Entropy-stable positivity-preserving DG schemes for Boltzmann-Poisson models of collisional electronic transport along energy bands

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Abstract

This work is related to the development of entropy-stable positivity-preserving Discontinuous Galerkin (DG) methods as a computational scheme for Boltzmann-Poisson systems modeling the probability density of collisional electronic transport along energy bands in semiconductors. We pose, in momentum coordinates representing spherical / energy-angular variables, the respective Vlasov-Boltzmann equation with a linear collision operator and a singular measure, modeling scatterings as functions of the bandstructure appropriately for hot electron nanoscale transport.

We show stability results of semi-discrete DG schemes under an entropy norm for 1D-position (2D-momentum) and 2D-position (3D-momentum), using dissipative properties of the collisional operator given its entropy inequality. The latter depends on an exponential of the Hamiltonian rather than the Maxwellian associated with only kinetic energy. For the 1D problem, knowing the analytic solution to the Poisson equation and convergence to a constant current is crucial to obtaining full stability (weighted entropy norm decreasing over time). For the 2D problem, specular reflection boundary conditions and periodicity are considered in estimating stability under an entropy norm.

Regarding the positivity-preservation proofs in the DG scheme for the 1D problem, inspired by [9], [10], and [11], [12], we treat collisions as a source and find convex combinations of the transport and collision terms which guarantee positivity of the cell average of our numerical probability density at the next time. The positivity of the numerical solution to the probability density in the domain is guaranteed by applying the limiters in [9] and [10] that preserve the cell average modifying the slope of the piecewise linear solutions to make the function non-negative. The use of a spherical coordinate system whose radial component is the momentum magnitude $|\vec{p}| (\mu = \cos \theta, \phi)$ is slightly different from choices in previous DG solvers for Boltzmann-Poisson, since the proposed DG formulation gives simpler integrals involving piecewise polynomials for both transport and collision.

1 Introduction

The Boltzmann-Poisson system is a model for electron transport in semiconductors representing the balance of transport and collisions in the $((\vec{x}, \vec{p})) \in \mathbb{R}^3_x \times \mathbb{R}^3_p$ position-momentum phase space for electrons in the gradient field of the electrostatic potential $\phi(\vec{x})$. In this work, we consider a variant of the system that accounts for collisions with acoustic phonons, modeled by a linear collision operator.

In the context of Boltzmann-Poisson systems, it is crucial to develop numerical methods that are not only accurate but also preserve key physical properties such as entropy stability and positivity of the probability density. The use of Discontinuous Galerkin schemes offers a powerful framework for such computations, especially when dealing with complex physical models like the Boltzmann equation.

The abstract highlights the focus of the work on developing entropy-stable positivity-preserving DG schemes for the Boltzmann-Poisson system. The key aspects include:

- **Entropy stability**: The schemes are designed to preserve the entropy inequality, a property that ensures the system evolves towards a state of minimum entropy, which is crucial for the long-time behavior of the system.

- **Positivity preservation**: The schemes guarantee that the numerical solutions remain non-negative, which is essential for maintaining the physical meaning of the probability density.

- **Spherical coordinates**: The use of spherical coordinates simplifies the integration of collision terms, making the numerical implementation more efficient.

The abstract sets the stage for the detailed analysis presented in the introduction, where the authors delve into the specifics of the problem formulation, the choice of coordinates, and the development of the DG schemes.
function (pdf) in the phase space for electrons in the conduction band, and at a given time, it is given by the negative gradient of the electric potential, $\partial_\phi \Phi(x, t) = -\frac{\partial_q \Phi(x, t)}{\epsilon}$, with the Hamiltonian $H(x, p, t) = \epsilon(p) - q\Phi(x, t)$, and collision

$$Q(f) = \int_{\Omega_p} S(p' \rightarrow p)f' dp' - f \int_{\Omega_p} S(p \rightarrow p') dp',$$

coupled to the Poisson equation for total charges

$$-\partial_\phi \cdot (\epsilon \partial_x \Phi)(x, t) = q \left[ N(x) - \int_{\Omega_p} f(x, p, t) dp \right], \quad \vec{E}(x, t) = -\partial_x \Phi(x, t),$$

for $x \in \Omega_x \subset \mathbb{R}^3$. The momentum variable is $p = \hbar \vec{k}$, $\vec{k}$ is the crystal momentum wave vector, $\epsilon(p)$ is the conduction energy band structure for electrons in the semiconductor, $f(x, p, t)$ is the probability density function (pdf) in the phase space for electrons in the conduction band at a given time,

$$\vec{v} = \frac{\partial_p \epsilon(p)}{\epsilon},$$

is the quantum mechanical electron group velocity, $q$ is the positive electric charge of a proton, $\Phi(x, t)$ 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), $\epsilon$ is the permittivity of the material, $N(x)$ is the doping background (assumed fixed) in the semiconductor material, and $S(p' \rightarrow p)$ is the scattering kernel that defines the gain and loss operators whose difference gives the collision integral operator $Q(f)$. We will assume in this work a linear collision operator, which is valid in the regime of low electron density, as the enforcement of the Pauli exclusion principle in this case via the collision operator structure is not needed. We assume $\Omega_x$ is $\Pi_\phi$ (a torus corresponding to periodic boundary conditions), a bounded domain where the Poisson problem is well posed, with periodic boundary conditions. That means the solution of our Boltzmann-Poisson problem is well posed and $f \in L^1, \Phi \in L^2$. We stress out that the transport terms have an underlying Hamiltonian structure, where this Hamiltonian transport vector is related to the group velocity $\vec{v}$ of the electron wave and the electric force $\vec{E}$ over it,

$$\alpha(x, p) = (\vec{v}, \vec{p}) = (\vec{v}(p), \vec{E}(x, t)) = (\partial_p \epsilon(p), q\partial_x \Phi(x, t)) = (\partial_p H, -\partial_x H) \in \Omega_x \times \mathbb{R}^3,$$

and then the transport part of the Boltzmann eq. for collisional electron transport in semiconductors has a Hamiltonian structure given by a Poisson bracket, as in

$$\partial_t f + \{f, H\} = Q(f), \quad \{f, H\} = \partial_z f \cdot \partial_p H - \partial_p f \cdot \partial_z H.$$

For many quantum collision mechanisms, such as in semiconductors, the scattering kernel $S(p' \rightarrow p)$ depends on the difference between energies $\epsilon(p) - \epsilon(p')$, as in collision operators of the form $\delta(\epsilon(p) - \epsilon(p')) + \hbar^2 v_p$ for electron - phonon collisions. This form is related to the energy conservation given by 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 $\epsilon(p)$ as
one of the variables \([1, 2, 3, 4, 5]\). 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 \((\mu, \varphi)\), the cosine of the polar angle and the azimuthal angle, respectively.

This gives both physical and mathematical motivations to pose the Boltzmann Equation for semiconductors in curvilinear coordinates for the momentum \(p(p_1, p_2, p_3) = \vec{p}(p_x, p_y, p_z)\), to later on choose a particular case of curvilinear coordinates such as \((\varepsilon, \mu, \varphi)\). We will assume in the rest of this paper that our system of curvilinear coordinates for the momentum is orthogonal. This happens in particular for the case \((\varepsilon, \mu, \varphi)\) in which \(\varepsilon(|\vec{p}|)\) is monotone increasing, so this set of coordinates is equivalent to the spherical coordinate representation \((|\vec{p}|, \mu, \varphi)\).

The Boltzmann Equation for semiconductors (and more general forms of linear collisional plasma models as well) can be written in orthogonal curvilinear coordinates for the momentum vector \(\vec{p}(p_1, p_2, p_3) = \vec{p}(p_x, p_y, p_z)\), under the velocity relation \((1.1)\), with \(h_j = \frac{|\vec{p}|}{|\vec{p}_j|}, j = 1, 2, 3\), generate the Jacobian determinant of the transformation by setting \(J := J_{\vec{p}\vec{p}} = h_1 h_2 h_3\) and \(\hat{e}_j\) the unitary vectors associated to each curvilinear coordinate \(p_j\) at the point \((p_1, p_2, p_3)\),

\[
\partial_t f + \partial_{\vec{v}} \cdot (J f \vec{v}) + q \nabla_x \Phi \cdot \nabla_v (J f) = C(f),
\]

with

\[
\nabla_x \Phi \cdot \nabla_v (J f) := \left[ \partial_{p_1} \left( J f \frac{\partial \Phi \cdot \hat{e}_{p_1}}{h_1} \right) + \partial_{p_2} \left( J f \frac{\partial \Phi \cdot \hat{e}_{p_2}}{h_2} \right) + \partial_{p_3} \left( J f \frac{\partial \Phi \cdot \hat{e}_{p_3}}{h_3} \right) \right],
\]

and a head on collisional form,

\[
C(f) := J Q(f) = \int_{\Omega_x} S(\vec{p}^u) \rightarrow \vec{p}^u J f \vec{v}' dp'_1 dp'_2 dp'_3 - \int_{\Omega_x} S(\vec{p} \rightarrow \vec{p}') J f dp'_1 dp'_2 dp'_3. \tag{1.9}
\]

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

\[
\partial_t (J f) + \partial_{\vec{v}} \cdot (J f \vec{v}(|\vec{p}|)) + \sum_{j=1}^3 \partial_{p_j} \left( J f \frac{q \partial_x \Phi \cdot \hat{e}_j}{h_j} \right) = C(f). \tag{1.10}
\]

For \(J \geq 0\), we can interpret \(J f(\vec{x}, p_1, p_2, p_3, t)\) as a probability density function in the phase space \((\vec{x}, p_1, p_2, p_3)\). This Boltzmann Eq. is a general form for orthogonal curvilinear momentum coordinates, from which previous energy-angular and spherical coordinate systems (such as in \([4, 5]\)) can be derived. For the spherical one in \([6]\), the orthogonal curvilinear system is

\[
(r \propto k^2, \mu = \cos \theta |p_x, \varphi = \arctan(p_z/p_y)), \tag{1.11}
\]

where \(\theta\) is the polar angle with respect to the \(p_x\)-axis, \(\varphi\) is the azimuthal angle, and \(r \propto k^2\), which is proportional to the energy in the limit as \(|k| \rightarrow 0\), approaching the conduction band local minimum. The energy-angular one in \([4]\) is

\[
(w \propto \varepsilon, \mu = \cos \theta |p_x, \varphi = \arctan(p_z/p_y)), \tag{1.12}
\]

with \(w \propto \varepsilon\), under the assumption that \(\varepsilon(|p|)\) is a Kane band model. The numerical method we will study in this work in connection to our Boltzmann - Poisson system is the Discontinuous Galerkin (DG) Finite Element Method (FEM), to be explained in Section 3. It was proposed by Reed and Hill \([7]\) for hyperbolic equations in the context of neutron transport. It is defined such that its numerics captures the mathematics of the hyperbolic transport by defining the so-called fluxes in such a way that the information propagates numerically in the same fashion as a hyperbolic equation propagates information analytically. In the particular context of electron collisional transport in semiconductors, the DG method has been used in works such
as [1, 3, 5] after an evolution of the numerical methods used to solve it that transitioned from Upwind Finite Differences [1] to WENO schemes [2, 3] and finally to mainly two schools, one related to the aforementioned development on DG methods for Boltzmann - Poisson, and the other related to Spherical Harmonics Expansions, for which a good overview can be found in [8]. There is a particular kind of DG methods, called Positivity Preserving (PPDG), which is designed to preserve the positivity of the functions that are the unknown to be solved for, usually having the interpretation of densities needed to be non-negative, such as fluid densities or probability density functions. These positivity preserving DG methods were developed by Zhang and Shu [9, 10]. The main idea is that, given a positive initial condition, PPDG is such that, after a time iteration, the cell averages are preserved to be positive and, if the function is negative for a given region, a limiter is applied in the interval(s) of interest, modifying the slope in such a way that after the modification the function is non-negative in the interval(s). It was designed in the context of the compressible Euler equations for fluids. Later works have incorporated this idea in different application contexts. Work related to our current problem was developed first in [11] for linear Vlasov - Boltzmann collisional transport equations in cartesian coordinates under quadratically confined electrostatic potentials, where the Boltzmann collision operator was linear (with bounded scattering functions), and later in [12] for a conservative phase space collisionless advection of neutral particles in curvilinear coordinates.

On the other hand, regarding works on entropy dissipation laws and stability under entropy norms for Boltzmann semiconductor models, analytical results have been obtained, for example, by [13], where moment closure hierarchies were studied for the Boltzmann - Poisson equation, getting a \( f \log f \) type entropy dissipation law. We would also like to mention the work on [14] that studies the relative entropies for kinetic equations in bounded domains, obtaining results on irreversibility, stationary solutions, and uniqueness. Regarding specifically numerical works on this kind of problems, [15] studies the semiconductor Boltzmann equation based on spherical harmonics expansions and entropy discretizations. The convergence of numerical moment methods for linear kinetic equations was studied in [16]. A mixed spectral-difference method for the steady state Boltzmann - Poisson system is presented in [17]. DG discretizations of first-order systems of conservation laws derivable as moments of the Boltzmann equation with Levermore closure were considered in [18] using energy analysis techniques; the problem does not include acceleration terms as no force field is considered. We should also mention the work in [19], where a high order DG scheme for solving nonlinear Fokker-Planck equations with a gradient flow structure was proposed, and it was shown to satisfy a discrete entropy dissipation law and to preserve steady-states, enforcing the positivity of the numerical solutions in the algorithm.

Our current work extends the contributions above mentioned by studying a Boltzmann - Poisson system for collisional electronic transport in which the momentum is studied in curvilinear coordinates determined by the energy band structure appearing both in the transport and the electron-phonon collision operator. The latter models the discrete energy jumps with a Dirac delta distribution scattering term, which is clearly not a smooth bounded function and therefore more complex than previous collision operators studied in the context of entropy stable and positivity preserving DG methods for collisional electron transport. We study semi-discrete stability properties (under an entropy norm) of the DG method for the Boltzmann - Poisson problem by means of the (semi-discrete) Hamiltonian energy functional, where, without loss of generality, we assume a suitable discretization for the Poisson equation, yielding an accurate mass preserving approximation for both the electrostatic potential and corresponding electric field, and later we present the proof of positivity preservation for the DG scheme for BP in the usual \( L_2 \) (Jacobian weighted) norm. For the positivity preserving work, we introduce the 1D-position with 3D-momenta space problem with azimuthal symmetry, which can be reduced to a 3-dimensional set of coordinates (1D in position, 2D in momentum) plus time when modeling a 1D diode under such symmetry assumptions in momentum space.

The type of approximations and numerical schemes implementations for the Poisson part of the Boltzmann - Poisson system (with the Boltzmann part in the usual \( L_2 \) Jacobian weighted norm, without enforcing the preservation of positivity) have been studied in [6, 5]. Our contribution is to show the stability of a DG scheme under an entropy norm for the Boltzmann - Poisson system with curvilinear momentum (the Boltz-
mann part using an \( L_2 \) norm weighted not only by the Jacobian but in addition by the exponential of the Hamiltonian) that incorporates the full time dependent Hamiltonian, in the corresponding curvilinear coordinates, obtaining a stability result that gives certain control over \( \partial_t f \) for the two dimensional position domain (and 3D in momentum) problem with specular reflection and periodic boundary conditions, and for the one dimensional space domain problem (with two dimensional momentum under symmetry assumptions) a full stability result, meaning specifically the decay of the entropy norm over time, using the knowledge of the convergence to a constant current in the limit of this time evolution problem and the solution to the Poisson problem in 1D.

1.1 Preliminaries: On the problem of energy - curvilinear coordinates

We would like to point out that the transport vector in curvilinear momentum coordinates (that usually represent either a spherical or energy-angular set of coordinates, and could equally represent an energy level set type of orthogonal system of coordinates)

\[
\beta = \mathbf{J} \left( \mathbf{	ilde{v}(\hat{p})}, \frac{F \cdot \hat{e}_{p_1}}{h_1}, \frac{F \cdot \hat{e}_{p_2}}{h_2}, \frac{F \cdot \hat{e}_{p_3}}{h_3} \right),
\]

with \( F(\vec{x}, t) = -q \mathbf{E}(\vec{x}, t) = q \partial_x \mathbf{\Phi} \), has two important properties in the curvilinear momentum space directly related to their Hamiltonian nature, namely \( \partial \cdot \beta = 0 \) and \( \beta \cdot \partial H = 0 \), defining \( \partial = \partial(\vec{x}, p_1, p_2, p_3) \) as the gradient in the curvilinear space.

Moreover, in the following sections we will present some physical examples to the reader in which it will be clear that the results on stability under an entropy norm for the DG scheme under study rely on these 2 properties. Once established for the general curvilinear momentum coordinate case, the same kind of entropy stability results to be proved in this paper would apply for any DG scheme under that formulation of a transformed Boltzmann equation. We therefore prove these two properties for the transport vector \( \beta \) (multiplied by the Jacobian) below. For \( \beta \cdot \partial H = 0 \), we have that

\[
\beta \cdot \partial H = \mathbf{J} \left( \nabla_{(p_x, p_y, p_z)} \mathbf{\epsilon}, \frac{F \cdot \hat{e}_{p_x}}{h_1}, \frac{F \cdot \hat{e}_{p_y}}{h_2}, \frac{F \cdot \hat{e}_{p_z}}{h_3} \right) \cdot (-F(\vec{x}, t), \partial(p_1, p_2, p_3)) \mathbf{\epsilon})
\]

\[
= \mathbf{J} \left[ -\nabla_{(p_x, p_y, p_z)} \mathbf{\epsilon} \cdot F + F \cdot \left( \frac{\hat{e}_{p_x}}{h_1} \partial_{p_1} \mathbf{\epsilon} + \frac{\hat{e}_{p_y}}{h_2} \partial_{p_2} \mathbf{\epsilon} + \frac{\hat{e}_{p_z}}{h_3} \partial_{p_3} \mathbf{\epsilon} \right) \right] = 0,
\]

because the formula that relates the gradients in the curvilinear (\( p_x, p_y, p_z \)) and in the curvilinear (\( p_1, p_2, p_3 \)) momentum coordinates is precisely

\[
\nabla_{(p_x, p_y, p_z)} \mathbf{\epsilon} = \frac{\partial \mathbf{\epsilon}}{\partial_{p_1} h_1} + \frac{\partial \mathbf{\epsilon}}{\partial_{p_2} h_2} + \frac{\partial \mathbf{\epsilon}}{\partial_{p_3} h_3}.
\]

The second property, related to the divergence of the transport field \( \beta \) in the phase space with curvilinear momentum, follows from the divergence free property of the transport vector in cartesian space. That is, we know that

\[
\nabla_{(\vec{x}, \hat{p})} \cdot (\mathbf{\tilde{v}(\hat{p})}, F(\vec{x}, t)) = 0
\]

trivially due to dependance in alternate coordinates. However, relating the divergence in the cartesian momentum space to the curvilinear one, we have

\[
0 = \nabla_{(p_x, p_y, p_z)} F(x, t) = \frac{1}{\mathbf{J}} \left[ \frac{\partial(F_1 J / h_1)}{\partial p_1} + \frac{\partial(F_2 J / h_2)}{\partial p_2} + \frac{\partial(F_3 J / h_3)}{\partial p_3} \right],
\]

with \( F_j = F \cdot \hat{e}_{p_j}, j = 1, 2, 3 \). So

\[
0 = \partial_{(p_1, p_2, p_3)} \cdot \left( J \left( F_1 / h_1, F_2 / h_2, F_3 / h_3 \right) \right)
\]

\[
= \partial_{(p_1, p_2, p_3)} \cdot \left( J \left( F \cdot \hat{e}_{p_1} / h_1, F \cdot \hat{e}_{p_2} / h_2, F \cdot \hat{e}_{p_3} / h_3 \right) \right)
\]

\[
= \partial_{(p_1, p_2, p_3)} \cdot \left( J \left( F \cdot \hat{e}_{p_1} / h_1, F \cdot \hat{e}_{p_2} / h_2, F \cdot \hat{e}_{p_3} / h_3 \right) + \nabla_{\vec{x}} \cdot (J \mathbf{\tilde{v}(\hat{p})}) = \partial \cdot \beta, \right.
\]

with \( \partial = \partial(\vec{x}, p_1, p_2, p_3) \), since \( J \) only depends on the momentum.
2 Stability of DG schemes under entropy norms

In this section we’ll study the stability of DG schemes under entropy norms, focusing on 3D & 5D plus time problems. We’ll make some comments as well on the problem in general for orthogonal curvilinear momentum coordinates.

2.1 1Dx-2Dp Diode Symmetric Problem

In the particular case of a 1D silicon diode problem, the main collision mechanisms are electron-phonon scatterings

\[ S(\vec{p}' \rightarrow \vec{p}) = \sum_{j=-1}^{1} c_j \delta(\varepsilon(\vec{p}')) - \varepsilon(\vec{p}) + j \hbar \omega), \quad c_1 = (n_{ph} + 1) K, \quad c_{-1} = n_{ph} K, \tag{2.1} \]

with \( \omega \) 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, \( \varepsilon(p) \), \( p = |\vec{p}| \), and that the initial condition for the pdf has azimuthal symmetry, \( f_{|t=0} = f_0(x,p,\mu,t), \partial_x f_0 = 0, \vec{p} = \hbar(\mu, \sqrt{1-\mu^2} \cos \varphi, \sqrt{1-\mu^2} \sin \varphi) \), then the dimensionality of the problem is reduced to 3D+time, that is, 1D in \( x \) and 2D in \( (p, \mu) \). Our curvilinear coordinates would be in this case

\[
\begin{align*}
p_1 &= |\vec{p}| = p, \\
p_2 &= \mu = \cos \theta |E(x,t)|, \\
p_3 &= \varphi = \arctan(p_z/p_y),
\end{align*}
\tag{2.2}
\]

since the polar axis (reference direction) \( p_x \) is chosen parallel to the direction of the 1D electric field \( E(x,t) \) in the \( x \)-direction, \( p_x|x \). The Jacobian determinant is

\[
J_{\vec{p}} = \left| \frac{\partial(p_x, p_y, p_z)}{\partial(p, \mu, \varphi)} \right| = -p^2,
\]

where the minus sign helps to transform the integral \( \int_0^{\pi} d\theta \cdots \int_0^1 d\mu \cdots \) as \( \mu = \cos \theta = v_x/|\vec{v}| \), where \( \vec{v}(\vec{p}) = (v_x, v_y, v_z) \). Then, the BP system for \( f(x,p,\mu,t) \) and \( \Phi(x,t) \) is written in spherical coordinates \( \vec{p}(p,\mu,\varphi) \) for the momentum (under azimuthal symmetry assumptions) as

\[
\begin{align*}
\partial_t f + \partial_x (f \partial_x \varepsilon) + \frac{\partial_y (f \mu \mu)}{p^2} + \frac{\partial_z (f (1 - \mu^2))}{p} q \partial_z \Phi(x,t) &= Q(f), \\
-\partial_x^2 \Phi &= \frac{q}{\epsilon} \left[ (N(x) - 2\pi \int_{-1}^{1} \int_0^{p_{max}} f p^2 dp d\mu, \right], \quad \Phi(0) = 0, \Phi(L) = \Phi_0, \tag{2.3}
\end{align*}
\]

where the charge density is given by

\[
\rho(x,t) = 2\pi \int_{-1}^{1} \int_0^{p_{max}} f(x,p,\mu,t)p^2 dp d\mu.
\]

We have assumed that the permittivity \( \epsilon \) is constant. The Poisson BVP with Dirichlet BC in 1D above has an analytic integral solution for \( \Phi(x,t) \) and for \( E(x,t) = -\partial_x \Phi(x,t) \) as well, which can be projected in the appropriate spaces for our numerical method. The solution is given by the integral formula [1]

\[
\begin{align*}
\Phi(x,t) &= \Phi_0 + \frac{q}{\epsilon} \int_0^L \left[ N(x') - \rho(t,x') \right] (L-x')dx' - \frac{q}{\epsilon} \int_0^x \left[ N(x') - \rho(t,x') \right] (x-x')dx', \\
E(x,t) &= -\left( \frac{\Phi_0}{L} + \frac{q}{\epsilon} \frac{1}{L} \int_0^L \left[ N(x') - \rho(t,x') \right] (L-x')dx' - \frac{q}{\epsilon} \int_0^x \left[ N(x') - \rho(t,x') \right] dx' \right) \tag{2.4}
\end{align*}
\]
Therefore, in this 1D problem we only need to concern ourselves with the Boltzmann Equation, since given the electron density we know the solution for the potential and electric field in Poisson.

The collision operator in this problem has the form

\[
Q(f) = 2\pi \left[ \sum_{j=-1}^{+1} c_j \int_{-1}^{+1} d\mu' f(x, p(x'), \mu') p^2(x') \frac{dp'}{d\omega'} \right] \chi(\varepsilon(p) + j\hbar\omega) \\
- f(x, p, \mu, t) \sum_{j=-1}^{+1} c_j 2p^2(\varepsilon') \frac{dp'}{d\omega'} \chi(\varepsilon(p) - j\hbar\omega)
\]

where \(\chi(\varepsilon)\) is 1 if \(\varepsilon \in [0, \varepsilon_{\text{max}}]\) and 0 if \(\varepsilon \notin [0, \varepsilon_{\text{max}}]\), with \(\varepsilon_{\text{max}} = \varepsilon(p_{\text{max}})\).

The domain of the Boltzmann Poisson problem is \(x \in [0, L], p \in [0, p_{\text{max}}], \mu \in [-1, +1], t > 0\). Moreover, since \(\varepsilon(p)\), then \(\partial p = \frac{dp}{dp}\). We assume that \(\frac{dp}{dp} > 0\) is well behaved enough such that \(p(\varepsilon)\) is a monotonic function for which \(\frac{dp}{dp} = (\frac{dp}{dp})^{-1}\) exists. The collision frequency is

\[
\nu(\varepsilon(p)) = \sum_{j=-1}^{+1} c_j 4\pi \chi(\varepsilon(p) - j\hbar\omega) p^2(\varepsilon') \frac{dp'}{d\omega'} \chi(\varepsilon(p) - j\hbar\omega) = \sum_{j=-1}^{+1} c_j n(\varepsilon(p) - j\hbar\omega),
\]

where the density of states with energy \(\varepsilon(p) - j\hbar\omega\) is

\[
n(\varepsilon(p) - j\hbar\omega) = \int_{\Omega_x} \delta(\varepsilon(p') - \varepsilon(p) + j\hbar\omega) dp'.
\]

### 2.2 RKDG Entropy preserving scheme for the 1Dx-2Dp Boltzmann-Poisson system

Before writing the weak form of the Transformed Boltzmann Equation and introducing an entropy preserving Runge-Kutta Discontinuous Galerkin (RKDG) scheme for the BP system \(2.3\), for \((x, p, \mu) \in \Omega = \Omega_x \times \Omega_{(p, \mu)} \subseteq \mathbb{R}^d\), we need to choose the choice of the cut-off domain in momentum space, since the probability density in momentum space may be supported in all its space of definition, while decaying at infinity fast enough to get mass, momentum, and energy bounded. The problem can also be restricted to the first position dimension \(x = (x, 0, 0)\), \(E(x, t) = (E(x, t), 0, 0)\). Since for \(f(x, p, \mu), g(x, p, \mu)\) we have that

\[
\int_{\Omega_x} \int_{\Omega_p} f g \, dp \, dx = 2\pi \int_{\Omega_x} \int_{\Omega_p} f g \, p^2 \, dp \, dx,
\]

we define our inner product of two functions \(f\) and \(g\) in the \((x, p, \mu)\) space as

\[
(f, g)_{X \times K} = \int_X \int_K f g \, p^2 \, dp \, dx,
\]

where \(X \subset [0, L]\) and \(K \subset [0, p_{\text{max}}] \times [-1, +1]\). The Boltzmann Equation for our problem can be written in weak form as

\[
(\partial_t f, g)_{\Omega_c} + (\partial_x (f \partial_p \varepsilon \mu), g)_{\Omega_c} + \left( \left( \frac{\partial_x (p^2 f \mu)}{p^2} + \frac{\partial_x (f (1 - \mu^2))}{p} \right) \right) q \partial_x \Phi(x, t), g \right)_{\Omega_c} \\
= (Q(f), g)_{\Omega_c},
\]

where \(\Omega = X \times K\). More specifically, we have that (assuming \(\partial_\mu \Phi = 0\))

\[
\int_{\Omega_c} Q(f) g p^2 dp \, dx = \partial_t \int_{\Omega_c} f g p^2 \, dp \, dx + \int_{\Omega_c} \partial_x (f \partial_p \varepsilon \mu) g p^2 \, dp \, dx \\
+ \int_{\Omega_c} \partial_p (p^2 f \mu) q \partial_x \Phi(x, t) \, g p \, dp \, dx + \int_{\Omega_c} \partial_\mu (f (1 - \mu^2)) q \partial_x \Phi(x, t) \, g \, p \, dp \, dx.
\]
2.2.1 The Cut-off-domain

Let’s start setting some notational components associated to the computational domain for the proposed DG scheme. The computational domain, in 1D in $x$-space and 2D in $\vec{p}$-space, is denoted by

$$\Omega_C := L_x \times \Omega_{\vec{p},t} = [0, L_x] \times [0, p_{\text{max}}] \times [-1, 1]_{\vec{p}}.$$  \hfill (2.7)

Thus, the domain in $\vec{p}$-momentum space needs to be cut-off and redefined by domain $\Omega_{\vec{p},t}$ in momentum space, as it depends on the electric field $E(x,t) = -\nabla \Phi(x,t)$ according to the mean-field BP flow in (2.3). The particular choice of diameter constant $p_{\text{max}}$ is chosen by taking

$$p_{\text{max}}^E = m^* L/T + T q E^*,$$  \hfill (2.8)

where $T$ is the time our physical evolution problem lasts, $m^*$ is the reduced mass of the electron, and $E_n(x) := E(x,t_n) = \int_0^x f_{\text{E}}(x,p,\mu) p^2 dp d\mu dx - C$, with $C$ a constant, where we denoted $f_{\text{E}}(x,p,\mu) := f(x,p,\mu,t_n)$ to be the pdf at the given time $t_n$ to be the discrete time evaluated in the RK method. Thus, $E^* \leq \int_{\Omega_{\vec{p},t}} f_{\text{E}}(x,p,\mu) p^2 dp d\mu dx+C$. In particular, this cut-off domain correction in momentum space allows the computational solution $f_h(x,p,\mu)$ of the Boltzmann flow along the Hamiltonian characteristic field, defined by $(x - v(p,\mu)t, p + qE_n(x,t_n), \mu)$, to keep its initial support transported by the characteristic curves inside the computational domain $\Omega_{\vec{p},t}$. This assumption on the cut-off domain depends on the magnitude of the electric field as well as on the support of the initial data. Under these conditions $\int f(x,p,\mu)|_{\partial\Omega_{\vec{p},t}} = 0$. We point out that using periodic boundary conditions in $x$-space set on $\Omega_x$ results in a uniform in time $E^*$, since the solution associated to the Vlasov - Poisson system in one dimension in $x$-space yields global uniformly bounded electric fields. That means the set $\Omega_{\vec{p},t}$ does not need to be updated with the time step evolution, regarding the transport process.

2.2.2 The DG-FEM scheme formulation for the transformed Boltzmann equation in the $(x,p,\mu)$-space computational domain.

The discretazation of the computational domain $\Omega_C$, defined in (2.7), is meshed as follows. Set

$$\Omega_C := \bigcup_{i,k,m} \Omega_{ikm}, \quad \Omega_{ikm} := X_i \times K_{k,m} = [x_{i_1}, x_{i_2}] \times [p_{k_1}, p_{k_2}] \times [\mu_{m_1}, \mu_{m_2}],$$

with the classical notation for mesh midpoint characterization

$$x_{i2} = x_{i1}/2, \quad p_{k2} = p_{k1}+1/2, \quad \mu_{m2} = \mu_{m1} \pm 1/2.$$  \hfill (2.9)

Denote by $T_h^x = I_x$ and $T_h^{p,m} = K_{p,m}$ the regular partitions of $\Omega_x$ and $\Omega_{(p,\mu)}$, respectively, with

$$T_h^x = \bigcup_{i=1}^{N_x} I_i \cup \bigcup_{1 \leq i \leq N_x} [x_{i_1}, x_{i_2}], \quad \text{and} \quad T_h^{p,m} = \bigcup_{k,m=1}^{N_p \times N_p} K_{k,m} = \bigcup_{k,m=1}^{N_p \times N_p} [p_{k_1}, p_{k_2}] \times [\mu_{m_1}, \mu_{m_2}],$$

with $x_{1/2} = 0, x_{N_x+1/2} = L; p_{1/2} = 0, p_{N_p+1/2} := p_{\text{max}}; \mu_{1/2} = -1, \mu_{N_p+1/2} := 1$, respectively. Then, $T_h = \{E : E = I_x \times K_k \subset \Omega | \forall I_x \subset T_h^x, \forall K_{k,m} \subset T_h^{p,m}\}$ defines a partition of $\Omega$. Denote by $e_x$ and $e_{k,m}$ the set of edges of $T_h^x$ and $T_h^{k,m}$, respectively. Then, the edges of $T_h$ will be $e = \{I_x \times e_k \subset T_h^x, \forall e_k \subset e_{k,m} \} \cup \{I_x \times K_{k,m} : \forall e_x, e_{k,m} \subset e_x \cup e_{k,m} \}$. In addition, $e_x = e_{x_1} \cup e_{x_2}$ with $e_{x_1}$ and $e_{x_2}$ being the interior and boundary edges, respectively (same for the domain of momentum variables). The mesh size is $h := \max(h_x, h_{k,m}) := \max_{e \in T_h^x} \text{diam}(E), \text{with } h_x \equiv \max_{I_x \subset T_h^x} \text{diam}(I_x)$ and $h_{k,m} \equiv \max_{K_{k,m} \in T_h^{k,m}} \text{diam}(K_{k,m})$. Hence, invoking the classical corresponding notation for their respective internal products in the described mesh becomes

$$(f,g)_{ikm} := \int_{ikm} fg p^2 dp d\mu dx.$$  \hfill (2.10)
The finite element space is defined as
\[ V_h^\kappa = \{ \phi_h \in L^2(\Omega_C) : \forall K \in T(\Omega_C), \phi_h|_K \in P^\kappa(K) \}, \]
where \( P^\kappa(K) \) is the set of polynomials of total degree at most \( \kappa \) on the simplex \( K \).

The semi-discrete Discontinuous Galerkin Formulation for our transformed Boltzmann Equation in curvilinear coordinates is to find \( f_h \in V_h^\kappa \) such that \( \forall g_h \in V_h^\kappa \) and \( \forall \Omega_{km} \),
\[
\partial_t \int_{\Omega_{km}} f_h g_h p^2 dp d\mu dx + \int_{\Omega_{km}} (1 - \mu_{m\pm}^2)(-qE f_h)|_{\mu_{m\pm}} g_h|_{\mu_{m\pm}} p dp d\mu dx \\
- \int_{\Omega_{km}} \vartheta_{\pm}(p) f_h \mu \partial_x g_h p^2 dp d\mu dx + \int_{\Omega_{km}} \vartheta_{\pm}(p) f_h \partial_x g_h|_{\mu_{m\pm}} p^2 dp d\mu \\
- \int_{\Omega_{km}} \vartheta_{\pm}(p) f_h(-qE)(x,t) \partial_x g_h p^2 dp d\mu dx + \int_{\Omega_{km}} \vartheta_{\pm}(p) f_h(-qE)(x,t) \partial_x g_h p^2 dp d\mu dx \\
- \int_{\Omega_{km}} (1 - \mu_{m\pm}^2)f_h(-qE)(x,t) \partial_x g_h p^2 dp d\mu dx = \int_{\Omega_{km}} Q(f_h) g_h p^2 dp d\mu dx.
\]

The Numerical Flux used in this scheme is the Upwind Rule, namely
\[
\tilde{f}_{h\mu}|_{\mu_{m\pm}} := \frac{\mu + |\mu|}{2} f_h|_{\mu_{m\pm}} + \frac{\mu - |\mu|}{2} f_h|_{\mu_{m\pm}}, \\
-\tilde{qE\mu}|_{\mu_{m\pm}} := \frac{-qE\mu + |qE\mu|}{2} f_h|_{\mu_{m\pm}} + \frac{-qE\mu - |qE\mu|}{2} f_h|_{\mu_{m\pm}}, \\
-\tilde{qE}|_{\mu_{m\pm}} := \frac{-qE + |qE|}{2} f_h|_{\mu_{m\pm}} + \frac{-qE - |qE|}{2} f_h|_{\mu_{m\pm}}.
\]

### 2.2.3 Stability of DG scheme under entropy norm for Periodic Boundary Conditions

We can prove the stability of the scheme under the entropy norm related to the interior product \( \int_{\Omega_c} f_h g_h e^{H(\tilde{p},\tilde{r})} p^2 dp d\mu dx \), inspired in the strategy of Cheng, Gamba, and Proft [11]. These 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 \( e^{H(\tilde{p},\tilde{r})} = \exp(\varepsilon(\tilde{p}) - q\Phi(\tilde{r},t)) \), which clearly has a Hamiltonian structure generating a divergence free characteristic field for the equations of motion.

Existence and uniqueness as well as regularity of initial-boundary value problems (IBVP) associated to the Vlasov-Boltzmann equation [11, 19] with periodic boundary conditions have been shown by Y. Guo [20, 21] for the non-linear Vlasov-Boltzmann-Poisson-Maxwell system with initial data near a global Maxwellian distribution. It also shows the regularity propagation of the initial behavior; and further, R. Strain [22], calculated almost exponential decay rates to such Maxwellian equilibrium. Additionally, in the particular case of the initial and boundary value problem, N. Ben-Abdallah and M. Tayeb [23] showed existence and uniqueness of solutions to the linear Vlasov-Boltzmann with a continuous in space-time field \( E(x,t) \) and non-negative initial and boundary conditions having the same polynomial decay in \( L^1 \cup L^\infty \) in one space dimension and higher dimensional phase-space (velocity). Such solution preserves the regularity and decay properties of the initial state. While this result uses low regularity of the integrating characteristic field \( E(x,t) \) with nonvanishing gradients, it is hoped that higher order Sobolev regularity may propagate for more regular fields, as well as more regular initial and boundary conditions satisfying at least polynomial decay. However, we are not aware, at this point, whether such result is available. We also mention that in [23] the authors showed the existence of weak solutions to Boltzmann-Poisson for incoming data with polynomial decay in the case of one phase-space dimension.

Hence, whenever the spatial domain is a rectangle, the assumption of periodic boundary data in \( \tilde{x} \)-space is the most suitable condition for stability of the transport flow along divergence free dynamics by means of

\[ 9 \]
entropy methods. Indeed, for \( f_h \in V_h^k \) such that \( \forall g_h \in V_h^k \) and \( \forall \Omega_{ikm} \),

\[
\int_{\Omega_{ikm}} \partial_t f_h g_h e^{H} p^2 dp d\mu dx + \int_{ik} (1-\mu^2_{m \pm}) - qE f_h |_{\mu_{m \pm}} g_h e^{H} |_{\mu_{m \pm}} dp dx
- \int_{ikm} \partial_p e(p) f_h \mu \partial_x (g_h e^{H}) p^2 dp d\mu dx + \int_{km} \partial_p e f_h |_{x \pm} g_h e^{H} |_{x \pm} p^2 dp d\mu \\
- \int_{ikm} p^2 (0 - qE)(x, t) f_h \mu \partial_p (g_h e^{H}) dp dx + \int \partial_p e f_h |_{x \pm} (0 - qE f_h) |_{\mu_{x \pm}} g_h e^{H} |_{\mu_{x \pm}} dp dx \\
- \int_{ikm} (1-\mu^2) f_h (0 - qE)(x, t) \partial_x (g_h e^{H}) p dp d\mu dx = \int_{ikm} Q(f_h) g_h e^{H} p^2 dp d\mu dx, \tag{2.13}
\]

where we are including as a factor the inverse of a Maxwellian along the characteristic flow generated by the Hamiltonian transport field \((\partial_{p'} e(p), q \partial_p \Phi(x, t))\),

\[
e^{H(x,p,t)} = \exp(e(p) - q\Phi(x, t)) = \left(e^{q\Phi(x,t) e^{-\epsilon(p)}}\right)^{-1}, \tag{2.14}
\]

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 some entropy inequalities related to the collision operator. Our collision operator satisfies the dissipative property

\[
\int_{\Omega_{C,\varphi}} Q(f) g d\vec{p} = -\frac{1}{2} \int_{\Omega_{\varphi}} S(\vec{p}' \rightarrow \vec{p}) e^{-\epsilon(p')} \left( \frac{f'}{e^{-H}} - \frac{f}{e^{-H}} \right) (g' - g) d\vec{p}' d\vec{p}, \tag{2.15}
\]

which can be also expressed as (multiplying and dividing by \( e^{-\Phi(x,t)} \))

\[
\int_{\Omega_{C,\varphi}} Q(f) g d\vec{p} = -\frac{1}{2} \int_{\Omega_{\varphi}} S(\vec{p}' \rightarrow \vec{p}) e^{-H'} \left( \frac{f'}{e^{-H'}} - \frac{f}{e^{-H}} \right) (g' - g) d\vec{p}' d\vec{p}. \tag{2.16}
\]

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,

\[
\int_{\Omega_{C,\varphi}} Q(f) \frac{f}{e^{-H}} d\vec{p} = -\frac{1}{2} \int_{\Omega_{\varphi}} S(\vec{p}' \rightarrow \vec{p}) e^{-H'} \left( \frac{f'}{e^{-H'}} - \frac{f}{e^{-H}} \right)^2 d\vec{p}' d\vec{p} \leq 0. \tag{2.17}
\]

So we have found the dissipative entropy inequality

\[
\int_{\Omega_{C,\varphi}} Q(f) fe^{H} p^2 dp d\mu d\varphi = \int_{\Omega_{C,\varphi}} Q(f) \frac{f}{e^{-H}} d\vec{p} \leq 0. \tag{2.18}
\]

As a consequence of this entropy inequality we obtain the following stability theorem of the scheme under an entropy norm.

**Theorem 1.** (Stability under the entropy norm \( \int f_h g_h e^{H} p^2 dp d\mu dx \) for a given periodic potential \( \Phi(x, t) \))

Consider the semi-discrete solution \( f_h \) to the DG formulation in \([2,3]\) for the BP system in momentum curvilinear coordinates. We have then that

\[
0 \geq \int_{\Omega_{c}} f_h \partial_t f_h e^{H(x,p,t)} p^2 dp d\mu dx = \frac{1}{2} \int_{\Omega_{c}} \partial_t f_h^2 e^{H(x,p,t)} p^2 dp d\mu dx. \tag{2.19}
\]

**Proof.** Choosing \( g_h = f_h \) in \([2,3]\), and considering the union of all the cells \( \Omega_{ikm} \), which gives us the whole
domain $\Omega = \Omega_x \times \Omega_{\rho, \mu}$ for integration, we have

$$0 \geq \int_{\Omega} Q(f_h) f_h e^H p^2 dpd\mu dx = \int_{\Omega} \partial_t f_h f_h e^H p^2 dpd\mu dx$$

$$- \int_{\partial \Omega} \partial_p \varepsilon(p) f_h \mu \partial_x (f_h e^H) p^2 dpd\mu dx + \int_{\partial \Omega} \partial_p \varepsilon f_h \mu f_h e^H p^2 dpd\mu$$

$$- \int_{\Omega} p^2 (qE) f_h \mu \partial_p (f_h e^H) dpd\mu dx + \int_{\partial \Omega} p^2 (-q \varepsilon f_h \mu) f_h e^H dpd\mu$$

$$- \int_{\Omega} (1 - \mu^2) f_h (-qE) \partial_p (f_h e^H) p dpd\mu dx + \int_{\partial \Omega} (1 - \mu^2) (-q \varepsilon f_h \mu) f_h e^H p dpd\mu .$$

We can express this in the more compact form

$$0 \geq \int_{\Omega} \partial_t f_h f_h e^H p^2 dpd\mu dx - \int_{\Omega} f_h \beta \cdot \partial(f_h e^H) dpd\mu dx + \int_{\partial \Omega} \hat{n} f_h e^H d\sigma,$$  \hspace{1cm} (2.20)

defining the transport vector

$$\beta = (p^2 \mu \partial_p \varepsilon(p), -qE p^2 \mu, -qEp(1 - \mu^2)).$$  \hspace{1cm} (2.21)

We integrate by parts again the transport integrals, obtaining that

$$\int_{\Omega} f_h \beta \cdot \partial(f_h e^H) dpd\mu dx = - \int_{\Omega} \partial (f_h \beta) f_h e^H dpd\mu dx + \int_{\partial \Omega} f_h \beta \cdot \hat{n} f_h e^H d\sigma$$

$$= - \int_{\Omega} (\beta \cdot \partial f_h) f_h e^H dpd\mu dx + \int_{\partial \Omega} f_h \beta \cdot \hat{n} f_h e^H d\sigma ,$$

but since

$$\beta \cdot \partial(f_h e^H) = \beta \cdot e^H \partial f_h + \beta \cdot f_h e^H \partial H = e^H \beta \cdot \partial f_h,$$  \hspace{1cm} (2.22)

we have then

$$\int_{\Omega} f_h \beta \cdot \partial(f_h e^H) dpd\mu dx = \int_{\Omega} f_h e^H \beta \cdot \partial f_h dpd\mu dx = \frac{\int_{\partial \Omega} f_h \beta \cdot \hat{n} f_h e^H d\sigma}{2}.$$  \hspace{1cm} (2.23)

We can express our entropy inequality then as

$$0 \geq \int_{\Omega} \partial_t f_h f_h e^H p^2 dpd\mu dx - \frac{1}{2} \int_{\partial \Omega} f_h \beta \cdot \hat{n} f_h e^H d\sigma + \int_{\partial \Omega} \hat{n} f_h e^H d\sigma ,$$  \hspace{1cm} (2.24)

remembering that we are integrating over the whole domain (the union of all cells defining our mesh). We distinguish between 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 rule \textbf{(2.12)} is such that $f_h = f_h^-$, we have that the solution value 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 solution value inside the cell close to that boundary is $f_h^+$. We have

$$0 \geq \int_{\Omega} \partial_t f_h f_h e^H p^2 dpd\mu dx - \frac{1}{2} \int_{\partial \Omega} f_h \beta \cdot \hat{n} f_h e^H d\sigma + \int_{\partial \Omega} f_h^+ \beta \cdot \hat{n} f_h e^H d\sigma$$

and

$$0 \geq \int_{\partial \Omega} \partial_k f_h f_h e^H p^2 dpd\mu dx - \frac{1}{2} \int_{\beta \cdot \hat{n} \geq 0} f_h^+ \beta \cdot \hat{n} f_h^- e^H d\sigma + \int_{\beta \cdot \hat{n} \leq 0} f_h^- \beta \cdot \hat{n} f_h^+ e^H d\sigma$$

$$+ \frac{1}{2} \int_{\beta \cdot \hat{n} \geq 0} f_h^+ \beta \cdot \hat{n} f_h^+ e^H d\sigma - \int_{\beta \cdot \hat{n} \leq 0} f_h^- \beta \cdot \hat{n} f_h^+ e^H d\sigma .$$
The notation $e_h$ is generic in finite elements, counting boundaries twice given that it indexes elements, so it must be balanced by a factor of 1/2. We have

\[
0 \geq \int_{\Omega_C} \partial_t f_h f_h e^H p^2 dpd\mu dx + \frac{1}{2} \left( -\frac{1}{2} \int_{\Omega_C} f_h^- |\beta \cdot \hat{n}| f_h^- e^H d\sigma + \int_{\Omega_C} f_h^- |\beta \cdot \hat{n}| f_h^- e^H d\sigma + \frac{1}{2} \int_{\Omega_C} f_h^+ |\beta \cdot \hat{n}| f_h^+ e^H d\sigma \right);
\]

\[
0 \geq \int_{\Omega_C} \partial_t f_h f_h e^H p^2 dpd\mu dx + \frac{1}{4} \int_{\Omega_C} (f_h^+ - f_h^-)^2 |\beta \cdot \hat{n}| e^H d\sigma.
\]

Since the second term is non-negative, we conclude that

\[
0 \geq -\frac{1}{4} \int_{\Omega_C} (f_h^+ - f_h^-)^2 |\beta \cdot \hat{n}| e^H d\sigma \geq \frac{1}{2} \int_{\Omega_C} \partial_t f_h^2 e^{H(x,p,t)} p^2 dpd\mu dx , \quad (2.25)
\]

and it is in this sense that the numerical solution has stability with respect to the considered entropy norm.

In addition, the following result holds.

**Corollary 2. (Stability under the entropy norm for a time independent Hamiltonian):** If $\Phi = \Phi(x)$, so $\partial_t H = 0$, the stability under our entropy norm gives us that for $t \geq 0$

\[
||f_h||_{L^2_{x,p}}^2 (t) = \int_{\Omega_C} f_h^2(x,p,\mu,t)e^{H(x,p)} p^2 dpd\mu dx \leq ||f_h||_{L^2_{x,p}}^2 (0) . \quad (2.26)
\]

**Proof.** The corollary follows from the fact that, since $\partial_t H = -\varrho \partial_t \Phi = 0$, we have

\[
0 \geq \int_{\Omega_C} \partial_t \left( f_h^2 e^{H(x,p)} \right) p^2 dpd\mu dx = \frac{d}{dt} \int_{\Omega_C} f_h^2(x,p,\mu,t)e^{H(x,p)} p^2 dpd\mu dx . \quad (2.27)
\]

Since the entropy norm decreases over time, our result follows immediately.

We perform further analysis of these discrete entropy inequalities applied to the Boltzmann - Poisson system \([1,11,5]\) for self consistent mean field charged transport, in the one space dimensional case, say $x \in [0,L]$, under the assumption for the electrostatic potential $\Phi(x)$ solving the Poisson equation that it satisfies periodic boundary conditions as much as the probability density $f(x,p,t)$. These boundary conditions on the electrostatic potential can be viewed as having neutral charges in a neighborhood containing the endpoints $\{0,L\}$ and zero potential bias, that is, the corresponding Poisson boundary value problem for the potential is

\[
-\partial_x^2 \Phi(x,t) = \frac{\varrho}{\epsilon} [N(x) - n_h(x,t)] ,
\]

\[
\Phi(0,t) - \Phi(L,t), \quad \partial_x \Phi(0,t) = \partial_x \Phi(L), \quad \forall \ t > 0 . \quad (2.28)
\]

Indeed, these boundary conditions for the homogeneous problem imply that solutions are determined up to a constant. Thus, in order to obtain existence of solutions, the Fredholm Alternative property indicates that existence holds provided the compatibility condition $\int_0^L [N(x') - n_h(x',t)] dx' = 0$, which yields neutral total charges for all times $t$. In addition, to obtain uniqueness, one needs to prescribe an extra condition on the $x$-space average of the solution $\int_0^L \Phi(x,t) dx$.

Therefore the following Theorem also holds for the semi-discrete Vlasov - Boltzmann - Poisson system in one $x$-space dimension, with spatial periodic boundary conditions, whose numerical solutions preserved the neutral charges for all times, where we take a compatible discretization of the periodic Poisson problem that is mass preserving as performed in \([5]\), and so preserves the above mentioned charge neutrality condition for all time.
**Theorem 3.** (Stability under the entropy norm for a time dependent Hamiltonian in the mean field limit): If \( \Phi = \Phi(x, t) \), solution of the boundary value problem (2.28) so the corresponding Hamiltonian is \( H(x, p, t) = \varepsilon(p) - q\Phi(x, t) \), then

\[
||f_h||^2_{L^2_{x,p}^2}(t) = \int_{\Omega_G} f_h^2(x, p, \mu, t)e^{H(x, p, t)}\, p^2\, dp d\mu dx \leq ||f_h||^2_{L^2_{x,p}^2}(0). \tag{2.29}
\]

**Proof.** Because of the divergence free structure of the Hamiltonian \( H(x, p, t) = \varepsilon(p) - q\Phi(x, t) \) for every \( t > 0 \), all estimates of Theorem 4 apply. In particular, starting from estimate (2.40), we perform the time differentiation with respect to \( t \) as we have assumed that the doping \( B_\varepsilon(x, t) \) is independent of time \( t \), which can be expressed more compactly as

\[
\partial_t \Phi(x, t) = \frac{q}{\varepsilon} \left[ \int_0^L \partial_t \rho_h(t, x')(L - x') dx' - \frac{x}{L} \int_0^L \partial_t \rho_h(t, x')(L - x') dx' \right]. \tag{2.30}
\]

Therefore, replacing this exact formula for \( \partial_t \Phi(x, t) \) into the inequality (2.30) yields a mean field, non-local, discrete entropy inequality.
\[
0 \geq \partial_t \int_{\Omega_c} f_h^c e^H p^2 dpd\mu dx - \frac{q}{\epsilon} \int_{\Omega_c} f_h^c e^H \left[ \int_0^L \partial_t \rho_h(t, x')(L - x') \left( \frac{x'}{2L} - \frac{x}{L} \right) dx' \right.
\]
\[
+ \int_0^x \partial_x \rho_h(t, x')(x - x') dx' \left. \right] p^2 dpd\mu dx.
\]

To this end, one can substitute the partial time derivative of the density by the right hand side of a conservation equation that can be derived simply by integration of the Boltzmann Eq. over the momentum domain. Therefore, since in 1D we have
\[
\partial_t \rho_h(x, t) + \partial_x J_h(x, t) = 0,
\]
with \(J_h(x, t) = \int_{\Omega_p} v(p) f_h(x, p, t) dp\), this yields
\[
0 \geq \partial_t \int_{\Omega_c} f_h^c e^H p^2 dpd\mu dx + \frac{q}{\epsilon} \int_{\Omega_c} f_h^c e^H \left[ \int_0^L \partial_x J(t, x')(L - x') \left( \frac{x'}{2L} - \frac{x}{L} \right) dx' \right.
\]
\[
+ \int_0^x \partial_x J_h(t, x')(x - x') dx' \left. \right] p^2 dpd\mu dx.
\]

We proceed with an integration by parts to simplify our second term. So
\[
0 \geq \partial_t \int_{\Omega_c} f_h^c e^H p^2 dpd\mu dx + \frac{q}{\epsilon} \int_{\Omega_c} f_h^c e^H \left[ J_h(t, 0) x - \int_0^L J_h(t, x') \frac{x - x' + L/2}{L} dx' \right.
\]
\[
- J_h(t, 0) x + \int_0^x J_h(t, x') dx' \left. \right] p^2 dpd\mu dx.
\]

This last term reduces to
\[
0 \geq \partial_t \int_{\Omega_c} f_h^c e^H p^2 dpd\mu dx + \frac{q}{\epsilon} \int_{\Omega_c} f_h^c e^H \left[ \int_0^x J_h(t, x') dx' \right.
\]
\[
- \int_0^L J_h(t, x') \left( \frac{x - x'}{L} + \frac{1}{2} \right) dx' \left. \right] p^2 dpd\mu dx,
\]
which can be written, equivalently, as
\[
0 \geq \partial_t \int_{\Omega_c} f_h^c e^H p^2 dpd\mu dx + \frac{q}{\epsilon} \int_{\Omega_c} f_h^c e^H \left[ \int_0^x J_h(t, x') \left( \frac{1}{2} - \frac{x - x'}{L} \right) dx' \right.
\]
\[
- \int_x^L J_h(t, x') \left( \frac{1}{2} + \frac{x - x'}{L} \right) dx' \left. \right] p^2 dpd\mu dx.
\]

The asymptotic and regular behaviour of our Boltzmann - Poisson problem as time approaches infinity in the spatial domain given by the interval \([0, L]\) is well known [23, 20, 21, 22], in particular convergence to a stationary state given by the balance of transport due to collisions, and so the corresponding current \(J(x, t)\) stabilizes over the whole interval domain to a constant value, i.e. \(\lim_{t \to \infty} J_h(x, t) = J_{0_h}\). Hence, by continuity, for any given \(\delta > 0\), there exists a finite time \(t_\delta > 0\) such that \(|J_h(x, t) - J_0| < \delta\) \(\forall x \in [0, L], \forall t > t_\delta\). Therefore, since

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\[ 0 \geq \partial_t \int_{\Omega_c} f_h^2 e^H p^2 \, dpd\mu dx + \frac{q}{\epsilon} \int_{\Omega_c} f_h^2 e^H \left[ \frac{J_h}{2L} \left[ (L/2 - x + x')^2_{0} + (x' - x - L/2)^2_{0} \right] \right. \\
\left. + \int_{0}^{x} (J_h - J_{0_h}) \left( \frac{1}{2} - \frac{x' - x}{L} \right) dx' + \int_{x}^{L} (J_h - J_{0_h}) \left( \frac{x' - x - L}{2} \right) dx' \right] p^2 dpd\mu dx, \]

and \( (L/2 - x + x')^2_{0} + (x' - x - L/2)^2_{0} = 0 \), our equation reduces to

\[ 0 \geq \partial_t \int_{\Omega_c} f_h^2 e^H p^2 \, dpd\mu dx + \frac{q}{\epsilon} \int_{\Omega_c} f_h^2 e^H \left[ \int_{0}^{x} (J_h - J_{0_h}) \left( \frac{1}{2} - \frac{x' - x}{L} \right) dx' + \int_{x}^{L} (J_h - J_{0_h}) \left( \frac{x' - x - L}{2} \right) dx' \right] p^2 dpd\mu dx. \]

Using our argument of convergence to a constant current as time goes to infinity,

\[ \left| \int_{\Omega_c} f_h^2 e^H \left[ \int_{0}^{x} (J_h - J_{0_h}) \left( \frac{1}{2} - \frac{x' - x}{L} \right) dx' + \int_{x}^{L} (J_h - J_{0_h}) \left( \frac{x' - x - L}{2} \right) dx' \right] p^2 dpd\mu dx \right| \]

\[ \leq \int_{\Omega_c} f_h^2 e^H \delta \left[ x \left\| \frac{1}{2} - \frac{x - x'}{L} \right\|_{\infty,[0,x]} + (L - x) \left\| \frac{x' - x}{L} - \frac{1}{2} \right\|_{\infty,[x,L]} \right] p^2 dpd\mu dx \]

\[ = \int_{\Omega_c} f_h^2 e^H \delta \left[ x \left( \frac{1}{2} + (L - x) \frac{1}{2} \right) \right] p^2 dpd\mu dx = \frac{\delta L}{2} \left| \int_{\Omega_c} f_h^2 e^H p^2 dpd\mu dx \right|. \]

Finally, choosing \( \delta > 0 \) such that for \( t_\delta > 0 \) we have

\[ \frac{\delta L}{2} \left| \int_{\Omega_c} f_h^2 e^H p^2 dpd\mu dx \right| < \frac{1}{2} \left| \partial_t \int_{\Omega_c} f_h^2 e^H p^2 dpd\mu dx \right|, \]

then

\[ 0 \geq \frac{d}{dt} \int_{\Omega_c} f_h^2 e^H p^2 dpd\mu dx \quad \forall t > t_\delta. \tag{2.34} \]

In particular, inequality (2.29) holds and Theorem 3 statement holds.

### 2.3 2DX-3DK Problem: DG scheme and Stability under an entropy norm for Periodic and Reflective Boundary Conditions

We consider now a 2D problem in position space (which requires a 3D dimensionality in momentum), using as momentum coordinates a normalized Kane energy band \( \omega \), a normalized polar component \( \mu \), and the azimuthal angle \( \varphi \) (the same as in [H]). This problem has the following semi-discrete DG formulation using an entropy norm: to find a function \( f_h \) such that for all \( g_h \) it holds that

\[ \int_{\Omega_c} Q(f_h) g_h e^H s(\omega) d\sigma d\bar{x} = \int_{\Omega_c} (\partial_t f_h g_h e^H s(\omega) - f_h \beta \cdot \partial(t g_h e^H)) d\sigma d\bar{x} + \int_{\partial\Omega_c} \hat{q} h \cdot \hat{n} g_h e^H d\sigma, \]
We integrate by parts again the transport integrals, obtaining

\[
\begin{align*}
\beta &= (\beta_1, \beta_2, \beta_3, \beta_4, \beta_5)(x, y, \omega, \mu, \varphi), \\
(\beta_1, \beta_2) &= c_x w(1 + \alpha K w)(\mu, \sqrt{1 - \mu^2} \cos \varphi), \\
\beta_3 &= -c_k 2 w(1 + \alpha K w) \left[ \mu E_x + \sqrt{1 - \mu^2} \cos \varphi E_y \right], \\
\beta_4 &= -c_k \sqrt{1 - \mu^2}(1 + 2 \alpha K w) \left[ \sqrt{1 - \mu^2} E_x - \mu \cos \varphi E_y \right], \\
\beta_5 &= -c_k - (1 + 2 \alpha K w) E_y \sin \varphi, \\
\frac{-\partial \cdot \beta / c_h}{1 + 2 \alpha K w} &= 2 \left( \mu E_x + \sqrt{1 - \mu^2} \cos \varphi E_y \right), \\
&= -2 \mu E_x - \left( \sqrt{1 - \mu^2} - \frac{\mu^2}{\sqrt{1 - \mu^2}} \right) \cos \varphi E_y - \frac{E_y \cos \varphi}{\sqrt{1 - \mu^2}},
\end{align*}
\]

which is zero since

\[
2 \left( \mu E_x + \sqrt{1 - \mu^2} \cos \varphi E_y \right) - 2 \mu E_x
\]

\[
= \left( \sqrt{1 - \mu^2} - \frac{\mu^2}{\sqrt{1 - \mu^2}} \right) \cos \varphi E_y - \frac{E_y \cos \varphi}{\sqrt{1 - \mu^2}}
\]

\[
= \sqrt{1 - \mu^2} \cos \varphi E_y + \frac{\mu^2}{\sqrt{1 - \mu^2}} \cos \varphi E_y - \frac{E_y \cos \varphi}{\sqrt{1 - \mu^2}}
\]

\[
= \frac{\cos \varphi E_y}{\sqrt{1 - \mu^2}} (1 - \mu^2 - 1) = 0.
\]

As we know, \( \partial \cdot \beta = 0 \) and \( \beta \cdot \partial H = 0 \). We state now our result regarding the stability under an entropy norm for this problem under periodic and specular reflection boundary conditions.

**Theorem 4.** (Stability under the entropy norm \( \int f_h g_h e^H s(\omega) d\omega d\bar{x} \) for a given potential \( \Phi(x, t) \)): Consider the semi-discrete solution \( f_h \) to the DG formulation for the BP system in radial energy-angular coordinates (assuming a Kane band model) under periodic and specular reflection boundary conditions. We have then

\[
0 \geq \int_{\Omega_c} f_h \partial_t f_h e^H s(\omega) d\omega d\bar{x} = \frac{1}{2} \int_{\Omega_c} \partial_t f_h^2 e^H s(\omega) d\omega d\bar{x}.
\]

**Proof.** Choosing \( g_h = f_h \) in the entropy inequality for the Boltzmann equation, and considering the union of all the cells (now \( \Omega_{x,y} \)), which gives us the whole domain \( \Omega = \Omega_{x,y} \times \Omega_{\omega,\mu,\varphi} \) for integration, we have

\[
0 \geq \int_{\Omega_c} Q(f_h) f_h e^H s(\omega) d\omega d\bar{x} = \int_{\Omega_c} \left( \partial_t f_h f_h e^H s(\omega) - f_h \beta \cdot \partial (f_h e^H) \right) d\omega d\bar{x} + \int_{\partial \Omega_c} \hat{n} f_h \beta \cdot \hat{n} f_h e^H d\sigma.
\]

We integrate by parts again the transport integrals, obtaining

\[
\int_{\Omega_c} f_h \beta \cdot \partial (f_h e^H) d\omega d\bar{x} = - \int_{\Omega_c} \partial \beta f_h e^H d\omega d\bar{x} + \int_{\partial \Omega_c} f_h \beta \cdot \hat{n} f_h e^H d\sigma
\]

\[
= - \int_{\Omega_c} \left( \beta \cdot \partial f_h \right) f_h e^H d\omega d\bar{x} + \int_{\partial \Omega_c} f_h \beta \cdot \hat{n} f_h e^H d\sigma,
\]

where the stability in the last line is proved.

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but since
\[
\beta \cdot \partial (f_h e^H) = \beta \cdot e^H \partial f_h + \beta \cdot f_h e^H \partial H = e^H \beta \cdot \partial f_h,
\]
we have then
\[
\int_{\Omega_C} f_h \beta \cdot \partial (f_h e^H) \, d\bar{x} d\tilde{\bar{x}} = \int_{\Omega_C} (\beta \cdot \partial f_h) f_h e^H \, d\bar{x} d\tilde{\bar{x}} = \frac{1}{2} \int_{\partial \Omega_C} f_h \beta \cdot \hat{n} f_h e^H \, d\sigma.
\]

We can express our entropy inequality then as
\[
0 \geq \int_{\Omega_C} \partial_t f_h f_h e^H s(\omega) \, d\bar{x} d\tilde{\bar{x}} - \frac{1}{2} \int_{\partial \Omega_C} f_h \beta \cdot \hat{n} f_h e^H \, d\sigma + \int_{\partial \Omega} \tilde{f}_h \beta \cdot \hat{n} f_h e^H \, d\sigma,
\]
(2.37)

remembering that we are integrating over the whole domain by considering the union of all the cells defining our mesh. We will distinguish between the internal edges and the external ones where periodic and specular reflection boundary conditions are applied, that is, \( \partial \Omega = IE \cup PB \cup RB \), so
\[
0 \geq \int_{\Omega_C} \partial_t f_h f_h e^H s(\omega) \, d\bar{x} d\tilde{\bar{x}} - \frac{1}{2} \int_{IE \cup PB} f_h \beta \cdot \hat{n} f_h e^H \, d\sigma + \int_{RB} \tilde{f}_h \beta \cdot \hat{n} f_h e^H \, d\sigma,
\]
The integrals with a factor of 1/2 vanish each other due to the specular reflection (after having done a transformation of coordinates from the inflow boundary to the outflow boundary), the remaining term being
\[
f(\bar{x}', \beta', t)|_- = f(\bar{x}, \beta, t)|_+.
\]

2.3.1 Specular Reflection Boundaries

We divide the reflection boundaries in inflow and outflow regions (remembering that we are dealing with hyper-surfaces)
\[
-\frac{1}{2} \int_{RB} f_h \beta \cdot \hat{n} f_h e^H \, d\sigma + \int_{RB} \tilde{f}_h \beta \cdot \hat{n} f_h e^H \, d\sigma = -\frac{1}{2} \int_{\beta \cdot \hat{n} > 0} f_h \beta \cdot \hat{n} f_h e^H \, d\sigma + \frac{1}{2} \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h \beta \cdot \hat{n} f_h e^H \, d\sigma,
\]
and remembering also that the specular reflection boundary condition relates the inflow and the outflow boundary by
\[
f(\bar{x}, \beta, t)|_- = f(\bar{x}', \beta', t)|_+.
\]

The integrals with a factor of 1/2 vanish each other due to the specular reflection (after having done a transformation of coordinates from the inflow boundary to the outflow boundary), the remaining term being
\[
\int_{\beta \cdot \hat{n} > 0} \tilde{f}_h \beta \cdot \hat{n} f_h e^H \, d\sigma - \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h \beta \cdot \hat{n} f_h e^H \, d\sigma = \int_{\beta \cdot \hat{n} > 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma - \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma =
\]
\[
\int_{\beta \cdot \hat{n} > 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma - \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma =
\]
\[
\int_{\beta \cdot \hat{n} > 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma - \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma =
\]
\[
\int_{\beta \cdot \hat{n} > 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma - \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma =
\]
\[
\int_{\beta \cdot \hat{n} > 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma - \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma =
\]
\[
\int_{\beta \cdot \hat{n} > 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma - \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma =
\]
\[
\int_{\beta \cdot \hat{n} > 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma - \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma =
\]
\[
\int_{\beta \cdot \hat{n} > 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma - \int_{\beta \cdot \hat{n} < 0} \tilde{f}_h |\beta \cdot \hat{n}| f_h e^H \, d\sigma =
\]
2.3.2 Internal Edges and Periodic Boundaries

Both internal edges and periodic boundaries are characterized by the fact that each edge has a pairing with another unique edge for which the conditions $\beta_{1} = -\beta_{2}$ and $\beta_{1} = \beta_{2}$ hold, so the idea behind these calculations is to recognize and consider jointly these pairs.

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 $f_{\hat{n}}$ is non-negative, we conclude therefore that $f_{\hat{n}} \geq 0$ and the ones for which $\beta \cdot \hat{n} \leq 0$ the value of the solution inside the cell close to that boundary is $f_{\hat{n}} = 0$. Then, it follows

\[ 0 \geq \int_{\Omega_{c}} f_{h} e^{\hat{H}} s(\omega) \partial_{t} f_{h} d\tilde{\omega} d\tilde{x} - \frac{1}{2} \int_{\Omega_{c}} f_{h} \beta \cdot \hat{n} f_{h} e^{\hat{H}} d\sigma - \int_{\partial \Omega_{c}} f_{h} \beta \cdot \hat{n} f_{h} e^{\hat{H}} d\sigma, \]

by using the upwind rule as numerical flux (2.12), denoting $z = (\tilde{x}, \tilde{p})$,

\[ \hat{f}_{h} = \lim_{\delta \to 0^{+}} f_{h}(z - \delta \beta(z)). \]

Thus, using a notation $e_{h}$ indexing each element (which counts twice element boundaries, and due to this allowed redundancy, is balanced by a factor of 1/2), we have

\[ 0 \geq \int_{\Omega_{c}} \partial_{t} f_{h} f_{h} e^{\hat{H}} s(\omega) d\tilde{\omega} d\tilde{x} + \frac{1}{2} \left( \int_{e_{h}} f_{h} \beta \cdot \hat{n} f_{h} e^{\hat{H}} d\sigma - \int_{e_{h}} f_{h} \beta \cdot \hat{n} f_{h} e^{\hat{H}} d\sigma \right), \]

\[ 0 \geq \int_{\Omega_{c}} \partial_{t} f_{h} f_{h} e^{\hat{H}} s(\omega) d\tilde{\omega} d\tilde{x} + \frac{1}{2} \left( \int_{e_{h}} f_{h} \beta \cdot \hat{n} f_{h} e^{\hat{H}} d\sigma - \int_{e_{h}} f_{h} \beta \cdot \hat{n} f_{h} e^{\hat{H}} d\sigma \right), \]

\[ 0 \geq \int_{\Omega_{c}} \partial_{t} f_{h} f_{h} e^{\hat{H}} s(\omega) d\tilde{\omega} d\tilde{x} + \frac{1}{4} \left( \int_{e_{h}} f_{h} f_{h} \beta \cdot \hat{n} e^{\hat{H}} d\sigma - 2 \int_{e_{h}} f_{h} f_{h} \beta \cdot \hat{n} e^{\hat{H}} d\sigma + \int_{e_{h}} f_{h} f_{h} \beta \cdot \hat{n} e^{\hat{H}} d\sigma \right), \]

Since the second term is non-negative, we conclude therefore that

\[ 0 \geq -\frac{1}{4} \int_{e_{h}} (f_{h} - f_{h})^{2} \beta \cdot \hat{n} e^{\hat{H}} d\sigma \geq \frac{1}{2} \int_{\Omega_{c}} \partial_{t} f_{h}^{2} e^{H(\xi, \eta, t)} s(\omega) d\tilde{\omega} d\tilde{x}, \quad (2.39) \]
and it is in this sense that the numerical solution has stability with respect to the entropy norm under consideration, namely

\[
\frac{1}{2} \int_{\Omega_c} \partial_t f_h^c e^{H(x,p,t)} s(\omega) d\omega d\vec{x} \leq \frac{1}{2} \int_{\Omega_c} \partial_t f_h^c(x,t,0) e^{H(x,p,0)} s(\omega) d\omega d\vec{x}.
\]

(2.40)

3 Error estimates for semi-discrete DG scheme with curvilinear momentum coordinates

We state in this section our main results regarding error estimation for our DG scheme in curvilinear momentum coordinates at the semi-discrete stage. We present in detail the proofs of those results in an Appendix at the end of this document.

**Theorem 5.** \(L^2\) error estimate: Consider the semi-discrete DG solution \(f_h\) to the linear Boltzmann equation (under cut-off and inflow BC)

\[
\left( \partial_t f_h, g_h \right) _{\Omega_h} + \mathcal{A}(f_h, g_h) = \mathcal{L}(g_h),
\]

\[
\left( \partial_t f_h, g_h \right) _{\Omega_h} = \sum_{ikm} \int_{ikm} \partial_t f_h g_h e^{H} s(w) d\omega d\vec{x}, \quad s(w) = p^2, \quad \vec{w} = (p, \mu),
\]

\[
\mathcal{A}(f_h, g_h) = - \sum_{ikm} \int_{ikm} \partial_p \varepsilon(p) f_h \mu \partial_\mu (g_h e^H) p^2 dpd\mu dx + \sum_{km} \int_{km} \partial_p \varepsilon f_h \mu \partial (g_h e^H) \mu \mu dx
\]

- \[
- \sum_{ikm} \int_{ikm} p^2 (-qE)(x,t) f_h \mu \partial_p (g_h e^H) dpd\mu dx + \sum_{n} \int_{n} (1 - \mu^2)(-qE f_h) \mu dx
\]

- \[
- \sum_{ikm} \int_{ikm} \mathcal{Q}(f_h) g_h e^H s(w) d\omega d\vec{x},
\]

where the primed sums for the boundary integrals indicate that the terms related to the cut-off and inflow boundaries are excluded, and finally,

\[
\mathcal{L}(g_h) = - \langle f^{in}, g_h \beta \cdot \hat{n} \rangle _{\Gamma}.
\]

denoting a surface integral over the inflow boundary. We have

\[
||f_h(t, \cdot, \cdot) - f(t, \cdot, \cdot)||_{L^2(\Omega_D)} \leq C \sqrt{t} e^{Cht} h^{k+1/2} ||f||_{L^\infty([0,t], H^{k+1}(\Omega_D))},
\]

with \(C = C(diam(\Omega_D), ||\beta||_{W^{1,\infty}(\Omega_D)})\) not depending on \(h\) or \(t\).

We also have the following result.

**Theorem 6.** If \(f_h\) is the semidiscrete DG solution to our Boltzmann equation with a linear collision operator in the semiconductor problem, then

\[
||f_h(t, \cdot, \cdot) - M||_{L^\infty([0,t], H^{k+1}(\Omega_D))} \leq C \sqrt{t} \exp(Cht) h^{k+1/2} ||f||_{L^\infty([0,t], H^{k+1}(\Omega_D))} + 3 \exp(-M) ||f_0 - M||_{B^2(\mathbb{R}^s)}
\]

with the constant \(C = C(diam(\Omega_D), ||\beta||_{W^{1,\infty}(\Omega_D)})\).
4 Conclusions

The work presented here relates to the development of entropy stable and positivity preserving DG schemes for BP models of collisional electron transport in semiconductors. Due to the physics of energy transitions 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 two previous BP models in different coordinate systems used in in [4] and [6] as particular cases. We consider first 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 choices in previous works in the literature, because its DG formulation gives simpler integrals involving just piecewise polynomial functions for both transport and collision terms, which is convenient for Gaussian quadrature. We have been able to prove the full stability of the semi-discrete DG scheme formulated under an entropy norm and the decay of this norm over time for a 3D plus time problem (1D in position and 2D in momentum), assuming periodic boundary conditions for simplicity. This highlights the importance of the dissipative properties of our collisional operator given by its entropy inequalities. The entropy norm depends on the full time dependent Hamiltonian rather than just the Maxwellian associated solely to the kinetic energy. We prove another stability result for a 5D plus time problem (2D in position, 3D in momentum) considering in this case not only periodic but also specular reflection boundary conditions, where the integral associated to each reflecting boundary vanishes by itself due to specularity. Regarding positivity preserving DG schemes, using the strategy in [9], [10], [11], we treat the collision operator as a source term, and find convex combinations of the transport and collision terms which guarantee the preservation 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 by applying the limiters in [9, 10] that preserve the cell average modifying the slope of the piecewise linear solutions to make the function non-negative.

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Appendix 1

We present in this appendix the detailed proofs of our statements in Section 3.

Theorem 7. \( L^2 \) error estimate: Consider the semi-discrete DG solution \( f_h \) to the linear Boltzmann equation (under cut-off and inflow BC)

\[
(\partial_t f_h, g_h)_{\tau_n} + A(f_h, g_h) = \mathcal{L}(g_h),
\]

\[
(\partial_t f_h, g_h)_{\tau_n} = \sum_{ikm} \int_{ikm} \partial_t f_h g_h e^H s(w) d\vec{w} d\vec{x}, \quad s(w) = p^2, \quad \vec{w} = (p, \mu),
\]

\[
A(f_h, g_h) = - \sum_{ikm} \int_{ikm} \partial_\vec{p} \varepsilon(p) f_h \mu \partial_x (g_h e^H) p^2 dpd\mu dx \pm \sum_{ikm} \int_{ikm} \partial_\vec{p} \varepsilon f_h^\perp |_{x^\perp} g_h e^H |_{x^\perp} p^2 dpd\mu
\]

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\[- \sum_{ikm} \int_{\Omega} p^2 (-qE)(x, t) f_{ikm} \partial_p (g_{h} e^H) d\mu dx \pm \sum_{im} \int_{\Omega} p^2 \pm (-qE h_{ikm} \mu) |p_{h+} g_{h} e^H|_{p_{h+}} \mu \int_{\mu} dx \]

\[- \sum_{ikm} \int_{\Omega} (1 - \mu^2) f_{ikm} (-qE)(x, t) \partial_p (g_{h} e^H) p \mu d\mu dx \pm \sum_{ik} \int_{\Omega} (1 - \mu^2) (-qE f_{ikm}) \mu |p_{h+} g_{h} e^H|_{p_{h+}} p d\mu dx \]

\[- \sum_{ikm} \int_{\Omega_c} Q(f_{ikm}) g_{h} e^H s(w) d\mu d\bar{w} \]

where the primed sums for the boundary integrals indicate that the terms related to the cut-off and inflow boundaries are excluded, and finally,

\[ \mathcal{L}(g_h) = - \langle f^{in}, g_h \beta \cdot \hat{n} \rangle_{\Gamma} \]

denoting a surface integral over the inflow boundary. We have

\[ \| f_{ikm}(t, \cdot) - f(t, \cdot) \|_{L^2(\partial \Omega_D)} \leq C \sqrt{e^{Ch_1 k_{h+1}/2}} |f|_{L^\infty([0, t], H^{k_{h+1}}(\Omega_D))}, \]

with \( C = C(diam(\Omega_D), \| \beta \|_{W^{1, \infty}(\partial \Omega_D)}) \) not depending on \( h \) or \( t \).

**Proof.** The classical (exact) solution \( f \) satisfies the weak formulation for the solution of the DG scheme. Therefore it also holds that

\[ (\partial_t f, g_h)_{\mathcal{T}} + \mathcal{A}(f, g_h) = \mathcal{L}(g_h) \]

for all test functions \( g_h \). The error is naturally defined as \( E = f - f_h \), so we have

\[ (\partial_t E, g_h)_{\mathcal{T}} + \mathcal{A}(E, g_h) = 0 \]

by linearity of the operator \( \mathcal{A} \). Now, the error will be decomposed in two parts,

\[ E = E + E_h, \]

with the first one related to the error in \( L^2 \) - projecting \( f \) in the DG-FEM space,

\[ E = f - \mathbb{P} f, \]

and the second part being the difference between this projection and the numerical solution to the DG scheme,

\[ E_h = \mathbb{P} f - f_h, \]

the latter error contribution belonging to the FEM space. Therefore we can choose \( g_h = E_h \), and then

\[ (\partial_t E, E_h)_{\mathcal{T}} + \mathcal{A}(E, E_h) = 0, \]

so the remainder equation is

\[ (\partial_t E, E_h)_{\mathcal{T}} + \mathcal{A}(E, E_h) + (\partial_t E_h, E_h)_{\mathcal{T}} + \mathcal{A}(E_h, E_h) = 0. \]

We have that \( (\partial_t E, E_h)_{\mathcal{T}} = 0 \). This happens because \( E = f - \mathbb{P} f \) is the \( L^2 \) - projection of \( f \) into the FEM space, and by definition \( \mathbb{P} f \) is the function in the FEM space whose \( L^2 \) - Fourier coefficients when represented in a basis for the FEM space are the same as the \( L^2 \) - inner products between \( f \) and the basis elements. Namely,

\[ (f, w_h)_{\mathcal{T}} = (\mathbb{P} f, w_h)_{\mathcal{T}} \]

as the equality above holds for all elements in the basis set and therefore for any \( w_h \) in the DG-FEM space. Therefore we get the equality we wanted to prove,

\[ (E, w_h)_{\mathcal{T}} = 0. \]
Now we consider the last term in the remainder equation,

\[ \mathcal{A}(E_h, E_h) = \frac{1}{4} \int_{q} (E^+_h - E^-_h)^2 |\beta \cdot \tilde{n}| e^H d\sigma - \int_{\Omega_C} Q(E_h) E_h e^H s(w) d\tilde{w} \]

which if we use in the remainder equation will give us

\[ \mathcal{A}(\mathcal{E}, E_h) + (\partial_t E_h, E_h)^T + \frac{1}{4} \int_{q} (E^+_h - E^-_h)^2 |\beta \cdot \tilde{n}| e^H d\sigma - \int_{\Omega_C} Q(E_h) E_h e^H s(w) d\tilde{w} = 0, \]

\[ \mathcal{A}(\mathcal{E}, E_h) + (\partial_t E_h, E_h)^T + \frac{1}{4} \int_{q} (E^+_h - E^-_h)^2 |\beta \cdot \tilde{n}| e^H d\sigma = \int_{\Omega_C} Q(E_h) E_h e^H s(w) d\tilde{w} \leq 0, \]

given the entropy inequality for our collisional operator. So

\[ (\partial_t E_h, E_h)^T + \frac{1}{4} \int_{q} (E^+_h - E^-_h)^2 |\beta \cdot \tilde{n}| e^H d\sigma \leq -\mathcal{A}(\mathcal{E}, E_h). \]

We will study the bound in this inequality. We have

\[
\mathcal{A}(\mathcal{E}, E_h) = - \sum_{ikm} \int_{km} \partial_p \mathcal{E} \mu \partial_x (E_h e^H) p^2 dpd\mu dx \pm \sum_{ikm} \int_{km} \partial_p \mathcal{E} \mu |x| \pm E_h e^H |x| p^2 dpd\mu
\]

\[
- \sum_{ikm} \int_{km} p^2 (-qE)(x,t) \mu \partial_p (E_h e^H) dpd\mu dx \pm \sum_{im} \int_{km} p^2 (-q\mathcal{E} \mu) |p| \pm E_h e^H |p| dpd\mu
\]

\[
- \sum_{ikm} \int_{km} (1-\mu^2) \mathcal{E}(-qE)(x,t) \partial_p (E_h e^H) dpd\mu dx \pm \sum_{ik} \int_{km} (1-\mu^2) (\mathcal{E}(-qE)|_{\mu} \pm E_h e^H |_{\mu} dpd\mu
\]

\[
- \sum_{ikm} \int_{\Omega_C} Q(\mathcal{E}) E_h e^H s(w) d\tilde{w} d\tilde{\tilde{w}},
\]

which we will decompose in three terms,

\[ T_1 = - \sum_{ikm} \int_{km} \partial_p \mathcal{E} \mu \partial_x (E_h e^H) p^2 dpd\mu dx \pm \sum_{ikm} \int_{km} p^2 (-qE)(x,t) \mu \partial_p (E_h e^H) dpd\mu dx
\]

\[ - \sum_{ikm} \int_{km} (1-\mu^2) \mathcal{E}(-qE)(x,t) \partial_p (E_h e^H) dpd\mu dx,
\]

\[ T_2 = \pm \sum_{ikm} \int_{km} \partial_p \mathcal{E} \mu |x| \pm E_h e^H |x| p^2 dpd\mu \pm \sum_{im} \int_{km} p^2 (-q\mathcal{E} \mu) |p| \pm E_h e^H |p| dpd\mu
\]

\[ \pm \sum_{ik} \int_{km} (1-\mu^2) (\mathcal{E}(-qE)|_{\mu} \pm E_h e^H |_{\mu} dpd\mu
\]

\[ T_3 = - \sum_{ikm} \int_{\Omega_C} Q(\mathcal{E}) E_h e^H s(w) d\tilde{w} d\tilde{\tilde{w}},
\]

so

\[ -\mathcal{A}(\mathcal{E}, E_h) \leq |\mathcal{A}(\mathcal{E}, E_h)| \leq |T_1| + |T_2| + |T_3|, \]
and we will bound the terms individually. For $T_1$, we first point out that the Hamiltonian is related to the transport vector since (using $K_B T$ units)

$$H(x, p, t) = \varepsilon(p) - qV(x, t), \quad \partial_\mu H = 0,$$

where the potential gives the electric field by $E(x, t) = -\partial_\mu V(x, t)$. So

$$T_1 = -\sum_{ikm} \int_{km} \partial_\mu \varepsilon(p) E\mu \partial_x (E_h e^H) p^2 dpd\mu dx - \sum_{ikm} \int_{km} p^2 (-qE(x, t)) E\mu \partial_\mu (E_h e^H) d\mu dx$$

$$- \sum_{ikm} \int_{km} (1 - \mu^2) E(-qE)(x, t) e^H \partial_\mu E_h dpd\mu dx =$$

$$- \sum_{ikm} \int_{km} \partial_\mu \varepsilon(p) E\mu (\partial_x E_h + E_h \partial_x e^H) p^2 dpd\mu dx$$

$$- \sum_{ikm} \int_{km} p^2 (-qE(x, t)) E\mu (\partial_\mu E_h e^H + E_h \partial_\mu e^H) d\mu dx +$$

$$\sum_{ikm} \int_{km} (1 - \mu^2) E qE(x, t) e^H \partial_\mu E_h dpd\mu dx = \sum_{ikm} \int_{km} \partial_\mu \varepsilon(p) E\mu (qE_h \partial_x V - \partial_x E_h) e^H p^2 dpd\mu dx$$

$$- \sum_{ikm} \int_{km} qE(x, t) E\mu (\partial_\mu E_h + E_h \partial_\mu e^H) e^H d\mu dx$$

$$- \sum_{ikm} \int_{km} (1 - \mu^2) E(-qE)(x, t) e^H \partial_\mu E_h dpd\mu dx =$$

$$= -\sum_{ikm} \int_{km} e^H \partial_\mu \varepsilon(p) E\mu \partial_x E_h p^2 dpd\mu dx + \sum_{ikm} \int_{km} qE(x, t) E\mu \partial_\mu E_h p^2 d\mu dx$$

$$+ \sum_{ikm} \int_{km} (1 - \mu^2) E qE(x, t) e^H \partial_\mu E_h dpd\mu dx =$$

$$= \sum_{ikm} \int_{km} E[-\partial_\mu \varepsilon(p) \mu \partial_x E_h + qE(x, t) \mu \partial_\mu E_h + (1 - \mu^2) qE(x, t) \partial_\mu E_h / p] p^2 dpd\mu dx$$

$$= \sum_{ikm} \int_{km} E(-\partial_\mu \varepsilon, qE\mu, qE(1 - \mu^2) / p) \cdot \partial E_h e^H p^2 dpd\mu dx,$$

where $\partial = \partial_{(x, p, \mu)}$ is understood. So we have expressed $T_1$ in the form

$$T_1 = \sum_{ikm} (E, \beta \cdot \partial E_h)_{ikm},$$

with the transport vector $\beta$ defined by

$$\beta = (-\partial_\mu \varepsilon, qE\mu, qE(1 - \mu^2) / p).$$

This vector depends on $(x, p, \mu)$, so we proceed to take an average of it over the elements, such that its projection over each one of the normals $\tilde{n} = \tilde{e}_x, \tilde{e}_p, \tilde{e}_\mu$ at the boundaries satisfies

$$< \beta^0 \cdot \tilde{n}, 1 >_{\partial K} = < \beta \cdot \tilde{n}, 1 >_{\partial K},$$

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so this constant vector is defined by
\[
\beta^0_{ikm} = \frac{-\partial_p \mu, 1 > _{km} \epsilon_p, \mu}{1 > _{km} \epsilon_p} + \frac{q \mu, 1 > _{im} \epsilon_p, \mu}{1 > _{im} \epsilon_p} + \frac{q (1 - \mu^2) \mu_{\text{min}}}{1 > _{ik} \epsilon_p}.
\]

By definition, the vector
\[
\beta^0 = \sum_{ikm} \chi_{ikm} \beta^0_{ikm}
\]
is such that \(\beta^0 \cdot \partial E_h\) is in the DG-FEM space, which implies that
\[
\sum_{ikm} (\mathcal{E}, \beta^0 \cdot \partial E_h)_{ikm} = (\mathcal{E}, \beta^0 \cdot \partial E_h)_{\mathcal{T}_h} = 0,
\]
and therefore
\[
T_1 = \sum_{ikm} (\mathcal{E}, \beta \cdot \partial E_h)_{ikm} = \sum_{ikm} (\mathcal{E}, (\beta - \beta^0) \cdot \partial E_h)_{ikm}.
\]

Now we can bound this term as
\[
|T_1| \leq \sum_{ikm} ||\mathcal{E}, (\beta - \beta^0) \cdot \partial E_h||_{ikm} \leq \sum_{ikm} ||\mathcal{E}||_{L^2_{ikm}} ||\beta - \beta^0||_{L^\infty_{ikm}} ||\partial E_h||_{L^1_{ikm}}.
\]

We will now bound the last factor by making use of the inverse inequality, which states that there’s a constant \(C_{ikm}\) s.t.
\[
||\partial E_h||_{L^2_{ikm}} \leq C_{ikm} ||E_h||_{L^2_{ikm}} / h_{ikm},
\]
which we use now to get
\[
|T_1| \leq \sum_{ikm} ||\mathcal{E}||_{L^2_{ikm}} ||E_h||_{L^2_{ikm}} C_{ikm} ||\beta - \beta^0||_{L^\infty_{ikm}} / h_{ikm}
\]
\[
\leq \{ \sum_{ikm} ||\mathcal{E}||_{L^2_{ikm}} ||E_h||_{L^2_{ikm}} \} \max_{ikm} C_{ikm} ||\beta - \beta^0||_{L^\infty_{ikm}} / h_{ikm},
\]
\[
|T_1| \leq ||\mathcal{E}||_{L^2_{\mathcal{T}_h}} ||E_h||_{L^2_{\mathcal{T}_h}} \max_{ikm} \{ C_{ikm} ||\beta - \beta^0||_{L^\infty_{ikm}} / h_{ikm} \},
\]
\[
|T_1| \leq ||\mathcal{E}||_{L^2_{\mathcal{T}_h}} ||E_h||_{L^2_{\mathcal{T}_h}} ||\beta||_{W^{(1,\infty)}(\mathcal{T}_h)},
\]

using the results in [24] for the last inequality. We proceed now to use a known estimate for \(L^2\)–projections,
\[
||\mathcal{E}||_{L^2_{ikm}} + h_{ikm}^{1/2} ||\mathcal{E}||_{L^2_{ikm}} + h_{ikm} ||\partial \mathcal{E}||_{L^2_{ikm}} \leq Ch_{ikm}^{k+1} ||f||_{H^{k+1}_{ikm}},
\]
therefore the 1st summand can be bounded over the triangulation and we’ll have
\[
|T_1| \leq Ch_{ikm}^{k+1} ||f||_{H^{k+1}_{(\mathcal{T}_h)}} ||E_h||_{L^2_{\mathcal{T}_h}} ||\beta||_{W^{(1,\infty)}(\mathcal{T}_h)}.
\]

Now we’ll proceed with the estimate of \(T_2\),
\[
T_2 = \pm \sum_{ikm} \int_{km} \partial_p \mathcal{E} \mu |_{x \epsilon E_h \in H} p \epsilon_{x \epsilon E_h \in H} |_{x \epsilon \mu} p^2 dpd\mu \pm \sum_{ikm} \int_{km} p^2 \epsilon_{x \epsilon \mu} (-q \mathcal{E} \mu) |_{x \epsilon \mu} E_h \in H |_{x \epsilon \mu} d\mu dx
\]
\[ \pm \sum_{ik} \int_{\Omega} \frac{1}{p} \frac{\mu^2_m}{p} (-q \ddot{E}E)_{\mu_m} |E_h e^H|_{\mu_m} \, p^2 \, dpdx, \]

which if we consider added over all the triangulation we have

\[ T_2 = - < E_h e^H, (-\partial_\mu \ddot{E}E, q \ddot{E}E \partial_\mu - \frac{\mu^2_m}{p} q \ddot{E}E) \cdot \hat{n} >_{\partial \Omega_T}, \]

and, if we remember that \( \beta = (-\partial_\mu \ddot{E}E, \partial_\mu \ddot{E}E)_{\mu_m} |E(1-\mu^2_m)_{\mu_m}/p), \)

\[ T_2 = - < E_h e^H, \ddot{E}E \cdot \hat{n} >_{\partial \Omega_T}, \]

therefore, using DG-FEM results related to volume and boundary integrals,

\[ |T_2| = | < E_h e^H, \ddot{E}E \cdot \hat{n} >_{\partial \Omega_T} | = \frac{1}{2} < E_h e^H |_{\partial \Omega_T}, |\ddot{E}E \cdot \hat{n}| >_{\partial \Omega_T}, \]

where the notation \( c_h \) indicates edge redundancy in counting, and therefore the factor of \( 1/2 \), and proceeding further,

\[ |T_2| \leq \frac{1}{8} ||(e^H E_h)\sqrt{|\ddot{E}E \cdot \hat{n}|} ||^2_{L^2(e_h)} + \frac{1}{2} ||E|| \sqrt{|\ddot{E}E \cdot \hat{n}|} ||^2_{L^2(e_h)}, \]

and bounding the second term, we have

\[ |T_2| \leq \frac{1}{8} ||(e^H E_h)\sqrt{|\ddot{E}E \cdot \hat{n}|} ||^2_{L^2(e_h)} + C ||\ddot{E}E \cdot \hat{n} ||^2_{L^2(e_h)}, \]

\[ |T_2| \leq \frac{1}{8} ||(e^H E_h)\sqrt{|\ddot{E}E \cdot \hat{n}|} ||^2_{L^2(e_h)} + C ||\ddot{E}E \cdot \hat{n} ||^2_{L^2(e_h)} + h^{2k+1} |f|^2 H^{k+1}(\Omega_T). \]

The only difference in this case is the appearance of the exponential of the Hamiltonian in one of the bounding terms. Finally, we proceed with \( T_3 \). We have

\[ T_3 = - \sum_{ikm} \int_{\Omega_c} Q(\mathcal{E}) E_h e^H s(w) d\bar{w} d\bar{x} = - (Q(\mathcal{E}), E_h)_{\Omega_T}, \]

by definition of the inner product under the entropy norm

\[ \langle g_h, f_h \rangle = \int_{\Omega_T} g_h f_h e^H s(w) d\bar{w} d\bar{x}, \]

where \( E_h \) belongs to the DG-FEM space. So

\[ |T_3| = | \sum_{ikm} \int_{\Omega_c} Q(\mathcal{E}) E_h e^H s(w) d\bar{w} d\bar{x} | = \| (Q(\mathcal{E}), E_h)_{\Omega_T} \| \leq \| Q(\mathcal{E}) \|_{L^2(\Omega_T)} \| E_h \|_{L^2(\Omega_T)} \]

by Cauchy-Schwarz. We only need to study the \( L^2 \)-norm of \( Q(\mathcal{E}) \). We have

\[ \| Q(\mathcal{E}) \|_{L^2(\Omega_T)} = (Q(\mathcal{E}), Q(\mathcal{E}))_{\Omega_T} = \sum_{ikm} \int_{\Omega_c} Q(\mathcal{E}) Q(\mathcal{E}) e^H s(w) d\bar{w} d\bar{x}, \]

but we know our collision operator has the following structure,

\[ \sum_{ikm} \int_{\Omega_c} Q(f) g e^H s(w) d\bar{w} d\bar{x} = - \frac{1}{2} \sum_{ikm} \int_{\Omega_c} S(\bar{p} T \bar{p} g e^{-H}) e^{-H T} (f' e^{-H} - f e^{-H}) g dp dq d\bar{w} d\bar{x}, \]
so if we apply it to our particular case, we have

$$\sum_{ikm} \int_{\Omega_c} Q(\mathcal{E})Q(\mathcal{E})e^{iH} s(w) d\tilde{w} d\tilde{x} = \frac{1}{2} \sum_{ikm} \int_{\Omega_c} S(\tilde{p} \to \tilde{p}) e^{-H} \left( \frac{\mathcal{E}'}{e^{-\mathcal{E}'}} - \frac{\mathcal{E}}{e^{-\mathcal{E}}} \right) (Q(\mathcal{E'}) - Q(\mathcal{E})) d\tilde{p} d\tilde{x}.$$

We therefore conclude that

$$||Q(\mathcal{E})||^2_{L^2(\mathcal{T}_h)} = (Q(\mathcal{E}), Q(\mathcal{E}))_{\mathcal{T}_n} = \sum_{ikm} \int_{\Omega_c} |Q(\mathcal{E})|^2 e^{iH} s(w) d\tilde{w} d\tilde{x} \leq$$

$$\sum_{ikm} \int_{\Omega_c} \left\{ \sum_{j=-1}^{+1} K_j \left| \frac{\partial \tilde{p}}{\partial (\epsilon, \mu', \phi')} \right|^2 (4\pi)^2 \left| e^{\frac{\Delta w_p}{T_h L}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{-\Delta w_p}{T_h L}} ||\mathcal{E}|| \right|^2 e^{iH} s(w) d\tilde{w} d\tilde{x} \leq$$

$$(4\pi)^2 \sum_{ikm} \int_{\Omega_c} \left\{ \sum_{j=-1}^{+1} K_j |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) \right\}^2 e^{iH} s(w) d\tilde{w} d\tilde{x} =$$

$$\sum_{ikm} \int_{\Omega_c} \left\{ K_0 |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) \right\}^2 e^{iH} s(w) d\tilde{w} d\tilde{x} +$$

$$\sum_{\pm} K_\pm |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||}} e^{iH} s(w) d\tilde{w} d\tilde{x},$$

but since

$$K_1 = K_{-1} = Kn_q e^{\frac{\Delta w_p}{T_h L}}, \quad n_q = (e^{\frac{\Delta w_p}{K_n T_h}} - 1)^{-1},$$

$$K_{\pm 1} = K e^{\frac{\Delta w_p}{T_h L}} = e^{\frac{\Delta w_p}{T_h L}} \sinh(\frac{\Delta w_p}{T_h L}),$$

then

$$||Q(\mathcal{E})||^2_{L^2(\mathcal{T}_h)} \leq (4\pi)^2 \sum_{ikm} \int_{\Omega_c} \left\{ K_0 |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) +$$

$$\sum_{\pm} K_\pm |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||}} e^{iH} s(w) d\tilde{w} d\tilde{x} =$$

$$(4\pi)^2 \sum_{ikm} \int_{\Omega_c} \left\{ K_0 |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) +$$

$$\sum_{\pm} K_\pm |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||}} e^{iH} s(w) d\tilde{w} d\tilde{x} =$$

$$(4\pi)^2 \sum_{ikm} \int_{\Omega_c} \left\{ K_0 |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) +$$

$$\sum_{\pm} K_\pm |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||}} e^{iH} s(w) d\tilde{w} d\tilde{x} =$$

$$(4\pi)^2 \sum_{ikm} \int_{\Omega_c} \left\{ K_0 |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) +$$

$$\sum_{\pm} K_\pm |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||}} e^{iH} s(w) d\tilde{w} d\tilde{x} =$$

$$(4\pi)^2 \sum_{ikm} \int_{\Omega_c} \left\{ K_0 |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) +$$

$$\sum_{\pm} K_\pm |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||}} e^{iH} s(w) d\tilde{w} d\tilde{x} =$$

$$(4\pi)^2 \sum_{ikm} \int_{\Omega_c} \left\{ K_0 |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) +$$

$$\sum_{\pm} K_\pm |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||}} e^{iH} s(w) d\tilde{w} d\tilde{x} =$$

$$(4\pi)^2 \sum_{ikm} \int_{\Omega_c} \left\{ K_0 |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) +$$

$$\sum_{\pm} K_\pm |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||}} e^{iH} s(w) d\tilde{w} d\tilde{x} =$$

$$(4\pi)^2 \sum_{ikm} \int_{\Omega_c} \left\{ K_0 |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) +$$

$$\sum_{\pm} K_\pm |J\chi|(|\mathcal{E}|^{\infty}(\epsilon', \mu', \phi') + |\mathcal{E}|) e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||_{L^{\infty}(\epsilon', \mu', \phi')} + e^{\frac{\pm w_p}{\epsilon^{\frac{1}{2}}} ||\mathcal{E}||}} e^{iH} s(w) d\tilde{w} d\tilde{x} =$$
\[+Kn_{q} \sum_{\pm} \pm [J\chi](\epsilon \pm \hbar \omega_{p})e^{\frac{\hbar \omega_{p}}{\hbar \omega_{p}+|E|}}|E|_{L^{\infty}(\epsilon',\mu',\phi')} + |E||]^{2}e^{H} s(w)d\vec{u}d\vec{x} =
\]
\[(4\pi)^{2} \sum_{ikm} \int_{\Omega_{C}} \{K_{0}[J\chi](\epsilon)||E||_{L^{\infty}(\epsilon',\mu',\phi')} + |E||]^{2}e^{H} s(w)d\vec{u}d\vec{x} =
\]
\[+Kn_{q}(J\chi)(\epsilon + \hbar \omega_{p}) - [J\chi](\epsilon - \hbar \omega_{p})e^{\frac{\hbar \omega_{p}}{\hbar \omega_{p}+|E|}}|E|_{L^{\infty}(\epsilon',\mu',\phi')} + |E||]^{2}e^{H} s(w)d\vec{u}d\vec{x},
\]
and using
\[K_{1} = K_{-1} = Kn_{q}e^{-\frac{h\omega_{p}}{2\pi}},
\]
then
\[||Q||^{2} L^{2}(\Omega_{C}) \leq (4\pi)^{2} \sum_{ikm} \int_{\Omega_{C}} \{K_{0}[J\chi](\epsilon)||E||_{L^{\infty}(\epsilon',\mu',\phi')} + |E||]^{2}e^{H} s(w)d\vec{u}d\vec{x} =
\]
\[K_{1}e^{\frac{-\hbar \omega_{p}}{\hbar \omega_{p}+|E|}}([J\chi](\epsilon + \hbar \omega_{p}) - [J\chi](\epsilon - \hbar \omega_{p}))e^{\frac{\hbar \omega_{p}}{\hbar \omega_{p}+|E|}}|E|_{L^{\infty}(\epsilon',\mu',\phi')} + |E||]^{2}e^{H} s(w)d\vec{u}d\vec{x} =
\]
\[(4\pi)^{2} \sum_{ikm} \int_{\Omega_{C}} \{K_{0}[J\chi](\epsilon)||E||_{L^{\infty}(\epsilon',\mu',\phi')} + |E||]^{2}e^{H} s(w)d\vec{u}d\vec{x} +
\]
\[\sum_{ikm} \int_{\Omega_{C}} \{K_{1}(J\chi)(\epsilon + \hbar \omega_{p}) - [J\chi](\epsilon - \hbar \omega_{p}))e^{\frac{\hbar \omega_{p}}{\hbar \omega_{p}+|E|}}|E|_{L^{\infty}(\epsilon',\mu',\phi')} + |E||]^{2}e^{H} s(w)d\vec{u}d\vec{x} +
\]
\[\sum_{ikm} \int_{\Omega_{C}} 2K_{0}K_{1}[J\chi](\epsilon)||E||_{L^{\infty}(\epsilon',\mu',\phi')} + |E||^{2}e^{H} s(w)d\vec{u}d\vec{x} =
\]
\[\sum_{ikm} \int_{\Omega_{C}} K_{1}^{2}(J\chi)(\epsilon)|E|_{L^{\infty}(\epsilon',\mu',\phi')} + |E||^{2}e^{H} s(w)d\vec{u}d\vec{x} +
\]
\[\sum_{ikm} \int_{\Omega_{C}} K_{0}^{2}[J\chi]^{2}(\epsilon)|E|_{L^{\infty}(\epsilon',\mu',\phi')} + |E||^{2}e^{H} s(w)d\vec{u}d\vec{x} +
\]
\[\sum_{ikm} \int_{\Omega_{C}} 2K_{0}K_{1}[J\chi](\epsilon)(J\chi)(\epsilon + \hbar \omega_{p}) - [J\chi](\epsilon - \hbar \omega_{p}))||E||_{L^{\infty}(\epsilon',\mu',\phi')} + |E||^{2}e^{H} s(w)d\vec{u}d\vec{x} =
\]
\[4\pi^{2} \sum_{ikm} \int_{\Omega_{C}} K_{0}^{2}|E|_{L^{\infty}(\epsilon',\mu',\phi')} ||E||^{2}e^{H} s(w)d\vec{u}d\vec{x} +
\]
\[\sum_{ikm} \int_{\Omega_{C}} 2K_{0}K_{1}[J\chi](\epsilon)(J\chi)(\epsilon + \hbar \omega_{p}) - [J\chi](\epsilon - \hbar \omega_{p}))e^{\frac{\hbar \omega_{p}}{\hbar \omega_{p}+|E|}}|E|_{L^{\infty}(\epsilon',\mu',\phi')}^{2}e^{H} s(w)d\vec{u}d\vec{x} +
\]
\[+ \sum_{ikm} \int_{\Omega_{C}} 2K_{0}K_{1}[J\chi](\epsilon)(J\chi)(\epsilon + \hbar \omega_{p}) - [J\chi](\epsilon - \hbar \omega_{p}))e^{\frac{\hbar \omega_{p}}{\hbar \omega_{p}+|E|}}|E|_{L^{\infty}(\epsilon',\mu',\phi')}^{2}e^{H} s(w)d\vec{u}d\vec{x} =
\]
\[27\]
$$(4\pi)^2\sum_{ikm} \int_{\Omega_c} \{K_0^2[J\chi]^2(\varepsilon) + K_1^2([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))\}^2 e^{\frac{\hbar\omega_p}{2K^2}} + 2K_0K_1\{[J\chi](\varepsilon)([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))\}^2 e^{\frac{\hbar\omega_p}{2K^2}} + 2\sum_{ikm} \int_{\Omega_c} \{K_0^2[J\chi]^2(\varepsilon) + K_1^2([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))\}^2 e^{\frac{\hbar\omega_p}{2K^2}} + 2\sum_{ikm} \int_{\Omega_c} \{K_0^2[J\chi]^2(\varepsilon) + K_1^2([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))\}^2 e^{\frac{\hbar\omega_p}{2K^2}} + 2K_0K_1\{[J\chi](\varepsilon)([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))\}^2 e^{\frac{\hbar\omega_p}{2K^2}}$$

Now we can try to bound as

$$||Q(\varepsilon)||^2_{L^2(\tau_n)} \leq 2\max\{[K_0[J\chi](\varepsilon) + K_1([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))]^2 + (4\pi)^2([\max\{K_0[J\chi](\varepsilon) + K_1([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))]^2 + 2K_0K_1\{[J\chi](\varepsilon)([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))\}^2 e^{\frac{\hbar\omega_p}{2K^2}} + 2\sum_{ikm} \int_{\Omega_c} \{K_0^2[J\chi]^2(\varepsilon) + K_1^2([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))\}^2 e^{\frac{\hbar\omega_p}{2K^2}} + 2K_0K_1\{[J\chi](\varepsilon)([J\chi](\varepsilon + \hbar\omega_p) - [J\chi](\varepsilon - \hbar\omega_p))\}^2 e^{\frac{\hbar\omega_p}{2K^2}}$$

If we define each of the maxima above as $M_i$, $i \in \{0, 1, 2\}$ respectively, we have

$$||Q(\varepsilon)||^2_{L^2(\tau_n)} \leq (4\pi)^2\{[M_0]^2 \sum_{ikm} \int_{\Omega_c} ||\varepsilon||^2 \int_{\varepsilon(\varepsilon', \varepsilon')} e^{H} s(w) dw dw + M_0^2 \sum_{ikm} \int_{\Omega_c} ||\varepsilon||_{L^\varepsilon(\varepsilon', \varepsilon')} e^{H} s(w) dw dw + 2M_2 \sum_{ikm} \int_{\Omega_c} ||\varepsilon||_{L^\varepsilon(\varepsilon', \varepsilon')} e^{H} s(w) dw dw + 2M_2 \sum_{ikm} \int_{\Omega_c} ||\varepsilon||_{L^\varepsilon(\varepsilon', \varepsilon')} e^{H} s(w) dw dw + 16\pi^2 (M_0^2 \sum_{ikm} \int_{\Omega_c} ||\varepsilon||^2_{L^\varepsilon(\varepsilon', \varepsilon')} e^{H} s(w) dw dw + M_0^2 \sum_{ikm} \int_{\Omega_c} ||\varepsilon||_{L^\varepsilon(\varepsilon', \varepsilon')} e^{H} s(w) dw dw)$$

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\[ M_f^2 \sum_{\text{odd, } k, m} \int_{\Omega_C} |E|^2 e^H s(w) d\bar{w} \bar{d}z + M_2 \sum_{\text{odd, } k, m} \int_{\Omega_C} ||E||_{L^\infty(z)} ||E||_{L^2(z, \bar{w})} \]
\[ = 16\pi^2 [M_f^2 (||E||_{L^\infty(z)})^2_{L^2(z, \bar{w})} + M_2^2 ||E||_{L^2(z, \bar{w})} + M_2 (||E||_{L^\infty(z)}, ||E||_{L^2(z, \bar{w})}). \]

If we combine the estimates of \( T_i \), \( i = 1, 2, 3 \) for our final estimate, we have that
\[ (\partial_t E_h, E_h)_{T_h} + \frac{1}{4} \int_{\Omega_C} \left( E_h^+ - E_h^- \right)^2 |\beta \cdot \hat{\eta}| e^H d\sigma \leq -\mathcal{A}(E, E_h), \]

with
\[ -\mathcal{A}(E, E_h) \leq |\mathcal{A}(E, E_h)| \leq |T_1| + |T_2| + |T_3|, \]

where
\[ |T_1| \leq C h^{k+1} ||f||_{H^{k+1}(T_h)} ||E_h||_{L^2_h} ||\beta||_{W^{1, \infty}(T_h)}, \]
\[ |T_2| \leq \frac{1}{8} ||e^H E_h|| \sqrt{||\beta \cdot \hat{\eta}||^2 L^2(e_h)} + C ||\beta||_{L^\infty_h} h^{2k+1} ||f||_{H^{k+1}(T_h)}, \]
\[ |T_3| = \sum_{\text{odd, } k, m} \int_{\Omega_C} Q(E) E_h e^H s(w) d\bar{w} \bar{d}z = ||Q(E), E_h)_{T_h} \| ||Q(E)||_{L^2(T_h)} \| ||E_h||_{L^2(T_h)} \]
\[ \|Q(E)\|_{L^2(T_h)} \leq 16\pi^2 [M_0^2 (||E||_{L^\infty(\omega^\rho)})^2_{L^2(\bar{w})} + M_2^2 ||E||_{L^2(\bar{w})} + M_2 (||E||_{L^\infty(\omega^\rho)}, ||E||_{L^2(\bar{w})})], \]

so we have
\[ (\partial_t E_h, E_h)_{T_h} + \frac{1}{4} \int_{\Omega_C} \left( E_h^+ - E_h^- \right)^2 |\beta \cdot \hat{\eta}| e^H d\sigma \leq |T_1| + |T_2| + |T_3| \leq \]
\[ C h^{k+1} ||f||_{H^{k+1}(T_h)} ||E_h||_{L^2_h} ||\beta||_{W^{1, \infty}(T_h)} + \frac{1}{8} ||e^H E_h|| \sqrt{||\beta \cdot \hat{\eta}||^2 L^2(e_h)} + C ||\beta||_{L^\infty_h} h^{2k+1} ||f||_{H^{k+1}(T_h)} \]
\[ + ||E_h||_{L^2(T_h)} \cdot 4\pi M \sqrt{||Q(E)||^2_{L^\infty(\omega^\rho)} ||E||^2_{L^2(\bar{w})} + ||E||^2_{L^2(\bar{w})} + ||Q(E)||^2_{L^2(\bar{w})} ||L^2(\bar{w}) \times ||E||_{L^2(\bar{w})}}, \]

with \( M = \max(M_0, M_1, \sqrt{M_2}) \).

We can get the following bound then,
\[ (\partial_t E_h, E_h)_{T_h} + \frac{1}{4} \int_{\Omega_C} \left( E_h^+ - E_h^- \right)^2 |\beta \cdot \hat{\eta}| e^H d\sigma \leq C h^{k+1} ||f||_{H^{k+1}(T_h)} ||E_h||_{L^2_h} ||\beta||_{W^{1, \infty}(T_h)} \]
\[ + \frac{1}{8} ||e^H E_h|| \sqrt{||\beta \cdot \hat{\eta}||^2 L^2(e_h)} + C ||\beta||_{L^\infty_h} h^{2k+1} ||f||_{H^{k+1}(T_h)} \]
\[ + 4\pi M ||E_h||_{L^2(T_h)} \sqrt{||Q(E)||^2_{L^\infty(\omega^\rho)} ||E||^2_{L^2(\bar{w})} + ||E||^2_{L^2(\bar{w})}} + 2 ||Q(E)||^2_{L^2(\bar{w})} ||L^2(\bar{w}) \times ||E||_{L^2(\bar{w})}}, \]
\[ = C h^{k+1} ||f||_{H^{k+1}(T_h)} ||E_h||_{L^2_h} ||\beta||_{W^{1, \infty}(T_h)} + \frac{1}{8} ||e^H E_h|| \sqrt{||\beta \cdot \hat{\eta}||^2 L^2(e_h)} + C ||\beta||_{L^\infty_h} h^{2k+1} ||f||_{H^{k+1}(T_h)} \]
\[ + 4\pi M ||E_h||_{L^2(T_h)} \sqrt{||Q(E)||^2_{L^\infty(\omega^\rho)} ||E||^2_{L^2(\bar{w})} + ||E||^2_{L^2(\bar{w})}}, \]

which is the result we want. Now, following similar arguments as in [11], if we assume that
\[ ||\beta||_{W^{1, \infty}(T_h)} \leq C', \]

which holds for quadratically confined electrostatic potentials [11], when
\[ \beta = (-\partial \varepsilon \mu, qE \mu, qE(1-\mu^2_m))_{\mu^m_{\mu^m_{\mu^m}}}/p), \quad E = -\partial_x V, \quad |V| \leq K|x - x_0|^2, \]

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with $K$, $x_0$ constants, we have then

$$(\partial_t E_h, E_h)_{T_h} + \frac{1}{4} \int_{\mathcal{C}_h} (E^+_h - E^-_h)^2 |\beta \cdot \tilde{n}| e^H dt \leq$$

$$C^* h^{k+1} |f|_{H^{k+1}(T_h)} ||E_h||_{L^2(T_h)} + \frac{1}{8} ||e^H E_h||_V \sqrt{||\beta \cdot \tilde{n}||^2_{L^2(\mathcal{C}_h)}} + C ||\beta||_{L^\infty(T_h)} h^{2k+1} |f|_{H^{k+1}(T_h)}^2 \left[ M' \right] ||E_h||_{L^2(T_h)} \left( ||\mathcal{E}\|_{L^\infty(\omega')} \right) ||E\|_{L^2(\tilde{x}, \tilde{w})} + ||\mathcal{E}\|_{L^2(\tilde{x}, \tilde{w})},$$

with $M' = 4\pi M$. So

$$(\partial_t E_h, E_h)_{T_h} + \frac{1}{4} \int_{\mathcal{C}_h} (E^+_h - E^-_h)^2 |\beta \cdot \tilde{n}| e^H dt \leq \frac{1}{8} ||e^H E_h||_V \sqrt{||\beta \cdot \tilde{n}||^2_{L^2(\mathcal{C}_h)}} \leq$$

$$+ C^* h^{k+1} |f|_{H^{k+1}(T_h)} ||E_h||_{L^2(T_h)} + C ||\beta||_{L^\infty(T_h)} h^{2k+1} |f|_{H^{k+1}(T_h)}^2 \left[ M' \right] ||E_h||_{L^2(T_h)} \left( ||\mathcal{E}\|_{L^\infty(\omega')} \right) ||E\|_{L^2(\tilde{x}, \tilde{w})} + ||\mathcal{E}\|_{L^2(\tilde{x}, \tilde{w})},$$

We have then that

$$(\partial_t E_h, E_h)_{T_h} \leq (\partial_t E_h, E_h)_{T_h} + \frac{1}{8} ||e^H E_h||_V \sqrt{||\beta \cdot \tilde{n}||^2_{L^2(\mathcal{C}_h)}} \leq$$

$$C^* h^{k+1} |f|_{H^{k+1}(T_h)} ||E_h||_{L^2(T_h)} + C ||\beta||_{L^\infty(T_h)} h^{2k+1} |f|_{H^{k+1}(T_h)}^2 \left[ M' \right] ||E_h||_{L^2(T_h)} \left( ||\mathcal{E}\|_{L^\infty(\omega')} \right) ||E\|_{L^2(\tilde{x}, \tilde{w})} + ||\mathcal{E}\|_{L^2(\tilde{x}, \tilde{w})},$$

therefore

$$\frac{1}{2} \frac{d}{dt} ||E_h||_{T_h}^2 \leq \frac{1}{2} \frac{d}{dt} (\partial_t E_h, E_h)_{T_h} = (\partial_t E_h, E_h)_{T_h} \leq$$

$$C^* h^{k+1} |f|_{H^{k+1}(T_h)} ||E_h||_{L^2(T_h)} + C ||\beta||_{L^\infty(T_h)} h^{2k+1} |f|_{H^{k+1}(T_h)}^2 \left[ M' \right] ||E_h||_{L^2(T_h)} \left( ||\mathcal{E}\|_{L^\infty(\omega')} \right) ||E\|_{L^2(\tilde{x}, \tilde{w})} + ||\mathcal{E}\|_{L^2(\tilde{x}, \tilde{w})},$$

with $E_h = 0$ at $t = 0$. We only need to proceed with a Gronwall inequality,

$$\frac{1}{2} \frac{d}{dt} ||E_h||_{T_h}^2 \leq C ||\beta||_{L^\infty(T_h)} h^{2k+1} |f|_{H^{k+1}(T_h)}^2 \left[ M' \right] ||E_h||_{L^2(T_h)} \left( ||\mathcal{E}\|_{L^\infty(\omega')} \right) ||E\|_{L^2(\tilde{x}, \tilde{w})} + ||\mathcal{E}\|_{L^2(\tilde{x}, \tilde{w})}.$$
Then
\[ \|E\|_{T_h} \leq \|E\|_{T_n} + \|E_h\|_{T_h} \]
and we expect the projection error to contribute as below,
\[ \|E\|_{T_h} \leq C'h^{k+1}. \]

Therefore we have
\[ \|E\|_{T_n} = \|E\|_{T_h} + \|E_h\|_{T_n} \]
\[ \leq C\sqrt{t} \exp(CH)h^{k+1/2} f_{L^\infty([0,t],H^{k+1}(Ω_D))} + t \times M'\{||E||_{L^\infty(ω')}\} ||E||_{L^2(ω')} + ||E||_{L^2(ω')} + C'h^{k+1}, \]
and if we simply take
\[ \bar{C} = \max\{C, M', C''\}, \]
then
\[ ||E||_{T_n} \leq \bar{C}\sqrt{t} \exp(CH)h^{k+1/2} f_{L^\infty([0,t],H^{k+1}(Ω_D))} + t ||E||_{L^\infty(ω')} ||E||_{L^2(ω')} + ||E||_{L^2(ω')} + h^{k+1}. \]

If we use the regularity property we get
\[ \|M^{-1/2}[f(t, \cdot, \cdot) - M]\|_{H^k} \leq K \exp(-\gamma t), \quad t \geq 0 \quad \Rightarrow \quad ||f(t)||_{H^{k+1}} \leq K. \]

Going back to our result, if \( t \geq Ch \), then we have (after a few time-steps)
\[ ||E||_{T_n} \leq \bar{C}\sqrt{t} \exp(CH)h^{k+1/2} f_{L^\infty([0,t],H^{k+1}(Ω_D))} + t ||E||_{L^\infty(ω')} ||E||_{L^2(ω')} + ||E||_{L^2(ω')} \]

This is interesting because we have square-root times exponential growth versus linear growth. It would seem the first one will win the latter for large times, after a few time steps again, and then we should have the \( L^2 \) error estimates of the DG solution,
\[ \|E\|_{T_n} \leq \bar{C}\sqrt{t} \exp(CH)h^{k+1/2} f_{L^\infty([0,t],H^{k+1}(Ω_D))}. \]

So although we get an extra term (not similar to any term reported in [11]), the terms analog to the ones appearing in [11] become more meaningful at long times, and since the other one is negligible for large times, we get a similar estimate as in [11]. Therefore, since \( E = f - f_h \), we have proved that for large times (i.e. after some transient time),
\[ \|f - f_h\|_{T_n} \leq \bar{C}\sqrt{t} \exp(CH)h^{k+1/2} f_{L^\infty([0,t],H^{k+1}(Ω_D))}. \]

We now present our second result regarding error estimation for our DG scheme with curvilinear momentum coordinates, at the semi-discrete stage.

**Theorem 8.** If \( f_h \) is the semidiscrete DG solution to our Boltzmann equation with a linear collision operator in the semiconductor problem, then
\[ \|f_h(t, \cdot, \cdot) - M\| \leq C\sqrt{t} \exp(CH)h^{k+1/2} f_{L^\infty([0,t],H^{k+1}(Ω_D))} + 3 \exp(-\lambda t) ||f_0 - M||_{B^2(\mathbb{R}^d)} \]
with the constant \( C = C(diam(Ω_D), ||β||_{W^{1,\infty}(Ω_D)}). \)

**Proof.** We have by triangle inequality
\[ ||f_h - M||_{L^2(Ω_D)} = ||f_h - f||_{L^2(Ω_D)} + ||f - M||_{L^2(Ω_D)} \leq ||f_h - f||_{L^2(Ω_D)} + ||f - M||_{B^2(Ω_D)}. \]

Since by definition
\[ ||f - M||_{B^2(Ω_D)}^2 = ||(f - M)M^{-1}||_{L^2(Ω_D)}^2 = ||(f - M)\exp(ε/K_BT)||_{L^2(Ω_D)}^2, \]

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and $\varepsilon \geq 0 \implies \exp(\varepsilon/KBT) \geq 1$, so

$$\|f - M\|_{L^2(\Omega_\delta)}^2 = \|(f - M) \exp(\varepsilon/KBT)\|_{L^2(\Omega_\delta)}^2 \geq \|(f - M)\|_{L^2(\Omega_\delta)}^2.$$  

We have then

$$\|f_h - M\|_{L^2(\Omega_\delta)} = \|f_h - f\|_{L^2(\Omega_\delta)} + \|f - M\|_{L^2(\Omega_\delta)} \leq \|f_h - f\|_{L^2(\Omega_\delta)} + \|f - M\|_{B^2(\Omega_\delta)} \leq C\sqrt{\text{exp}(C\varepsilon)} h^{k+1/2} \|f\|_{L^\infty(\Omega_\delta)} + \|f - M\|_{B^2(\Omega_\delta)},$$

and we only need to justify that

$$\|f - M\|_{B^2(\Omega_\delta)} \leq 3 \exp(-\lambda t) \|f_0 - M\|_{B^2(\Omega_\delta)},$$

with $f_0$ the initial condition. This is simply a consequence of the work in [25] (as referenced in [11]). So both inequalities hold and we get the desired result. Therefore, for large times (again, after some transient time),

$$\|f_h(t, \cdot, \cdot) - M\| \leq C\sqrt{\text{exp}(C\varepsilon)} h^{k+1/2} \|f\|_{L^\infty(\Omega_\delta)} + 3 \exp(-\lambda t) \|f_0 - M\|_{B^2(\Omega_\delta)}$$

as expected.  

\[\square\]

**Appendix 2**

6  **Positivity Preservation in DG Scheme for BP**

6.1  **1Dx-2Dp problem: Preliminaries**

Using the notation in [12], the semi-discrete DG formulation is written in the form below.

Find $f_h \in V_h^k$ such that $\forall g_h \in V_h^k$ and $\forall \Omega_{ikm}$

\[
\int_{\Omega_{ikm}} Q(f_h) g_h p^2 dp d\mu dx = \partial_t \int_{\Omega_{ikm}} f_h g_h p^2 dp d\mu dx \\
- \int_{\Omega_{ikm}} H(x) f_h \partial_p g_h p^2 dp d\mu dx \pm \int_{\Omega_{ikm}} H^{(x)} f_h |_{x_\pm} g_h |_{x_\pm}^2 p^2 dp d\mu \\
- \int_{\Omega_{ikm}} p^2 H^{(p)} f_h \partial_p g_h dp d\mu dx \pm p_{km}^2 \int_{\Omega_{ikm}} H^{(p)} f_h |_{p_\pm} g_h |_{p_\pm} dp d\mu = \int_{\Omega_{ikm}} (1 - \mu^2) H^{(\mu)} f_h \partial_\mu g_h dp d\mu dx \pm (1 - \mu_{km}^2) \int_{\Omega_{ikm}} H^{(\mu)} f_h |_{\mu_{\pm}} g_h |_{\mu_{\pm}} dp d\mu dx,
\]

where we have defined the following terms (taking in account that $\partial_\mu(\mu) > 0$)

\[
H^{(x)} = \mu \partial_\mu \varepsilon, \quad H^{(x)} f |_{x_\pm} = \partial_\mu \varepsilon f_{h_\pm} \mu_{x_\pm}; \quad \Omega^{(x)}_{km} = [r_{k-}, r_{k+}] \times [\mu_{m-}, \mu_{m+}] = \partial_\mu \Omega_{km},
\]

\[
H^{(p)} = -qE \mu, \quad H^{(p)} f |_{p_\pm} = -q \varepsilon \eta_{h_\pm} \mu_{p_\pm}; \quad \Omega^{(p)}_{km} = [x_{i-}, x_{i+}] \times [\mu_{m-}, \mu_{m+}] = \partial_\mu \Omega_{km},
\]

\[
H^{(\mu)} = -qE, \quad H^{(\mu)} f |_{\mu_{\pm}} = -q \varepsilon \eta_{h_\pm} \mu_{\mu_{\pm}}; \quad \Omega^{(\mu)}_{ik} = [x_{i-}, x_{i+}] \times [r_{k-}, r_{k+}] = \partial_\mu \Omega_{ik}.
\]

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The weak form of the collisional operator in the DG scheme is, specifically,

\[
\int_{\Omega_{ikm}} Q(f_h) g_h p^2 \, dp \, d\mu \, dx = \int_{\Omega_{ikm}} \left[ G(f_h) - \nu(\epsilon(p)) f_h \right] g_h p^2 \, dp \, d\mu \, dx = 2\pi \times 
\]

\[
\int_{\Omega_{ikm}} \sum_{j=-1}^{1} c_j \chi(\epsilon(p) + j\hbar) \int_{\Omega_{ikm}} f_h(x, p(\epsilon'), \mu') p^2(\epsilon') \frac{dp'}{d\epsilon} |_{\epsilon(p)+j\hbar} g_h p^2 \, dp \, d\mu \, dx 
\]

\[-4\pi \int_{\Omega_{ikm}} f_h(x, p, \mu, t) \sum_{j=-1}^{1} c_j \chi(\epsilon(p) - j\hbar) p^2(\epsilon') \frac{dp'}{d\epsilon} |_{\epsilon(p)-j(h\omega)} g_h p^2 \, dp \, d\mu \, dx.\]

The cell average of \( f_h \) in \( \Omega_{ikm} \) is

\[
\bar{f}_{ikm} = \frac{\int_{\Omega_{ikm}} f_h \, dp \, d\mu \, dx}{\int_{\Omega_{ikm}} p^2 \, dp \, d\mu \, dx} = \frac{\int_{\Omega_{ikm}} f_h \, dV}{V_{ikm}}, \quad (6.1)
\]

where, for our particular spherical curvilinear coordinates,

\[
V_{ikm} = \int_{\Omega_{ikm}} dV, \quad dV = \tau \prod_{d=1}^{3} z_d, \quad (z_1, z_2, z_3) = (x, p, \mu), \quad \tau = \sqrt{\gamma}, \quad \gamma = 1, \quad \lambda = p^2.
\]

The time evolution of the cell average in the DG scheme is given by

\[
\partial_t \bar{f}_{ikm} = -\frac{1}{V_{ikm}} \left[ \int_{\partial_{s,\Omega_{ikm}}} H^{(x)} f_h |_{x,=} p^2 dp \, d\mu - \int_{\partial_{s,\Omega_{ikm}}} H^{(e)} f_h |_{x,=} p^2 dp \, d\mu \right] 
\]

\[+ \frac{\mu^2}{\tau} \int_{\partial_{\mu,\Omega_{ikm}}} H^{(p)} f_h |_{\mu,=} dp \, dx - \int_{\partial_{\mu,\Omega_{ikm}}} H^{(p)} f_h |_{\mu,=} dp \, dx 
\]

\[+ (1 - \mu^2_{m+}) \int_{\partial_{\mu,\Omega_{ikm}}} H^{(\mu)} f_h |_{\mu,=} dp \, dx - (1 - \mu^2_{m-}) \int_{\partial_{\mu,\Omega_{ikm}}} H^{(\mu)} f_h |_{\mu,=} dp \, dx 
\]

\[+ 2\pi \sum_{j=-1}^{1} \int_{\Omega_{ikm}} c_j \chi(\epsilon(p) + j\hbar) \int_{\Omega_{ikm}} f_h(x, p(\epsilon'), \mu') p^2(\epsilon') \frac{dp'}{d\epsilon} |_{\epsilon(p)+j(h\omega)} p^2 dp \, d\mu \, dx.\]

Regarding the time discretization, we will apply a TVD RK-DG scheme. These schemes are convex combinations of Euler methods. Therefore, it suffices if we consider the time evolution of the cell average in the DG scheme using a Forward Euler Method, so \( \partial_t \bar{f}_{ikm} \approx \frac{\bar{f}_{ikm}^{n+1} - \bar{f}_{ikm}^{n}}{\Delta t^n} \), and

\[
\bar{f}_{ikm}^{n+1} = \bar{f}_{ikm}^{n} - \Delta t^n \int_{\partial_{s,\Omega_{ikm}}} H^{(x)} f_h |_{x,=} p^2 dp \, d\mu - \int_{\partial_{s,\Omega_{ikm}}} H^{(e)} f_h |_{x,=} p^2 dp \, d\mu 
\]

\[-\frac{\Delta t^n (1 - \mu^2_{m+})}{V_{ikm}} \int_{\partial_{\mu,\Omega_{ikm}}} H^{(p)} f_h |_{\mu,=} dp \, dx - (1 - \mu^2_{m-}) \int_{\partial_{\mu,\Omega_{ikm}}} H^{(p)} f_h |_{\mu,=} dp \, dx 
\]

\[-\frac{\Delta t^n \mu^2}{V_{ikm}} \int_{\partial_{\mu,\Omega_{ikm}}} H^{(p)} f_h |_{\mu,=} dp \, dx - \frac{\mu^2}{\tau} \int_{\partial_{\mu,\Omega_{ikm}}} H^{(p)} f_h |_{\mu,=} dp \, dx + 
\]

\[\int_{\Omega_{ikm}} \frac{2\pi \Delta t^n}{V_{ikm}} c_j \chi(\epsilon(p) + j\hbar) \int_{\Omega_{ikm}} f_h(x, p, \mu') p^2(\epsilon') \frac{dp'}{d\epsilon} |_{\epsilon(p)+j(h\omega)} p^2 dp \, d\mu \, dx 
\]

\[-4\pi \Delta t^n \int_{\Omega_{ikm}} f_h(x, p, \mu, t) \sum_{j=-1}^{1} c_j \chi(\epsilon(p) - j\hbar) p^2(\epsilon') \frac{dp'}{d\epsilon} |_{\epsilon(p)-j(h\omega)} p^2 dp \, d\mu \, dx.\]
or more briefly, \( \tilde{f}_{ikm}^{n+1} = \tilde{f}_{ikm}^{n} + \Gamma_T + \Gamma_C \), where the transport and collision terms for the cell average time evolution are

\[
\Gamma_T = -\frac{\Delta t^n}{V_{ikm}} \left[ \int_{\partial_{k}\Omega_{km}} H^{(x)} f_{h}|_{x_{i}+} p^2 dp d\mu - \int_{\partial_{k}\Omega_{km}} H^{(x)} f_{h}|_{x_{i}-} p^2 dp d\mu \right] + p_k^2 \int_{\partial_{k}\Omega_{km}} \left[ \hat{H}(\nu) f_{h}|_{pk_{+}} dp - \hat{p}_k \right] \int_{\partial_{k}\Omega_{km}} \left[ \hat{H}(\nu) f_{h}|_{pk_{-}} dp \right] + (1 - \mu_{m+}^2) \int_{\partial_{k}\Omega_{km}} \left[ \hat{H}(\nu)f_{h}|_{\mu_{m+}} dpdx - (1 - \mu_{m-}^2) \int_{\partial_{k}\Omega_{km}} \left[ \hat{H}(\nu)f_{h}|_{\mu_{m-}} dpdx \right] \right]
\]

\[
\Gamma_C = \frac{2\pi\Delta t^n}{V_{ikm}} \int_{\Omega_{ikm}} \sum_{j=-1}^{1} c_j \chi(\epsilon(p) + j\hbar\omega) \int_{-1}^{1} dp' \int_{-1}^{1} \frac{p'^2(\epsilon')}{d\epsilon'} dp' \left| \epsilon(p) + j\hbar\omega \right| p^2 dp d\mu dx \]

\[
- \frac{4\pi\Delta t^n}{V_{ikm}} \int_{\Omega_{ikm}} \sum_{j=-1}^{1} c_j \chi(\epsilon(p) - j\hbar\omega) p^2(\epsilon') \left| \frac{dp'}{d\epsilon'} \right| \epsilon(p) - j\hbar\omega \right| p^2 dp d\mu dx.
\]

### 6.2 Positivity preservation for 1Dx-2Dp DG scheme

We use the strategy of Zhang & Shu in [9, 10] for conservation laws, applied as well in [12] for conservative phase space collisionless transport in curvilinear coordinates, and in [11] for a Vlasov - Boltzmann problem with linear non-degenerate collisional forms, to preserve the positivity of the probability density function in our DG scheme treating the collision term as a source, this being possible since our collisional form is mass preserving. We will use a convex combination parameter \( \eta \in [0, 1] \)

\[
\tilde{f}_{ikm}^{n+1} = \eta \cdot I + (1 - \eta) \cdot II, \quad I = \tilde{f}_{ikm}^{n} + \frac{\Gamma_T}{\eta}, \quad II = \tilde{f}_{ikm}^{n} + \frac{\Gamma_C}{(1 - \eta)},
\]

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 [9,10] that preserve the cell average but modify the slope of the piecewise linear solutions in order to make the function non-negative. Regarding \( I \), we derive its positivity conditions below.

\[
I = \tilde{f}_{ikm}^{n} + \frac{\Gamma_T}{\eta} = \frac{\tilde{f}_{ikm}^{n} f_{h} p^2 dp dx}{V_{ikm}} \frac{\Delta t^{n}/\eta}{V_{ikm}} \left[ \int_{\partial_{k}\Omega_{km}} (H^{(x)} f_{h}|_{x_{i}+} - \hat{H}^{(x)} f_{h}|_{x_{i}-}) p^2 dp d\mu \right] + p_k^2 \int_{\partial_{k}\Omega_{km}} (\hat{H}(\nu) f_{h}|_{pk_{+}} - \hat{H}(\nu) f_{h}|_{pk_{-}}) dp d\mu \right] + \int_{\partial_{k}\Omega_{km}} \left[ (1 - \mu_{m+}^2) H^{(\nu)} f_{h}|_{\mu_{m+}} - (1 - \mu_{m-}^2) \hat{H}(\nu) f_{h}|_{\mu_{m-}} \right] dp dx.
\]
We will split the cell average convexly, as in \( \{s_i\}_{i=1}^3 \). Then

\[
I = \frac{1}{V_{ikm}} \left[ (s_1 + s_2 + s_3) \int_{\Omega_{ikm}} f_h p^2 \, dp \, dx \right] \\
- \frac{\Delta t^n}{\eta} \left( \int_{\partial_\Omega_{ikm}} \hat{H}(x) f_{h|_{x^+}} p^2 \, dp \, dx - \int_{\partial_\Omega_{ikm}} \hat{H}(x) f_{h|_{x^-}} p^2 \, dp \, dx \right) \\
+ \left( 1 - \mu_{m+}^2 \right) \int_{\partial_{\mu_{ik}^+}} \hat{H}(x) f_{h|_{\mu_{m+}}} p \, dp \, dx - \left( 1 - \mu_{m-}^2 \right) \int_{\partial_{\mu_{ik}^-}} \hat{H}(x) f_{h|_{\mu_{m-}}} p \, dp \, dx \\
= \frac{1}{V_{ikm}} \left[ \int_{\partial_\Omega_{km}} \left\{ s_1 \int_{x_{i-}}^{x_{i+}} \hat{f}_h p^2 \, dx - \frac{\Delta t^n}{\eta} \sum_{\pm} \pm \hat{H}(x) f_{h|_{x^\pm}} p^2 \right\} \, dp \, dx \right] \\
+ \int_{\partial_{\mu_{ik}^+}} \left\{ s_2 \int_{p_{\mu_{ik}^+}}^{p_{\mu_{ik}+}} f_{h|_{p_{\mu_{ik}+}}} p^2 \, dp \right\} \, d\mu \, dx \\
+ \int_{\partial_{\mu_{ik}^-}} \left\{ s_3 \int_{p_{\mu_{ik}^-}}^{p_{\mu_{ik}+}} f_{h|_{p_{\mu_{ik}+}}} p^2 \, dp \right\} \, d\mu \, dx.
\]

We can integrate all the functions above by Gauss-Lobatto quadrature. We use it for the integrals of \( f_h p^2 \) over intervals, so that the endpoints values can balance the flux terms of boundary integrals, obtaining then CFL conditions. So

\[
I = \frac{1}{V_{ikm}} \left[ \int_{\partial_\Omega_{km}} \left\{ s_1 \sum_{q=1}^N \bar{w}_q f_{h|_{x_q}} p^2 \Delta x_i - \frac{\Delta t^n}{\eta} \left( \hat{H}(x) f_{h|_{x^+}} p^2 - \hat{H}(x) f_{h|_{x^-}} p^2 \right) \right\} \, dp \, dx \right] \\
+ \int_{\partial_{\mu_{ik}^+}} \left\{ s_2 \sum_{\tau=1}^N \bar{w}_\tau f_{h|_{p_{\tau}}} p^2 \Delta p_{\tau} - \frac{\Delta t^n}{\eta} \left( \sum_{\pm} \pm \hat{H}(x) f_{h|_{p_{\pm}}} p^2 \right) \right\} \, d\mu \, dx \\
+ \int_{\partial_{\mu_{ik}^-}} \left\{ s_3 \sum_{\kappa=1}^N \bar{w}_\kappa f_{h|_{\mu_{\kappa}}} p^2 \Delta \mu_{\kappa} - \frac{\Delta t^n}{\eta} \left( \sum_{\pm} \pm (1 - \mu_{m_{\pm}}^2) \hat{H}(x) f_{h|_{\mu_{m_{\pm}}}} p \right) \right\} \, d\mu \, dx = p^2 \, dp \, d\mu \times

\[
\left[ \int_{\partial_\Omega_{km}} s_1 \Delta x_i \sum_{q=1}^N \bar{w}_q f_{h|_{x_q}} \left( \bar{w}_1 f_{h|_{x_q^+}} + \bar{w}_N f_{h|_{x_q^-}} \right) - \frac{\Delta t^n}{\eta s_1} \Delta x_i \left( \hat{H}(x) f_{h|_{x^+}} - \hat{H}(x) f_{h|_{x^-}} \right) \right] \\
+ \int_{\partial_{\mu_{ik}^+}} s_2 \Delta p_{\tau} \left( \bar{w}_1 f_{h|_{p_{\tau}^+}} + \bar{w}_N f_{h|_{p_{\tau}^+}} + \bar{w}_N f_{h|_{p_{\tau}^-}} + \bar{w}_N f_{h|_{p_{\tau}^-}} \right) \, d\mu \, dx \\
- \frac{\Delta t^n}{\eta s_2} \Delta p_{\tau} \left( p_{\mu_{ik}^+}^2 \hat{H}(x) f_{h|_{p_{\mu_{ik}^+}}} - p_{\mu_{ik}^-}^2 \hat{H}(x) f_{h|_{p_{\mu_{ik}^-}}} \right) \, d\mu \, dx \\
+ \int_{\partial_{\mu_{ik}^-}} s_3 \sum_{\kappa=1}^N \bar{w}_\kappa f_{h|_{\mu_{\kappa}}} \left( \bar{w}_1 f_{h|_{\mu_{\kappa}^+}} + \bar{w}_N f_{h|_{\mu_{\kappa}^+}} \right) + \sum_{\kappa=1}^{N-1} \bar{w}_\kappa f_{h|_{\mu_{\kappa}^-}} \, d\mu \, dx \\
- \frac{\Delta t^n}{\eta s_3} \Delta \mu_{\kappa} \left( \sum_{\pm} \pm (1 - \mu_{m_{\pm}}^2) \hat{H}(x) f_{h|_{\mu_{m_{\pm}}}} \right) \, d\mu \right] = \frac{1}{V_{ikm}}.
\]
We reorganize the terms involving the endpoints, which are in parenthesis. So

\[
I = \frac{1}{V_{k,m}} \int_{\partial_s \Omega_{k,m}} s_1 \Delta x_i \left\{ \left( \hat{w}_1 f_{h|x}^{+} + \frac{\Delta t^n}{\eta_1 \Delta x_i} \hat{H}^{(x)} f_{h|x}^{-} \right) \\
+ \left( \hat{w}_N f_{h|x}^{-} - \frac{\Delta t^n}{\eta_1 \Delta x_i} \hat{H}^{(x)} f_{h|x}^{+} + \sum_{q=2}^{N-1} \hat{w}_q f_{h|x}^{q} \right) \right\} p^2 dp d\mu + \\
\int_{\partial_p \Omega_{k,m}} s_2 \Delta p_k \left\{ \sum_{i=2}^{N-1} \hat{w}_i f_{h|p}^{i} p_i^2 + p_k^2 \left( \hat{w}_1 f_{h|p}^{+} + \frac{\Delta t^n}{\eta_2 \Delta p_k} \hat{H}^{(p)} f_{h|p}^{-} \right) \\
+ \Delta t^n \left( \frac{\Delta t^n}{\eta_2 \Delta p_k} \hat{H}^{(p)} f_{h|p}^{+} \right) \right\} d\mu dx + \\
\int_{\partial_s \Omega_{k,i}} dx dp^2 s_3 \Delta \mu_m \left\{ \sum_{i=2}^{N-1} \hat{w}_i f_{h|\mu}^{i} + \left( \hat{w}_1 f_{h|\mu}^{+} + \frac{\Delta t^n}{\eta_3 \Delta \mu_m} \hat{H}^{(\mu)} f_{h|\mu}^{-} \right) \\
+ \Delta t^n \left( \frac{\Delta t^n}{\eta_3 \Delta \mu_m} \hat{H}^{(\mu)} f_{h|\mu}^{+} \right) \right\} ,
\]

To guarantee the positivity of \( I \), assuming that the terms \( f_{h|x}, f_{h|p}, f_{h|\mu} \) 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

\[
0 \leq \hat{w}_N f_{h|x|_{\pm}} + \frac{\Delta t^n}{\eta_1 \Delta x_i} \hat{H}^{(x)} f_{h|x|_{\pm}}, \\
0 \leq \hat{w}_N f_{h|p|_{\pm}} + \frac{\Delta t^n}{\eta_2 \Delta p_k} \hat{H}^{(p)} f_{h|p|_{\pm}}, \\
0 \leq \hat{w}_N f_{h|\mu|_{\pm}} + \frac{\Delta t^n}{\eta_3 \Delta \mu_m} \hat{H}^{(\mu)} f_{h|\mu|_{\pm}} .
\]

We have used the notation below for the numerical flux, given by the upwind rule

\[
\hat{H}^{(x)} f_{h|x|_{\pm}} = \partial p e f_{h|\mu|_{\pm}} = \partial p e \left( \frac{\mu + |\mu|}{2} f_{h|x|_{\pm}} + \frac{\mu - |\mu|}{2} f_{h|x|_{\pm}} \right), \\
\hat{H}^{(p)} f_{h|p|_{\pm}} = -q \hat{E} f_{h|\mu|_{\pm}} = q \left( \frac{|\mu| - E \mu}{2} f_{h|p|_{\pm}} - \frac{E \mu + |E\mu|}{2} f_{h|p|_{\pm}} \right), \\
\hat{H}^{(\mu)} f_{h|\mu|_{\pm}} = -q \hat{E} f_{h|\mu|_{\pm}} = q \left( \frac{-E + |E|}{2} f_{h|\mu|_{\pm}} + \frac{E - |E|}{2} f_{h|\mu|_{\pm}} \right).
\]

We have assumed the positivity of the pdf evaluated at Gauss-Lobatto points, which include endpoints, so we know that \( f_{h|x|_{\pm}}, f_{h|p|_{\pm}}, f_{h|\mu|_{\pm}} \) are positive. The worst case scenario for positivity is having negative flux terms. In this case,

\[
0 \leq \hat{w}_N f_{h|x|_{\pm}} - \frac{\Delta t^n}{\eta_1 \Delta x_i} \partial p e |\mu| f_{h|x|_{\pm}} = f_{h|x|_{\pm}} \left( \hat{w}_N - \frac{\Delta t^n}{\eta_1 \Delta x_i} \partial p e |\mu| \right), \\
0 \leq \hat{w}_N f_{h|p|_{\pm}} - \frac{\Delta t^n}{\eta_2 \Delta p_k} q E(x,t)|\mu| f_{h|p|_{\pm}} = f_{h|p|_{\pm}} \left( \hat{w}_N - \frac{\Delta t^n}{\eta_2 \Delta p_k} q E(x,t)|\mu| \right), \\
0 \leq \hat{w}_N f_{h|\mu|_{\pm}} - \frac{\Delta t^n}{\eta_3 \Delta \mu_m} q E(x,t)|\mu| f_{h|\mu|_{\pm}} = f_{h|\mu|_{\pm}} \left( \hat{w}_N - \frac{\Delta t^n}{\eta_3 \Delta \mu_m} q E(x,t)|\mu| \right).
\]

We need then for the worst case scenario that

\[
\hat{w}_N \geq \frac{\Delta t^n}{\eta_1 \Delta x_i} \partial p e |\mu|, \quad \hat{w}_N \geq \frac{\Delta t^n}{\eta_2 \Delta p_k} q E(x,t)|\mu|, \quad \hat{w}_N \geq \frac{\Delta t^n}{\eta_3 \Delta \mu_m} q E(x,t)|\mu| ,
\]

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or equivalently,
\[ \frac{\eta s_1 \Delta t}{\partial \nu \epsilon |\nu|} \geq \Delta t^n, \quad \frac{\eta s_2 \Delta p_k}{q |\epsilon| t \mu} \geq \Delta t^n, \quad \frac{\eta s_3 \Delta \mu_m p}{1 - \mu_m^2} \geq \Delta t^n. \]

Therefore the CFL conditions imposed to satisfy the positivity of \( I \) are
\[
\frac{s_1 \Delta t}{\max \epsilon \partial \nu \epsilon |\nu| \max |\mu_m^2|} \geq \Delta t^n, \quad \frac{s_2 \Delta p_k}{q \max \epsilon |\epsilon| t \mu \max |\mu_m^2|} \geq \Delta t^n.
\]

Regarding \( II \), there are several ways to guarantee its positivity. One possible way to guarantee it is 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. We would need an additional set of points in which to impose positivity in order to guarantee positivity of \( II \) as a whole, since

\[
II = f_{ikm} + \frac{\Gamma_C}{1 - \eta} = f_{ikm} + \frac{\epsilon \Delta t^n}{1 - \eta} \int_{\Omega_{ikm}} \sum_{j=1}^{1} c_j \epsilon (\epsilon + j \epsilon \omega) \int_{-1}^{1} dp \int_{-1}^{1} dp' f_h p^2 (p') \frac{dp'}{d \epsilon} |_{\epsilon + j \epsilon \omega} \int_{\epsilon + j \epsilon \omega}^{p} p^2 dp d\mu dx \\
\]

\[
- 2 \int_{\Omega_{ikm}} f_h \sum_{j=1}^{1} c_j \epsilon (\epsilon + j \epsilon \omega) \int_{-1}^{1} dp \int_{-1}^{1} dp' f_h p^2 (p') \frac{dp'}{d \epsilon} |_{\epsilon + j \epsilon \omega} \int_{\epsilon + j \epsilon \omega}^{p} p^2 dp d\mu dx \\
+ \int_{\Omega_{ikm}} f_h dV - \frac{4 \pi \Delta \tau^n}{1 - \eta} \int_{\Omega_{ikm}} f_h \left( \sum_{j=1}^{1} c_j \epsilon (\epsilon + j \epsilon \omega) p^2 (p') \frac{dp'}{d \epsilon} |_{\epsilon + j \epsilon \omega} \int_{\epsilon + j \epsilon \omega}^{p} p^2 dp d\mu dx \right) \\
= \frac{1}{V_{ikm}} \left[ \frac{2 \pi \Delta t^n}{1 - \eta} \sum_{j=1}^{1} c_j \int_{\epsilon + j \epsilon \omega}^{p} p^2 (p') \frac{dp'}{d \epsilon} |_{\epsilon + j \epsilon \omega} \int_{\epsilon + j \epsilon \omega}^{p} p^2 dp d\mu dx + \right. \\
\left. \int_{\Omega_{ikm}} f_h (1 - \frac{4 \pi \Delta \tau^n}{1 - \eta}) \sum_{j=1}^{1} c_j \epsilon (\epsilon + j \epsilon \omega) p^2 (p') \frac{dp'}{d \epsilon} |_{\epsilon + j \epsilon \omega} \int_{\epsilon + j \epsilon \omega}^{p} p^2 dp d\mu dx \right] \\
= \frac{1}{V_{ikm}} \left[ \frac{2 \pi \Delta t^n}{1 - \eta} \sum_{j=1}^{1} c_j \int_{\epsilon + j \epsilon \omega}^{p} p^2 (p') \frac{dp'}{d \epsilon} |_{\epsilon + j \epsilon \omega} \int_{\epsilon + j \epsilon \omega}^{p} p^2 dp d\mu dx + \right. \\
\left. \int_{\Omega_{ikm}} f_h (1 - \frac{4 \pi \Delta \tau^n}{1 - \eta}) \sum_{j=1}^{1} c_j \epsilon (\epsilon + j \epsilon \omega) p^2 (p') \frac{dp'}{d \epsilon} |_{\epsilon + j \epsilon \omega} \int_{\epsilon + j \epsilon \omega}^{p} p^2 dp d\mu dx \right] \\
> 0 \Rightarrow \text{Additional point set for positivity}
\]

where the notation for the measure of the elements is
\[
|\Omega_{ikm}| = \Delta x_i \Delta p_k \Delta \mu_m.
\]
Another possible way to guarantee positivity for \( II \) is by considering the collision term as a whole. The difference between the gain and loss integrals will give us a smaller source term, and therefore a more relaxed CFL condition for \( \Delta t^n \). We have

\[
II = \int_{\Omega_{km}} f^n_{ikm} + \frac{\Gamma_C}{1 - \eta} = \int_{\Omega_{km}} f_h dV + \frac{\Delta t^n}{(1 - \eta)} \int_{\Omega_{km}} Q(f_h) dV = \int_{\Omega_{km}} f_h dV + \frac{\Delta t^n}{(1 - \eta)} \int_{\Omega_{km}} Q(f_h) dV = \frac{1}{V_{km}} \int_{\Omega_{km}} f_h dV
\]

\[
\left[ \frac{1}{2} \int_{\Omega_{km}} \int_{j=1}^{+1} c_j \chi(\varepsilon(p) + j\hbar\omega) \int_{-1}^{1} dp' f_h p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \bigg|_{\varepsilon(p)+j\hbar\omega} \right] \nu(p) = \frac{1}{V_{km}} \times \frac{\Delta t^n}{(1 - \eta)} \int_{\Omega_{km}} \left\{ \int_{j=1}^{+1} c_j \chi(\varepsilon(p) + j\hbar\omega) \int_{-1}^{1} dp' f_h p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \bigg|_{\varepsilon(p)+j\hbar\omega} \right\} \nu(p)
\]

\[
\left[ \frac{2\pi \Delta t^n}{(1 - \eta)} \int_{\Omega_{km}} \int_{j=1}^{+1} c_j \chi(\varepsilon(p) + j\hbar\omega) \int_{-1}^{1} dp' f_h p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \bigg|_{\varepsilon(p)+j\hbar\omega} \right] \nu(p) = \frac{4\pi}{V_{km}} \int_{\Omega_{km}} \left\{ \int_{j=1}^{+1} c_j \chi(\varepsilon(p) + j\hbar\omega) \int_{-1}^{1} dp' f_h p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \bigg|_{\varepsilon(p)+j\hbar\omega} \right\} \nu(p)
\]

We have then

\[
II = \int_{\Omega_{km}} f^n_{ikm} + \frac{\Gamma_C}{1 - \eta} = \int_{\Omega_{km}} f_h dV + \frac{\Delta t^n}{(1 - \eta)} \int_{\Omega_{km}} Q(f_h) dV = \frac{1}{V_{km}} \int_{\Omega_{km}} f_h dV + \frac{\Delta t^n}{(1 - \eta)} \int_{\Omega_{km}} Q(f_h) dV
\]

\[
Q(f_h) = 2\pi \int_{\Omega_{km}} \int_{j=1}^{+1} c_j \chi(\varepsilon(p) + j\hbar\omega) \int_{-1}^{1} dp' f_h(x, p) \eta' p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \bigg|_{\varepsilon'=\varepsilon(p)+j\hbar\omega} - f_h \nu(p)
\]

\[
\nu(p) = 4\pi \int_{\Omega_{km}} \int_{j=1}^{+1} c_j \chi(\varepsilon(p) + j\hbar\omega) \int_{-1}^{1} dp' f_h(x, p) \eta' p^2(\varepsilon') \frac{dp'}{d\varepsilon'} \bigg|_{\varepsilon'=\varepsilon(p)+j\hbar\omega} = \nu(p)
\]

We want \( II \) to be positive. If the collision operator part was negative, we choose the time step \( \Delta t^n \) 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 the following,

\[
II = \int_{\Omega_{km}} \int_{\Omega_{km}} f_h(x, p, \mu, t) + \frac{\Delta t^n}{(1 - \eta)} Q(f_h)(x, p, \mu, t) p^2 d\mu dy dx \geq 0
\]

\[
II = \frac{\Omega_{km}}{V_{km}} \sum_{q,r,s} w_q w_r w_s \int_{\Omega_{km}} f_h(x_q, p_r, \mu_s, t) + \frac{\Delta t^n}{(1 - \eta)} Q(f_h)(x_q, p_r, \mu_s, t) p^2 \geq 0
\]

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If \( 0 > Q(f_h) \) for any of the points \((x_q, p_r, \mu_s)\) at time \( t = t^n \), then choose \( \Delta t^n \) s. t.

\[
0 \leq f_h(x_q, p_r, \mu_s, t) + \frac{\Delta t^n}{(1 - \eta)} Q(f_h)(x_q, p_r, \mu_s, t),
\]

\[
0 \leq f_h(x_q, p_r, \mu_s, t) - \frac{\Delta t^n}{(1 - \eta)} Q(f_h)(x_q, p_r, \mu_s, t),
\]

\[
\Delta t^n \leq \frac{(1 - \eta) f_h(x_q, p_r, \mu_s, t)}{|Q(f_h)(x_q, p_r, \mu_s, t)|}.
\]

Our CFL condition in this case would be then

\[
\Delta t^n \leq (1 - \eta) \min_{Q(f_h)(x_q, p_r, \mu_s, t^n) < 0} \left\{ \frac{f_h(x_q, p_r, \mu_s, t^n)}{|Q(f_h)(x_q, p_r, \mu_s, t^n)|} \right\}. \tag{6.4}
\]

The minimum for the CFL condition is taken over the subset of Gaussian Quadrature points \((x_q, p_r, \mu_s)\) inside the cell \( \Omega_{ikm} \) over which \( Q(f_h)(x_q, p_r, \mu_s, t^n) < 0 \).

This subset of points might be different for each time \( t^n \).

We have figured out the respective CFL conditions for the transport and collision parts. Finally, we only need to choose the optimal parameter \( \eta \) that gives us the most relaxed CFL condition for \( \Delta t^n \) such that positivity is preserved for the cell average at the next time, \( f_{ikm}^{n+1} \). The positivity of the whole numerical solution to the pdf, not just its cell average, can be guaranteed by applying the limiters in [9, 10], 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.

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