaries that allows redundancy, balanced

then by a factor of $1/2$, we have

$$\begin{aligned}
0 &\geq \int_\Omega \partial_t f_h \, f_h e^H \, p^2 \, dpd\mu dx - \frac{1}{2}\left(\frac{1}{2}\int_{e_h} f_h^- |\beta\cdot\hat{n}| f_h^- e^H \, d\sigma + \int_{e_h} f_h^- |\beta\cdot\hat{n}| \, f_h^- e^H \, d\sigma \right. \\
&+ \left. \frac{1}{2}\int_{e_h} f_h^+ |\beta\cdot\hat{n}| f_h^+ e^H \, d\sigma - \int_{e_h} f_h^- |\beta\cdot\hat{n}| \, f_h^+ e^H \, d\sigma\right) \\
0 &\geq \int_\Omega \partial_t f_h \, f_h e^H \, p^2 \, dpd\mu dx + \frac{1}{2}\left(\frac{1}{2}\int_{e_h} f_h^- |\beta\cdot\hat{n}| f_h^- e^H \, d\sigma \right. \\
&+ \left. \frac{1}{2}\int_{e_h} f_h^+ |\beta\cdot\hat{n}| f_h^+ e^H \, d\sigma - \int_{e_h} f_h^- |\beta\cdot\hat{n}| \, f_h^+ e^H \, d\sigma\right) \\
0 &\geq \int_\Omega \partial_t f_h \, f_h e^H \, p^2 \, dpd\mu dx \\
&+ \frac{1}{4}\left(\int_{e_h} f_h^- f_h^- |\beta\cdot\hat{n}| e^H \, d\sigma - 2\int_{e_h} f_h^- f_h^+ |\beta\cdot\hat{n}| \, e^H \, d\sigma + \int_{e_h} f_h^+ f_h^+ |\beta\cdot\hat{n}| e^H \, d\sigma \right) \\
0 &\geq \int_\Omega \partial_t f_h \, f_h e^H \, p^2 \, dpd\mu dx + \frac{1}{4}\int_{e_h} (f_h^+ - f_h^-)^2 |\beta\cdot\hat{n}| e^H \, d\sigma \, . \qquad (5.35)
\end{aligned}$$

Since the second term is non-negative, we conclude therefore that

$$0 \geq \int_\Omega f_h \partial_t f_h \, e^{H(x,p,t)} \, p^2 \, dpd\mu dx = \frac{1}{2}\int_\Omega \partial_t f_h^2 e^{H(x,p,t)} \, p^2 \, dpd\mu dx \, , \qquad (5.36)$$

and in this sense is that the numerical solution has stability with respect to the considered entropy norm. □

As a remark, we obtain the following corollary:

Corollary 5.4.2. (Stability under the entropy norm for a time independent Hamiltonian): *If $V = V(x)$, so $\partial_t H = 0$, the stability under our entropy norm gives us that, for $t \geq 0$,*

$$||f_h||^2_{L^2_{e^H p^2}}(t) = \int_\Omega f_h^2(x,p,\mu,t) e^{H(x,p)} \, p^2 \, dpd\mu dx \leq ||f_h||^2_{L^2_{e^H p^2}}(0) \, . \qquad (5.37)$$

Proof. The corollary follows from the fact that, since $\partial_t H = -q\partial_t V = 0$, we have

$$0 \geq \int_\Omega \partial_t \left(f_h^2 e^{H(x,p)} \right) \, p^2 \, dpd\mu dx = \frac{d}{dt} \int_\Omega f_h^2(x,p,\mu,t) e^{H(x,p)} \, p^2 \, dpd\mu dx \quad (5.38)$$

Since the entropy norm is a decreasing function of time, our result follows immediately. □

Chapter 6

Conclusions

The work presented in this dissertation is related to several lines of research in the area of deterministic DG numerical methods for computational electronic transport in semiconductor physics.

The first line of research is the use of EPM related energy bands in order to increase the accuracy of the physical modeling of the energy band structure and its partial derivatives, via a spherical average of an EPM band structure and the spline interpolation of its derivatives, as these functions drive the mechanisms of collision (electron - phonon scattering) and transport (via the electron group velocity). The balance of these two mechanisms is the core of the modeling of electron transport in semiconductors by means of Boltzmann - Poisson. The values of the energy band obtained from the spherical average of the EPM full band structure and its derivatives interpolated by splines, gives a quantitative correction in kinetic moments (averages) related to the energy band model, such as average velocity, energy, and particularly the momentum (proportional to the current) given by our numerical solver. This highlights the importance of band models and features such as anisotropy and interpolation of their derivatives in the BP numerical modeling of electron transport via DG

schemes. Work in progress is related to the computational implementation of a DG scheme with the full EPM band structure and the spline interpolation of its partial derivatives. Future work will focus on DG methods for Boltzmann - Poisson systems with multi - bands, for the modeling of electron and hole transport or multi-valley modeling.

We have considered in the second line of research the mathematical and numerical modeling of Reflective Boundary Conditions in 2D devices and their implementation in DG-BP schemes. We have studied the specular, diffusive and mixed reflection BC on the boundaries of the position domain of the device. We developed a numerical equivalent of the pointwise zero flux condition at the position domain boundaries for the case of a more general mixed reflection with a momentum dependant specularity parameter $p(\vec{k})$. We compared the influence of these different reflection cases in the computational prediction of moments after implementing numerical BC equivalent to the respective reflective BC, each one satisfying a mathematical zero flux condition at insulating boundaries. There are effects due to the inclusion of diffusive reflection boundary conditions over the moments of the probability density function and over the electric field and potential, whose influence is not only restricted to the boundaries but actually to the whole domain. Expected effects of the inclusion of diffusivity in kinetic moments are the increase of the density close to the reflecting boundary, the decrease of the mean energy over the domain and the increase of the momentum x-component over the domain. Future research will consider the inclusion of surface roughness scat-

tering mechanisms in the collision operator for our diffusive reflection problem in silicon devices, for example. Another line of work of our interest for future research will be the more general case of a $p(\vec{x}, \vec{k})$ specular probability dependant on momentum and position as well, considering its mathematical and numerical aspects, and its respective computational simulations, intending to use as input experimental values of $p(\vec{x}, \vec{k})$.

The third line of research is related to the development of positivity preserving DG schemes for BP semiconductor models. Due to the physics of energy conservation given by Planck's law and to reduce the dimension of the associated collision operator given its mathematical form, we pose the Boltzmann Equation for electron transport in curvilinear coordinates for the momentum. This is a more general form that includes the two other BP models used in the previous lines of research as particular cases. We consider the 1D diode problem with azimuthal symmetry assumptions, which give us a 3D plus time problem. We choose for this problem the spherical coordinate system $\vec{p}(p, \mu, \varphi)$, slightly different to the previous choices, because its DG formulation gives simpler integrals involving just (piecewise) polynomial functions for both transport and collision terms. Using the strategy in [63], [64], [36] we treat the collision operator as a source term, and find convex combinations of the transport and collision terms which guarantee the propagation of positivity of the cell average of our numerical probability density function at the next time step. The positivity of the numerical solution to the pdf in the whole domain can be guaranteed just by applying the limiters in [63], [64] that preserve the

cell average but modify the slope of the piecewise linear solutions in order to make the function non - negative. We have been able to prove as well the stability of the semi-discrete DG scheme formulated under an entropy norm, assuming periodic boundary conditions for simplicity. For the simpler case of a time dependent Hamiltonian, the decay of the entropy norm of the numerical solution over time follows as a corollary. This highlights the importance of the dissipative properties of our collisional operator given by its entropy inequalities. In this case, the entropy norm depends on the full time dependent Hamiltonian rather than just the Maxwellian associated solely to the kinetic energy.

Bibliography

[1] C. W. Shu, *Discontinuous Galerkin methods: general approach and stability*, Numerical Solutions of Partial Differential Equations, S. Bertoluzza, S. Falletta, G. Russo and C. W. Shu, Advanced Courses in Mathematics CRM Barcelona, Birkhauser, Basel, 2009, pp.149-201.

[2] A. Jüngel, *Transport Equations for Semiconductors*, Springer-Verlag (2009).

[3] W.H. Reed and T.R. Hill, *Triangular mesh methods for the neutron transport equation*, Tech. Report LA-UR-73-479, Los Alamos Scientific Laboratory (1973).

[4] E. Kane, *Band structure of Indium Antimonide*, J. Phys. Chem. Solids, vol. 1, pp. 249-261, (1957).

[5] X. Zhang and C.-W. Shu. *On maximum-principle-satisfying high order schemes for scalar conservation laws*, J. Comput. Phys., 229:30913120 (2010).

[6] M. G. Crandall and L. Tartar. *Some relations between nonexpansive and order preserving mappings*, Proc. Amer. Math. Soc., 78:385390 (1980).

[7] P. Ciarlet. *The finite element method for elliptic problems*, North-Holland, Amsterdam (1975).

[8] C.-W. Shu and S. Osher. *Efficient implementation of essentially non-oscillatory shock-capturing schemes*, J. Comput. Phys., 77:439471 (1988).

[9] Y. Cheng, *Deterministic Numerical Methods for the Boltzmann-Poisson System*, Tutorial of ICERM workshop on 'Novel Applications of Kinetic Theory and Computation' (2011).

[10] A. Majorana, *The Boltzmann-Poisson System: Model Document (Version D: Full Bands)* , U. Catania.

[11] F. Register, *Semiconductor Physics Graduate Course Notes*, U. Texas - Austin, 2012.

[12] L. Reggiani, *Hot-Electron Transport in Semiconductors*, Springer-Verlag Berlin Heidelberg, 1985.

[13] A. Majorana, S.A. Marano, *Space homogeneous solutions to the Cauchy problem for semiconductor Boltzmann equations.* SIAM J. Math. Anal., 1997, 28 (6), 1294–1308.

[14] A. Majorana, S.A. Marano, *On the cauchy problem for spatially homogeneous semiconductor Boltzmann equations: existence and uniqueness.* Annali di Mat. Pura e Appl., **2005**, 184, 275–296.

[15] D.K. Ferry, *Semiconductors*, Maxwell MacMillian: New-York, 1991.

[16] K. Tomizawa, *Numerical simulation of sub micron semiconductor devices*, Artech House: Boston, 1993.

[17] P. Markowich, C. Ringhofer and C. Schmeiser, *Semiconductor Equations*, Springer-Verlag, 1990.

[18] M. Lundstrom, *Fundamentals of Carrier Transport*, Cambridge University Press, 2000.

[19] C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation*, Spring-Verlag: Wien-New York, 1989.

[20] E. Fatemi and F. Odeh, *Upwind finite difference solution of Boltzmann equation applied to electron transport in semiconductor devices*, Journal of Computational Physics, 108 (1993) 209-217.

[21] A. Majorana and R. Pidatella, *A finite difference scheme solving the Boltzmann Poisson system for semiconductor devices*, Journal of Computational Physics, 174 (2001) 649-668.

[22] J.A. Carrillo, I.M. Gamba, A. Majorana and C.-W. Shu, *A WENO-solver for 1D non-stationary Boltzmann-Poisson system for semiconductor devices*, Journal of Computational Electronics, 1 (2002) 365-375.

[23] J.A. Carrillo, I.M. Gamba, A. Majorana and C.-W. Shu, *A direct solver for 2D non-stationary Boltzmann-Poisson systems for semiconductor devices: a MESFET simulation by WENO-Boltzmann schemes*, Journal of Computational Electronics, 2 (2003) 375-380.

[24] J.A. Carrillo, I.M. Gamba, A. Majorana and C.-W. Shu, *A WENO-solver for the transients of Boltzmann-Poisson system for semiconductor devices.*

Performance and comparisons with Monte Carlo methods, Journal of Computational Physics, 184 (2003) 498-525.

[25] M.J. Caceres, J.A. Carrillo, I.M. Gamba, A. Majorana and C.-W. Shu, *Deterministic kinetic solvers for charged particle transport in semiconductor devices*, in Transport Phenomena and Kinetic Theory Applications to Gases, Semiconductors, Photons, and Biological Systems. Series: Modeling and Simulation in Science, Engineering and Technology. C. Cercignani and E. Gabetta (Eds.), Birkhäuser (2006) 151-171.

[26] J.A. Carrillo, I.M. Gamba, A. Majorana and C.-W. Shu, *2D semiconductor device simulations by WENO-Boltzmann schemes: efficiency, boundary conditions and comparison to Monte Carlo methods*, Journal of Computational Physics, 214 (2006) 55-80.

[27] M. Galler and A. Majorana, *Deterministic and stochastic simulation of electron transport in semiconductors*, Bulletin of the Institute of Mathematics, Academia Sinica (New Series), 6th MAFPD (Kyoto) special issue Vol. 2 (2) (2007) 349-365.

[28] Z. Chen, B. Cockburn, C. Gardner and J. Jerome, *Quantum hydrodynamic simulation of hysteresis in the resonant tunneling diode*, Journal of Computational Physics, 274 (1995) 274-280.

[29] Z. Chen, B. Cockburn, J. W. Jerome and C.-W. Shu, *Mixed-RKDG finite element methods for the 2-d hydrodynamic model for semiconductor device simulation*, VLSI Design, 3 (1995) 145-158.

[30] Y.-X. Liu and C.-W. Shu, *Local discontinuous Galerkin methods for moment models in device simulations: formulation and one dimensional results*, Journal of Computational Electronics, 3 (2004) 263-267.

[31] Y.-X. Liu and C.-W. Shu, *Local discontinuous Galerkin methods for moment models in device simulations: Performance assessment and two dimensional results*, Applied Numerical Mathematics, 57 (2007) 629-645.

[32] Y. Cheng, I.M. Gamba, A. Majorana and C.-W. Shu, *Discontinuous Galerkin Solver for the Semiconductor Boltzmann Equation*, SISPAD 07, T. Grasser and S. Selberherr, editors, Springer (2007) 257-260.

[33] Y. Cheng, I. Gamba, A. Majorana and C.-W. Shu, *Discontinuous Galerkin solver for Boltzmann-Poisson transients*, Journal of Computational Electronics, 7 (2008) 119-123.

[34] Y. Cheng, I. M. Gamba, A. Majorana and C.-W. Shu *A discontinuous Galerkin solver for Boltzmann-Poisson systems in nano-devices*, Computer Methods in Applied Mechanics and Engineering, 198 (2009) 3130-3150.

[35] Y. Cheng, I. M. Gamba, A. Majorana and C.W. Shu *A discontinuous Galerkin solver for Full-Band Boltzmann-Poisson Models*, IWCE13 (13th International Workshop on Computational Electronics) (2009).

[36] Y. Cheng, I. M. Gamba and J. Proft, *Positivity-preserving discontinuous Galerkin schemes for linear Vlasov-Boltzmann transport equations*, Mathematics of Computation, 81 (2012) 153-190.

[37] J. Chelikowsky, and M. Cohen, *Electronic structure of silicon*, Physical Review B, 10 (1974) 5095-5107.

[38] M L. Cohen and J.R. Chelikowsky, *Electronic Structure and Optical Properties of Semiconductors*, Springer Series in Solid-State Sciences 75 (1989).

[39] M. C. Vecchi, D. Ventura, A. Gnudi, and G.Baccarani, *Incorporating full band-structure effects in spherical harmonics expansion of the Boltzmann transport equation,* Proceedings of NUPAD V Conference, vol. 8, pp. 55–58, 1994.

[40] S. Smirnov and C. Jungemann, *A full band deterministic model for semiclassical carrier transport in semiconductors*, Journal of Applied Physics, 99 (2006) 063707.

[41] C. Jungemann, A.T. Pham, B. Meinerzhagen, C. Ringhofer and M. Bollhöfer, *Stable discretization of the Boltzmann equation based on spherical harmonics, box integration, and a maximum entropy dissipation principle*, Journal of Applied Physics, 100 (2006) 024502.

[42] A. Majorana, *A comparison between bulk solutions to the Boltzmann equation and the spherical harmonic model for silicon devices*, Progress in Industrial Mathematics at ECMI 2000 - Mathematics in Industry, 1 (2002) 169-173.

[43] B. Cockburn and C.-W. Shu, *TVB Runge-Kutta local projection discontinuous Galerkin finite element method for conservation laws II: general*

framework, Mathematics of Computation, 52 (1989) 411-435.

[44] B. Cockburn, S.-Y. Lin and C.-W. Shu, *TVB Runge-Kutta local projection discontinuous Galerkin finite element method for conservation laws III: one dimensional systems*, Journal of Computational Physics, 84 (1989) 90-113.

[45] B. Cockburn, S. Hou and C.-W. Shu, *The Runge-Kutta local projection discontinuous Galerkin finite element method for conservation laws IV: the multidimensional case*, Mathematics of Computation, 54 (1990) 545-581.

[46] B. Cockburn and C.-W. Shu, *The Runge-Kutta local projection P1-discontinuous Galerkin finite element method for scalar conservation laws*, Mathematical Modelling and Numerical Analysis, 25 (1991) 337-361.

[47] B. Cockburn and C.-W. Shu, *The Runge-Kutta discontinuous Galerkin method for conservation laws V: multidimensional systems*, Journal of Computational Physics, 141 (1998) 199-224.

[48] B. Cockburn and C.-W. Shu, *Runge-Kutta discontinuous Galerkin methods for convection-dominated problems*, Journal of Scientific Computing, 16 (2001) 173-261.

[49] B. Cockburn and C.-W. Shu, *The local discontinuous Galerkin method for time-dependent convection-diffusion systems*, SIAM Journal on Numerical Analysis, 35 (1998) 2440-2463.

[50] D. Arnold, F. Brezzi, B. Cockburn, and L. Marini, *Unified analysis of discontinuous Galerkin methods for elliptic problems*, SIAM Journal on Numerical Analysis, 39 (2002) 1749-1779.

[51] C. Cercignani, I.M. Gamba, C.L. Levermore, *A Drift-Collision Balance asymptotic for a Boltzmann-Poisson System in Bounded Domains*, SIAM J. Appl. Math., Vol 61, No. 6, (2001) 1932-1958.

[52] Y. Sone, *Molecular Gas Dynamics: Theory, Techniques, and Applications*, Birkhauser (2007).

[53] C. Cercignani, *The Boltzmann Equation and Its Applications*, Springer-Verlag, Appl. Math. Sc. 67, (1988).

[54] C. Cercignani, I. M. Gamba, C.D. Levermore, *High Field Approximations to a Boltzmann - Poisson System and Boundary Conditions in a Semiconductor*, Appl. Math. Lett. **10**, 4, 111-117 (1997).

[55] S. Soffer, *Statistical Model for the size effect in Electrical Conduction*, Journal of Applied Physics 38 1710 (1967).

[56] K. Fuchs, Proc. Cambridge Phil. Soc. 34 100 (1938).

[57] R. F. Greene, *Boundary Conditions for Electron Distributions at Crystal Surfaces*, Physical Review 141 687 (1966).

[58] R. F. Greene, R. W. O'Donnell, *Scattering of Conduction Electrons by Localized Surface Charges*, Physical Review 147 599 (1966).

[59] V. D. Borman, S. Yu. Krylov, A. V. Chayanov, *Theory of nonequilibrium phenomena at a gas-solid interface*, Sov. Phys. JETP 67 (10), 1988.

[60] Brull, Charrier, Mieussens, *Gas-surface interaction and boundary conditions for the Boltzmann equation*, Kinetic & Related Models (2014).

[61] Struchtrup, H. *Maxwell boundary condition and velocity dependent accommodation coefficient*, Phys. Fluids 25, 112001 (2013).

[62] B. Ghosh, S. Banerjee (Supervisor), F. Register (Co-Supervisor), *Semiclassical Monte Carlo simulation of nano-scaled semiconductor devices*, UT Electronic Theses and Dissertations, (2007).

[63] X. Zhang and C.-W. Shu, *Positivity-preserving high order discontinuous Galerkin schemes for compressible Euler equations with source terms*, J. Comput. Phys., 230 (2011) 1238-1248.

[64] X. Zhang and C.-W. Shu, *On positivity-preserving high order discontinuous Galerkin schemes for compressible Euler equations on rectangular meshes*, J. Comput. Phys., 229 (2010) 8918-8934.

[65] Eirik Endeve, Cory Hauck, Yulong Xing, Anthony Mezzacappa, *Bound-preserving discontinuous Galerkin methods for conservative phase space advection in curvilinear coordinates*, Journal of Computational Physics, 2015.

[66] I. M. Gamba, A. Majorana, J. Morales and C.W. Shu *A fast approach to discontinuous Galerkin solvers for Boltzmann-Poisson transport systems for full electronic bands and phonon scattering*, IWCE15, 1-4 (2012).

[67] J.A. Morales Escalante, I.M. Gamba, A. Majorana, Y. Cheng, C.-W. Shu, and J.R. Chelikowsky, *Deterministic DG Solvers for EPM-Boltzmann-Poisson Transport*, IWCE16 Abstracts, 2013.

[68] J. Morales Escalante, I.M. Gamba, *Boundary conditions effects by Discontinuous Galerkin solvers for Boltzmann-Poisson models of electron transport*, Proceedings Paper, 17th IWCE, 2014.

[69] J. A. Morales Escalante, I.M. Gamba, A. Majorana , Y. Cheng, C.-W. Shu, and J. Chelikowsky, *Discontinuous Galerkin Deterministic Solvers for a Boltzmann-Poisson Model of Hot Electron Transport by Averaged Empirical Pseudopotential Band Structures*, submitted to CMAME, 2016.

[70] J. Morales Escalante, I.M. Gamba, *Reflective Boundary conditions in Discontinuous Galerkin solvers for Boltzmann-Poisson models of electron transport in semiconductors and Zero Flux Condition for General Mixed Reflection*, preprint.

[71] J. Morales Escalante, E. Endeve, C. Hauck, I.M. Gamba, *Positivity Preserving DG schemes for a Boltzmann - Poisson model of electrons in semiconductors in curvilinear momentum coordinates*, preprint.

Vita

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