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entitled
Legendre Polynomial Expansion of the Electron Boltzmann
Equation Applied to the Discharge in Argon

by
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An Abstract of

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The main effort of the present dissertation is to establish a framework for construction of the numerical solution of the system of partial differential equations for the coefficients in the N-term expansion of the solution of the Boltzmann equation in Legendre polynomials, also known as the $P_N$ approximation of the Boltzmann equation. The key feature of the discussed solution is the presence of multiple waves moving in opposite directions in both velocity and spatial domains, which requires transformation of the expansion coefficients to characteristic variables and a directional treatment (up/down winding) of their velocity and spatial derivatives. After the presence of oppositely directed waves in the general solution is recognized, the boundary conditions at the origin of velocity space are formulated in terms of the arriving and reflected waves, and the meaning of the characteristic variables is determined, then the construction proceeds employing the standard technique of operator splitting. Special effort is made to insure numerically exact particle conservation in treatment of the advection and scattering processes.
The constructed numerical routine has been successfully coupled with a solver for the Poisson equation in a self-consistent model of plasma discharge in argon for a two parallel-plate bare electrode geometry. The results of this numerical experiment were presented at the workshop on “Nonlocal, Collisionless Electron Transport in Plasmas” held at Plasma Physics Laboratory of Princeton University on August 2-4, 2005.
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To my parents, my sister and my wife.
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Notations

Vector in the coordinate space

\[ \mathbf{r} = r_x e_x + r_y e_y + r_z e_z = x e_x + y e_y + z e_z. \]  \hfill (0.1)

Vector in the velocity space and its absolute value

\[ \mathbf{v} = v_x e_{v_x} + v_y e_{v_y} + v_z e_{v_z} \]
\[ v = (v_x^2 + v_y^2 + v_z^2)^{\frac{1}{2}}. \] \hfill (0.3)

Cosine of the polar angle \( \theta \) in the velocity space

\[ \zeta = \cos \theta = \frac{v_z}{v}. \] \hfill (0.4)

Matrix

\[ A = \begin{bmatrix}
A_{1,1} & A_{1,2} & \cdots & A_{1,N} \\
A_{2,1} & A_{2,2} & \cdots & A_{2,N} \\
\vdots & \vdots & \ddots & \vdots \\
A_{N,1} & A_{N,2} & \cdots & A_{N,N}
\end{bmatrix} = [A_{i,j}] \] \hfill (0.5)

Matrix element

\[ [A]_{i,j} = A_{i,j}. \] \hfill (0.6)

Column matrix, given in italic to discriminate it from a vector,

\[ \mathbf{a} = \begin{bmatrix}
a_1 \\
a_2 \\
\vdots \\
a_N
\end{bmatrix} = [a_1 \ a_2 \ \cdots \ a_N]^T. \] \hfill (0.7)

Raw matrix

\[ \tilde{\mathbf{a}} = [a_1 \ a_2 \ \cdots \ a_N]. \] \hfill (0.8)

Diagonal matrix

\[ \text{diag}(A_i) = [A_i \delta_{i,j}]. \] \hfill (0.9)

Gradient

\[ \frac{\partial f}{\partial \mathbf{r}} = \text{grad}_r f = e_x \frac{\partial f}{\partial x} + e_y \frac{\partial f}{\partial y} + e_z \frac{\partial f}{\partial z}. \] \hfill (0.10)

Divergence

\[ \frac{\partial \mathbf{f}}{\partial \mathbf{r}} = \text{div}_r \mathbf{f} = \frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z}. \] \hfill (0.11)

Imaginary

\[ i = \sqrt{-1}. \] \hfill (0.12)

Complex conjugate

\[ \bar{z} = x - iy \quad \text{for} \quad z = x + iy \] \hfill (0.13)
Kronecker delta

\[
\delta_{i,j} = \begin{cases} 
1 & \text{for } i = j \\
0 & \text{for } i \neq j 
\end{cases}
\] (0.14)

Dirac delta function

\[
\delta(x) : \int dx \, \delta(x - a)f(x) = f(a)
\] (0.15)

Range of integer numbers

\[
\mathbb{N}, \mathbb{M} = N, N + 1, ... M - 1, M
\] (0.16)
Chapter 1

Introduction

This study discusses the method to obtain a numerical solution of the $P_N$ approximation of the Boltzmann equation. Due to the author’s present involvement into the numerical simulations of barrier and glow discharges, the application of the method is illustrated with the examples coming from the area of low temperature plasmas.

The Boltzmann equation (see references [8] and [31])

\[
\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{r}} + \mathbf{a} \frac{\partial f}{\partial \mathbf{v}} = S(f)
\]  

(1.1)

describes statistically the evolution of a system of identical particles, whose dynamics is governed by the laws of classical mechanics in terms of the distribution function $f(t, \mathbf{r}, \mathbf{v})$. The distribution function is defined in a six-dimensional domain $D_r \times D_v$, called the configuration space, which consists of all the possible pairs ($\mathbf{r}, \mathbf{v}$) of the coordinates and velocities that a particle in the system can achieve. Considered separately $D_r$ and $D_v$ are called the coordinate space and the velocity space domains.
In equation 1.1, \( \mathbf{a}(\mathbf{r}) = \mathbf{F}(\mathbf{r})/m \) is the acceleration of a particle in the system with mass \( m \) at the spatial position \( \mathbf{r} \) caused by an external force \( \mathbf{F}(\mathbf{r}) \). The term \( S(f) \), later referred to as a collision operator, describes the interaction of the particles comprising the system among themselves or with objects not included in the system.

When the distribution function is normalized to unity

\[
\int_{\mathcal{D}_r} d^3\mathbf{r} \int_{\mathcal{D}_v} d^3\mathbf{v} f = 1, \tag{1.2}
\]

the value of \( f(t, \mathbf{r}, \mathbf{v})d^3\mathbf{v}d^3\mathbf{r} \) determines the probability to find a particular particle of the system in a volume \( d^3\mathbf{v}d^3\mathbf{r} \) of the configuration space. The probabilistic nature of the distribution function indicates that \( f \) has to be positive at every point of the configuration space.

In the absence of external forces, collisions with the outside objects and energy losses in particle collisions (for example photon emission), the distribution function of a system relaxes (“thermalizes”) to the Maxwellian distribution

\[
f_M = \frac{1}{V} \left( \frac{m}{2\pi kT} \right)^{3/2} e^{-\frac{mv^2}{2kT}} \tag{1.3}
\]

due to the energy exchange among the particles during collisions. Here \( V = \int_{\mathcal{D}_r} d^3\mathbf{r} \) is the physical volume of the system, \( m \) is the mass of the particle, \( T \) is the temperature of the system, and \( k \) is Boltzmann’s universal constant. The Maxwellian distribution function \( f_M \) is only dependent on the absolute value of the velocity \( v \) and not on the velocity orientation, being spherically symmetric in \( \mathbf{v} \). For the Maxwellian distri-
bution (or any other distribution that does not depend on the velocity orientation) the average velocity of the particle \( \langle v \rangle = \int d^3v \, v f_M = 0 \), implying the absence of macroscopic currents in the system. Equation 1.1 suggests two possible mechanisms that can affect the shape of the distribution function. The more evident one involves the term \( a \frac{\partial f}{\partial v} \) and is caused by the application of an external force creating acceleration. The other one influences the distribution function through the spatial variance in its shape and is induced by the term \( v \frac{\partial f}{\partial r} \). In both cases the distribution function becomes different from the spherically symmetric form. If the difference is caused by the application of a small external force or spatial variance, it is reasonable to assume that the resultant change from the spherically symmetric shape will also be small.

Using the spherical coordinates in velocity space (see appendix A) and assuming the distribution function to be a smooth function of angles \( \theta \) and \( \phi \), it can be expanded into associated Legendre polynomials (or into spherical harmonics), and when it does not depend on \( \phi \) into Legendre polynomials

\[
f(t, z, v, \theta) = \sum_{n=0}^{N \to \infty} f_n(t, z, v) P_n(\cos \theta).
\]

Here the spatial dependence of the distribution function has to be reduced to one spatial coordinate (see appendix A). In practical calculations, one often has to use the truncated expansion with a finite \( N \). Following the established tradition in the theory of neutron transport (see references [34], [5], [9] and [24]), we will call the truncated sum 1.4 a \( P_N \) approximation of the distribution function \( f \). For the Maxwellian distribution, \( f_0 = f_M \) determines the spherically symmetric component and the rest
of the expansion coefficients \( f_{n>0} = 0 \). If the distribution function is only slightly different from a Maxwellian, it is reasonable to expect that most of the difference is due to the presence of the first non-spherically symmetric term \( f_1P_1 \) in the expansion \( 1.4 \), and it is possible to obtain a relevant description of the system with a simple truncated “two-term” (or \( P_1 \)) approximation \( f = f_0 + f_1 \cos \theta \). The spherical harmonics produce a similar expansion of the distribution function: \( f = f_0 + f_1 \frac{v}{v} \).

In the case of large forces or large spatial deviations of the distribution function, the expansion has to contain many terms to satisfactorily resolve the deviation of the distribution function from a simple spherically symmetric form. The examples can be found in the treatments of semiconductor devices (see reference [4]) and plasmas of glow and barrier discharges (see references [45] and [33]). For many of the mentioned systems the thermalization time is much longer than the time scales on which the system is influenced by the external forces or collisions with the external objects, so that the collision operator can be considered linear in \( f \). To deal with the general case, the Boltzmann equation \( 1.1 \) can be converted to spherical coordinates (see appendix A)

\[
\frac{\partial f}{\partial t} + v \cos \theta \frac{\partial f}{\partial z} + a_z(z) \left( \cos \theta \frac{\partial f}{\partial v} - \frac{\sin \theta}{v} \frac{\partial f}{\partial \theta} \right) = S(f) \tag{1.5}
\]

and its distribution function can be expanded into spherical harmonics in the velocity space. In this dissertation, we consider the case when by use of expansion \( 1.4 \) for the distribution function \( f \), equation \( 1.5 \) can be transformed into a system of differential
equations for the expansion coefficients $f_n$ (see appendix C):

\[
\frac{\partial f_n}{\partial t} + \left\{v \frac{\partial f_{n+1}}{\partial z} + a_z \left(\frac{\partial f_{n+1}}{\partial v} + \frac{f_{n+1}}{v} (n+2)\right)\right\} \frac{n+1}{2n+3} + \left\{v \frac{\partial f_{n-1}}{\partial z} + a_z \left(\frac{\partial f_{n-1}}{\partial v} - \frac{f_{n-1}}{v} (n-1)\right)\right\} \frac{n}{2n-1} = S_n(f_0...f_N).
\] (1.6)

During the last fifty years, the system of equations 1.6 and a similar system obtained for the expansion of the distribution function into spherical harmonics (see article [19] or book [34] p.129) have found numerous applications in the areas of neutron and radiation transport, solid state physics, and physics of plasmas. Relevant problems of the neutron and radiation transport are discussed in books [34], [5], [9] and in the references of article [24]. Examples of the recent applications in the physics of semiconductors are given in book [13] and the references therein. This author is more familiar with the works in the field of plasma physics. For $N \leq 7$, stationary solutions of equation 1.6 without spatial terms were considered by A. V. Phelps, L. C. Pitchford, W. A. Allis and coworkers in the first part of 1980-s, in the series of works [42], [43], [2], [41] about the properties of electron-swarms in $N_2$ and model gases. The review of the developments in the solution of the Boltzmann equation expanded into spherical harmonics until 1986 can be found in the article [47]. Solutions of the Boltzmann equation expanded into spherical harmonics were considered by K. Ness, R. Robson, R. White and coworkers. Their progress until 2001 is summarized in the review [56]. R. Winkler, D. Loffhagen, F. Sigeneger, G. Petrov and coworkers mainly considered solutions of the Legendre polynomial expansions of the Boltzmann equation. Review [57] presents the developments made until 2004 with this approach.
Relevant to the topic of this dissertation are works discussing numerical solutions of the time and space dependent Boltzmann equation coupled with the Poisson equation. At present in both industry and academia, the two-term spherical harmonic expansions of the distribution function are routinely used for numerical solution of this problem. For an example of a recent algorithm of this type see article [21]. Examples of numerical solutions of the Boltzmann equation 1.1 that use Cartesian geometry in the velocity space are less frequent. Examples related to plasma discharges can be found in the article [10] and references therein. More works have been devoted recently to the numerical simulations of instabilities in the coupled Vlasov(Boltzmann equation missing the collision operator)-Poisson systems (see references [52] and [6]).

The motivation of the study presented in this dissertation came from the author’s efforts to obtain a numerical description for the behavior of the plasma electrons governed by equations 1.6 with the methods currently described in the literature. In modeling of plasma discharges, the equations that determine the motion of ions and electrons have to be solved together with the Poisson equation to obtain a complete (self-consistent) numerical model. The one-dimensional Poisson equation

\[
\frac{\partial E_z}{\partial z} = \frac{q}{\varepsilon_0},
\]

(1.7)

where \(\varepsilon_0\) is the vacuum dielectric constant, allows one to obtain the electric field \(E_z\) for a known charge density \(q = e(n^i - n^e)\), where \(n^i\) and \(n^e\) are the spatial densities of ions and electrons respectively. When electrons are described by the Boltzmann
equation, their spatial density can be found as

$$n^e = \int_{D_v} d^3\mathbf{v} = 4\pi \int_0^V dv \, v^2 f_0,$$  \hspace{1cm} (1.8)

where $V$ is the maximum absolute value of the velocity that the electron can achieve.

The electric field, found from the Poisson equation

$$E_z = \frac{1}{\epsilon_0} \int_0^z dz' (n^i - \int_{D_v} d^3\mathbf{v} f) + E_{ext},$$  \hspace{1cm} (1.9)

where $E_{ext}$ is an applied external field, determines the acceleration of the electrons and drift velocities of the ions (assuming a drift-diffusion model of ion motion). Notice that $a_z = \frac{eE_z}{m_e}$ is dependent on $f$ and being substituted into equation 1.6, makes the equation non-linear in $f$. It is reasonable to suppose that a numerical solution of the equations 1.6 and 1.9 coupled together would be quite sensitive to a particular implementation due to the mentioned nonlinearity. Hence, along with the requirements formulated for the methods of solution of the coupled Vlasov and Poisson equations (see article [6]), the author’s minimal requirements on the numerical methods describing the motion of ions and electrons are the conservation of particles and the absence of negative densities. With these requirements in mind, the author has implemented the methods for the solution of equation 1.6 currently available in the literature.

The finite-difference method, used for the numerical solution of equation 1.6 without spatial dependence by D. Loffhagen, R. Winkler and coworkers, can be found in article [32]. It is an implicit in time, second-order method with a “straightforward”
calculation of the velocity derivative \( \left( \frac{\partial f_n}{\partial v} \right)_{s+1/2} = \frac{1}{2} \left( f_{n+1,i}^{s+1} - f_{n,i}^{s+1} + f_{n,i+1}^{s+1} - f_{n,i}^{s+1} \right) \),

where \( s \) and \( i \) are the temporal and velocity indices and \( \nu \) is the length of the velocity mesh. The author has conducted the matrix and Von Neumann (finite Fourier series) stability analysis for this method, following the procedure of the book [14] vol.1, p.79.

The results suggest that the finite-difference scheme of article [32] is unstable in some vicinity of \( v = 0 \) irrespective of the specific form of the temporal derivative \( \left( \frac{\partial f_n}{\partial t} \right)_{s+1/2} \), the scattering term \( S \) in the equation 1.6, and its boundary conditions. More to the author’s surprise has been the finding that at least a dozen different numerical methods that the author tried to use to approximate the velocity and temporal derivatives have shown the same type of instability. The evidence of the instability of the above method is also indicated in a recent article [7]. In addition, the boundary conditions that can be found in article [32]: \( f_{n=odd}^{s+1/2} (v = 0) = 0 \), suggest a non-removable discontinuity of the distribution function at \( v = 0 \). The boundary conditions, in turn, seem to be a matter of disagreement among researchers. For example, the authors of article [7] use the boundary conditions \( \left( \frac{\partial f_n}{\partial v} \right)_{v=0} = 0 \) and \( f_{n>0} (v = 0) = 0 \) (and cite article [32] as their source).

K. Ness, R. Robson, R. White, and coworkers have used a Galerkin-type method whose description can be found in the review [56]. In brief, they use an additional expansion of the coefficients \( f_n(t, v) = \sum_{i=1}^{N_v} f_{n,i} \varphi_i(v) \), where \( \varphi_i(v) \) is a set of \( N_\varphi \), in general, arbitrary functions. After substitution of the expansion for \( f_n(t, v) \) into equation 1.6, the result can be multiplied by \( \varphi_j(v) \) and integrated over \( v \) yielding a system of \( N \times N_\varphi \) ordinary differential equations. It is noted in review [56], that the result of the calculations is largely dependent on the particular choice of \( \varphi_i(v) \), may
require large $N_\varphi$ for convergence, or the method may simply fail. The author has also implemented this method for several different sets of $\varphi_i(v)$ and has two additional remarks: Firstly, the implementation of particle conservation, although in principle possible, would be a much more difficult task with this method than with any of the finite-difference methods. Secondly, the proper behavior of the distribution function at $v = 0$ (see formula 3.39) is achievable with the right choice of $\varphi_i(v)$.

The conclusion of review [56] and the introduction of review [57] state the need for better numerical methods to solve the Boltzmann equation expanded into spherical harmonics, as well as the need for a clear formulation of the boundary conditions to properly address the full plasma problem (for the Boltzmann equation expanded into spherical harmonics coupled with Maxwell’s equations for the electric and magnetic fields).

The main feature of equation 1.6 that has to be properly addressed by a numerical method is it’s “wave” character (see subsection 3.1.1). It intrinsically contains multiple pairs of “waves” going in opposite directions in both $v$ and $z$ so that the velocity derivative $\frac{\partial f_n}{\partial v}$ and spatial derivative and $\frac{\partial f_n}{\partial z}$ have to be discretized in a special manner to produce a numerically stable finite-difference method. The waves appear in pairs because of the transition to a half-line $v \geq 0$ that has to be done in order to convert equation 1.1 into its spherical coordinate form 1.5. To produce a meaningful solution, the amplitudes of the waves coming to and leaving the point $v = 0$ have to be matched appropriately.

The following example, suggested to the author by A. Shvydky and displayed in figure 1-1, illustrates how a pair of waves originates. Consider the equation
\[ \frac{\partial f}{\partial t} + a \frac{\partial f}{\partial v} = 0, \]
serving in this example as a simplified model of equation 1.1, with \( a > 0 \)
and \( v \) defined over the entire real line from \(-\infty \) to \(+\infty \). Its solution is a wave \( f(v-at) \)
going toward the positive direction of \( v \) as shown by the graph on the left. Imagine
the left graph being drawn on a piece of transparency and animated so that we can
see the motion of the wave. Let’s fold the transparency in two along the vertical axis
to make a half. The result is shown by the right graph. Two waves appear on the
folded transparency. One wave \( f_-(v+at) \) is moving toward the origin \( v = 0 \) and the
other wave \( f_+(v-at) \) is moving in the opposite direction. Both waves are restricted to
positive values of \( v \). At the origin, \( f_- \) reflects and transforms into \( f_+ \). Algebraically,
the folding is done by the coordinate transformation \( v = xc \) with \( c = \mp 1 \) that serves
as a transformation to the (one-dimensional) spherical coordinates. In this simplified
model, \( c = \mp 1 \) defines only two directions. The coordinate transformation restricts
the domain of definition for the original equation to half-line \( v \geq 0 \) and produces
two equations:
\[ \frac{\partial f_-}{\partial t} - a \frac{\partial f_-}{\partial x} = 0 \quad \text{and} \quad \frac{\partial f_+}{\partial t} + a \frac{\partial f_+}{\partial x} = 0. \]
Their solutions \( f_-(v+at) \) and \( f_+(v-at) \) need the boundary condition \( f_+ = f_- \) at \( v = 0 \) in order to be equivalent
to the solution \( f(v - at) \) of the original equation \( \frac{\partial f}{\partial t} + a \frac{\partial f}{\partial v} = 0 \).
Being unable to find an appropriate method for the solution of system 1.6, the author was left with no other option but to develop his own. The choice had to be made about a numerical method to use for the description of the two-dimensional advective motion present in each of the equations of the system 1.6. A recent comparison review of the numerical methods for the two-dimensional advection problems [18] provided the answer: a fast, accurate and easily implementable algorithm can be obtained by combining the method of operator-splitting (see appendix G) and an accurate method for the solution of the one-dimensional advection problem. Comparison of the different methods for solution of the one-dimensional advection equation, provided in book [37], p.323 and study [25], pointed towards Leonard’s high-order conservative flux-limited method as the best choice. Fortunately, article [28] by the same author considers the application of the operation-splitting technique to problems of two-dimensional advection.

An important feature of the method of operator-splitting is that it allows decoupling of the physical processes present in system 1.6. Thus, a numerical procedure for each process can be developed and tested separately.

In chapter 2, the analytical solution of equation 1.6 without the collision term $S$ is constructed on the half-line $v \geq 0$. The author decided not to discuss the analytical solution of this problem on the interval $0 \leq v \leq V$, due to its increasing complexity. One can develop the analytical solution on the interval using the results of sections 2.1, 2.2 and appendix E. The analytical solution, constructed in this chapter, serves as a reference for the later numerical consideration of the same problem. It also demonstrates the main disadvantage of the truncated expansion - the distribution
function 1.4 may become negative in some regions of the velocity space.

In chapter 3, the method of operator splitting is consecutively applied to decouple various physical processes described by equation 1.6 and to obtain relevant numerical procedures for their modeling. Special attention is paid to the ability of each procedure to conserve particles. The obtained numerical routines are further assembled into the procedure for the solution of equation 1.6 without spatial dependence. The addition of spatial terms and the consequent discussion on a parallel implementation completes the development of the method.

Chapter 4 presents the results of application of the obtained method to a model of the discharge in the argon gas that consists of equation 1.6 for electrons, a fluid equation for the argon ions, and the Poisson equation 1.7.
Chapter 2

Solution of $P_N$ approximation of advection equation.

In this chapter we derive the formal solution of the advection equation in the velocity space under conditions appropriate for the application of the $P_N$ approximation, that is when $\mathbf{a} = a_z \mathbf{e}_{v_z}$, where $\mathbf{e}_{v_z}$ is a unit vector pointing along $v_z$ axis (see Appendix A). We omit the term $\mathbf{v} \frac{\partial f}{\partial r}$ in equation 1.1 and consider the simplest case of $a_z = \text{const}$, to obtain the advection equation in the velocity space,

$$\frac{\partial f}{\partial t} + a_z \mathbf{e}_{v_z} \frac{\partial f}{\partial v} = \frac{\partial f}{\partial t} + a_z \frac{\partial f}{\partial v_z} = 0. \quad (2.1)$$
In the $P_N$ approximation, the system of equations for the expansion coefficients $f_n$ corresponding to equation 2.1 is (see Appendix C)

$$\frac{\partial f_n}{\partial t} + a_z \left( \frac{\partial f_{n+1}}{\partial v} + f_{n+1}(n+2) \right) \frac{n+1}{2n+3} + a_z \left( \frac{\partial f_{n-1}}{\partial v} - f_{n-1}(n-1) \right) \frac{n}{2n-1} = 0,$$

(2.2)

where

$$0 \leq n \leq N.$$  

(2.3)

Introducing a column matrix for the expansion coefficients $f_n$

$$f = [f_0 \ f_1 \ \cdots \ f_N]^T$$

(2.4)

and matrices

$$A_{k,s} = \delta_{k,s-1} \frac{k+1}{2k+3} + \delta_{k,s+1} \frac{k}{2k-1},$$

(2.5)

$$B_{k,s} = \delta_{k,s-1} \frac{(k+2)(k+1)}{2k+3} - \delta_{k,s+1} \frac{(k-1)k}{2k-1},$$

(2.6)

equations 2.2 can be rewritten in matrix form

$$\frac{\partial f}{\partial t} + a_z \left( A \frac{\partial f}{\partial v} + \frac{1}{v} B f \right) = 0.$$  

(2.7)

The above equation can be reexpressed as

$$\left[ \frac{\partial}{\partial t} + a_z L(v) \right] f = 0,$$

(2.8)
where we introduced an operator

\[
L(v) = A \frac{\partial}{\partial v} + \frac{1}{v} B,
\]  

(2.9)

By determination of the eigenfunctions of the operator \( L(v) \), equation 2.7 can be solved by separation of variables.

### 2.1 Eigensystem of \( L(v) \)

The eigenvalue problem for the operator \( L(v) \) (see formula 2.9) is given by

\[
L(v)f = i\lambda f,
\]

(2.10)

or in component form

\[
\left( \frac{\partial f_{n+1}}{\partial v} + \frac{f_{n+1}}{v} (n + 2) \right) \frac{n + 1}{2n + 3} + \left( \frac{\partial f_{n-1}}{\partial v} - \frac{f_{n-1}}{v} (n - 1) \right) \frac{n}{2n - 1} = i\lambda f_n.
\]

(2.11)

For further convenience, we assume that the eigenvalues of \( L(v) \) are pure imaginary numbers \( i\lambda \). The above equation can be written as

\[
v^{-(n+2)} \frac{\partial (v^{n+2} f_{n+1})}{\partial v} \frac{n + 1}{2n + 3} + v^{n-1} \frac{\partial (v^{-(n-1)} f_{n-1})}{\partial v} \frac{n}{2n - 1} = i\lambda f_n.
\]

(2.12)
On the basis of the recurrence relations for the Bessel functions $J_\nu(v)$ (see reference [3], p.671)

$$v^{-\nu}\frac{\partial}{\partial v}\left(v^\nu J_\nu(v)\right) = J_{\nu-1}(v) \quad \text{and} \quad v^{-\nu}\frac{\partial}{\partial v}\left(v^{-\nu}J_\nu(v)\right) = -J_{\nu+1}(v), \quad (2.13)$$

one can hope to simplify equation 2.12 with the substitution

$$f_n(v) = i^n v^{s_n} J_{\nu_n}(v) \varphi_n, \quad (2.14)$$

where $\varphi_n$ are coefficients, undetermined at this point. Equating the same powers of $v$ and indices of the Bessel functions in equation 2.12 with the recurrence relations 2.13, requires

$$n + 2 + s_{n+1} = \nu_{n+1} \quad \text{and} \quad n - 1 - s_{n-1} = \nu_{n-1}, \quad (2.15)$$

or

$$\nu_n = n + \frac{1}{2} \quad \text{and} \quad s_n = -\frac{1}{2}. \quad (2.16)$$

The determined values for $\nu_n$ and $s_n$ suggest that

$$f_n(v) = i^n j_n(v) \varphi_n \text{ or } i^n n_n(v) \varphi_n, \quad (2.17)$$

$$j_n(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} J_{n+\frac{1}{2}}(x) \quad \text{and} \quad (2.18)$$

$$n_n(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} N_{n+\frac{1}{2}}(x) = (-1)^{n+1} \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} J_{-n-\frac{1}{2}}(x) \quad (2.19)$$

\[ v^{-n-1} \frac{d}{dv} \left( v^{n+1} j_n(v) \right) = j_{n-1}(v) \] and \[ v^n \frac{d}{dv} \left( v^{-n} j_n(v) \right) = -j_{n+1}(v), \] (2.20)

where \( j_n(v) \) can be interchanged with \( n_n(v) \). In further derivations, we use \( j_n(x) \) and ignore \( n_n(x) \). We will assume that \( j_n(x) \) can be interchanged by a linear combination of \( j_n(x) \) and \( n_n(x) \), unless stated otherwise. Substituting the above value of \( f_n \) into equation 2.11 (or 2.12) and simplifying (but not dropping anything), we obtain

\[ i^{n+1} j_n(v) \left( \frac{n+1}{2n+3} \varphi_{n+1} + \frac{n}{2n-1} \varphi_{n-1} \right) = \lambda i^{n+1} j_n(v) \varphi_n, \] (2.21)

or in matrix form

\[ L(v) f = L(v) J(v) \varphi = i J(v) A \varphi = i \lambda J(v) \varphi = i \lambda f, \] (2.22)

where we introduced

\[ \varphi = [\varphi_0 \ \varphi_1 \ \cdots \ \varphi_N]^T \] and

\[ J(x) = \text{diag}(i^n j_n(x)). \] (2.23)

The second equality in the formula 2.22 suggests that

\[ L(v) J(v) = i J(v) A. \] (2.25)
Note that operator $L(v)$ has the following scaling property

$$L(v) = A \frac{\partial}{\partial v} + \frac{1}{v} B = q(A \frac{\partial}{\partial (qv)} + \frac{1}{qv} B) = qL(qv), \text{ for } q \neq 0.$$ \hspace{1cm} (2.26)

Introducing the eigensystem of matrix $A$ (discussed in Appendix D), that is $\alpha_\ell$ and $a_\ell$ satisfying $A\alpha_\ell = a_\ell \alpha_\ell$, and using the properties of the operator $L(v)$ given by formulas 2.25 and 2.26 yields

$$L(v)J(qv)\alpha_\ell = qL(qv)J(qv)\alpha_\ell = iqJ(qv)A\alpha_\ell = ia_\ell qJ(qv)\alpha_\ell.$$ \hspace{1cm} (2.27)

Comparison with equation 2.22 suggests that

$$f = \xi_\ell(qv) = J(qv)\alpha_\ell \text{ or } f = \eta_\ell(qv) = N(qv)\alpha_\ell,$$ \hspace{1cm} (2.28)

are eigenfunctions and a corresponding eigenvalue of the operator $L(v)$. Here we introduce

$$N(x) = \text{diag}(v^n n_\ell(x)).$$ \hspace{1cm} (2.30)

In the derivation of the above result, we use the scaling property 2.26, which holds for $q \neq 0$. The eigenvalues of matrix $A$ are distinct from zero for $P_{\text{odd}}$. For $P_{\text{even}}$, one of the eigenvectors has a zero eigenvalue. The only possibility of $\lambda = 0$ for the eigenfunctions given by equation 2.28 is when $a_\ell = 0$ for $P_{\text{even}}$. Later, we refer to $\xi_0(qv)$ as the eigenfunctions associated with a zero eigenvalue of matrix $A$. To see
whether solutions different from $\xi_0(qv)$ are possible, we need to consider the case of $\lambda = 0$ separately.

### 2.2 Kernel of $L(v)$

To find eigenfunctions corresponding to zero eigenvalue of $L(v)$ and distinct from those given by equation 2.28, we have to solve the equation

$$L(v)f = A \frac{\partial f}{\partial v} + \frac{1}{v} B f = 0. \quad (2.31)$$

For odd $N$, the number of equations is $N + 1 = l_{\text{even}}$ and matrix $A$ is regular (see appendix D). Hence equation 2.31 has $l_{\text{even}}$ linearly independent solutions.

Let’s start with an even number of equations and later consider the case of an odd number of equations. Rewriting equation 2.31 in component form yields a system of $l_{\text{even}}$ equations with the $n$-th equation ($0 \leq n \leq N$) given by

$$\left( \frac{\partial f_{n+1}}{\partial v} + \frac{f_{n+1}(n + 2)}{v} \right) \frac{n + 1}{2n + 3} + \left( \frac{\partial f_{n-1}}{\partial v} - \frac{f_{n-1}(n - 1)}{v} \right) \frac{n}{2n - 1} = 0, \quad (2.32)$$

where $f_{N+1} = 0$ to satisfy the closure requirement for the $P_N$ approximation (see formula C.9). Looking for a solution in the form

$$f_n(v) = c_n v^s \text{ for } s = 0, 1, 2... \quad (2.33)$$

and substituting it into equation 2.32 gives the $n$-th relation for the coefficients $c_{n+1}$
and $c_{n-1}$

$$(s + n + 2)\frac{n + 1}{2n + 3} c_{n+1} + (s - n + 1)\frac{n}{2n - 1} c_{n-1} = 0. \tag{2.34}$$

Note that for the above relations and for the later relations 2.38 $c_1 = c_{N+1} = 0$.

For $n = s + 1$, relation 2.34 becomes

$$(2s + 3)\frac{s + 2}{2s + 5} c_{s+2} + 0 \cdot c_s = 0. \tag{2.35}$$

This means that $c_s$ is arbitrary. Relations 2.34 further determine that coefficients $..., c_{s-4}, c_{s-2}$ are proportional to $c_s$, while $c_{s+2} = c_{s+4} = c_{s+6} = ... = 0$ and $..., c_{s-1}, c_{s+1}, ...$ are proportional to each other.

If $s$ is even, the odd relations 2.34 define the sequence of coefficients with even indices $c_0, ..., c_{s-2}, c_s$, while $c_{s+2} = c_{s+4} = ... = c_{N+1} = 0$ and $c_1 = c_3 = ... = c_N = 0$.

If $s$ is odd, the even relations determine the sequence of coefficients with odd indices resulting in $c_1 = c_3 = ... c_s = 0$, while $c_{s+2} = c_{s+4} = ... = c_N = 0$ and $c_0 = c_2 = ... = c_{N+1} = 0$. Thus we constructed $l_{\text{even}}/2$ solutions of the form

$$f = \chi_{k/2+1} = [c_0 \ 0 \ c_2 \ 0 \ \cdots \ c_k \ 0 \ \cdots \ 0]^T v^k \text{ for } k = 0, 2, ..., N - 1, \tag{2.36}$$

where non-zero coefficients have even indices and are related to each other by formula 2.34.

Let’s further consider a solution in the form

$$f_n(v) = c_n v^{-s} \tag{2.37}$$
that transforms the $n$-th relation for the coefficients $c_i$ into

$$(-s + n + 2) \frac{n + 1}{2n + 3} c_{n+1} - (s + n - 1) \frac{n}{2n - 1} c_{n-1} = 0. \quad (2.38)$$

Relation 2.38 for $n = s - 2$ becomes

$$0 \cdot c_{s-1} - (2s - 3) \frac{s - 2}{2s - 5} c_{s-3} = 0, \quad (2.39)$$

leaving $c_{s-1}$ arbitrary. Relations 2.38 set $c_{s-3} = c_{s-5} = ... = 0$ while making coefficients $c_{s-1}, c_{s+1}, ...$ proportional to each other as it also does for ..., $c_s, c_{s+2}, ...$.

If $s - 1$ is odd, the even relations 2.38 define the sequence of coefficients with odd indices $c_{s-1}, c_{s+1}, ..., c_N$, while $c_1 = c_3 = ... = c_{s-3} = 0$ and $c_0 = c_2 = ... = c_{N+1} = 0$.

If $s - 1$ is even, the odd relations will determine the sequence of coefficients with even indices resulting in $c_{s-1} = c_{s+1} = ... = c_{N+1} = 0$, while $c_0 = c_2 = ... c_{s-3} = 0$ and $c_1 = c_3 = ... = c_N = 0$. This way we find $l_{\text{even}}/2$ additional solutions of the form

$$f = \chi_{-\frac{k}{2}+1} = \begin{bmatrix} 0 & \cdots & 0 & c_k & \cdots & 0 & c_{N-1} & 0 & c_N \end{bmatrix}^T \begin{bmatrix} v^{-k-1} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix} \text{ for } k = 1, 3, ..., N, \quad (2.40)$$

where non-zero coefficients have odd indices and are related by formula 2.38.

The constructed $l_{\text{even}}$ solutions 2.36 and 2.40 are linearly independent and are the only solutions of system 2.32. Because even equations of the system 2.32 interconnect $f_n$ with odd indices and odd equations interconnect $f_n$ with even indices, expression 2.36 solves the subsystem of odd equations and expression 2.40 solves the subsystem of even equations.
Let’s now increase the number of equations by one to study the \( P_{N+1} \) case. The number of equations becomes equal to \( N + 2 = l_{\text{odd}} \) and the matrix \( A \) becomes singular (see equation D.8). To obtain the solutions of the system 2.32 for the \( P_{N+1} \) case, we compare the \( P_{N+1} \) case with the \( P_N \) case just considered. As before, even and odd equations can be studied separately.

There are \((N + 1)/2 + 1\) even equations in the \( P_{N+1} \) system of which \((N + 1)/2\) are the same as even equations of the \( P_{N+1} \) system. An additional last equation for the \( P_{N+1} \) system interconnects \( f_N \) and \( f_{N+2} = 0 \). The number of equations in the \( P_{N+1} \) system exceeds by one the number of dependent variables, comprising an overdetermined system. From the study of the \( P_N \) case we already know that the first \((N + 1)/2\) even equations of the \( P_{N+1} \) system are well determined and we have constructed their solutions 2.40. To find solutions of the system with the extra equation we just need to eliminate the solutions 2.40 that do not satisfy the additional equation. In the the process of finding the solutions 2.40, we determined the sequence of coefficients with odd indices: \( c_{s-1}, c_{s+1}, c_{s+3}, ..., c_N \) starting from an arbitrary coefficient \( c_{s-1} \). In the \( P_{N+1} \) case, the last of the even relations 2.38 interconnects \( c_N \) and \( c_{N+2} = 0 \), setting \( c_{s-1} = c_{s+1} = ... = c_N = 0 \). Hence for the \( P_{N+1} \) case, the system of even equations has only a trivial solution.

The systems of odd equations in the \( P_N \) and \( P_{N+1} \) cases have the same number of equations with a difference in the last equation. The last odd equation for the \( P_{N+1} \) case interconnects \( f_{N-1} \) with \( f_{N+1} \) which had to be set to zero in the \( P_N \) case. The number of dependent variables in the \( P_{N+1} \) system of odd equations exceeds by one the number of equations, forming an underdetermined system. From the
study of the $P_N$ case, we know that when $f_{N+1} = 0$ the odd equations form a well
determined homogeneous system with solutions given by 2.36. Addition of terms
associated with $f_{N+1}$ form an inhomogeneous system where $f_{N+1}$ can be considered
an arbitrary function. A particular solution of the inhomogeneous system can be
found by recalling that (see section 2.1)

$$f_n(v) = i^n j_n(v) \rho_n$$

(2.41)

substituted into equation 2.32 yields

$$i^{n+1} j_n(v) \left( \frac{n+1}{2n+3} \rho_{n+1} + \frac{n}{2n-1} \rho_{n-1} \right) = 0.$$  (2.42)

Using the scaling property of the operator $L(v)$ (see formula 2.26), we find a particular
solution of the inhomogeneous system to be

$$f = \sum_q \varphi(q) \left[ j_0(qv) \rho_0 \quad -j_2(qv) \rho_2 \quad 0 \quad \cdots \quad 0 \quad i^{N+1} j_{N+1}(qv) \rho_{N+1} \right]^T.$$  (2.43)

where $\rho_{n-1}$ and $\rho_{n-1}$ are related by 2.42, $\varphi(q)$ is an arbitrary function of $q$, and $j_n(qv)$
can be interchanged with $n_n(qv)$.

An additional solution that we did not mention yet can be found by noticing that
the additional terms can be set to zero: $\frac{\partial f_{N+1}}{\partial v} + \frac{f_{N+1}}{v}(N+2) = 0$, while the remaining
functions $f_{n<N+1} = 0$. The corresponding solution is

$$f = \chi_0 = \begin{bmatrix} 0 & \cdots & 0 & c_{N+1} \end{bmatrix}^T v^{-N-2}.$$  (2.44)
The general solution for the system of odd equations in the $P_{N+1}$ case, is a linear combination of the $(l_{odd} - 1)/2$ solutions 2.36, solution 2.44 and solutions 2.43. Solution 2.43 is identical to the eigenfunction of the operator $L(v)$ corresponding to a zero eigenvalue of matrix $A$ (see section 2.1).

### 2.3 Properties of the eigenfunctions

We want to use the eigenfunctions of $L(v)$ to construct $P_N$ expansions of smooth enough real functions $f$ (see reference [3], p.893 for the discussion of required smoothness):

\[
\begin{align*}
f(v, \cos \theta) & \approx \sum_{n=0}^{N} f_n(v) P_n(\cos \theta) = \\
& \sum_{n=0}^{N} \left( \sum_{q \neq 0, \ell} f_{q,\ell} \xi_{n,\ell}(qv) + \sum_{q \neq 0, \ell} f_{1,\ell}^{1} \eta_{n,\ell}(qv) + \sum_{s} f_{s}^{0} \chi_{n,s}(v) \right) P_n(\cos \theta). \quad (2.45)
\end{align*}
\]

Here $\xi_{n,\ell}$ and $\chi_{n,s}$ are eigenfunctions of $L(v)$ defined in the sections 2.1 and 2.2, $f_{q,\ell}$, $f_{1,\ell}^{1}$ and $f_{s}^{0}$ are the expansion coefficients, $q$ is real, index $\ell$ goes over the range given by formula D.12 and $s$ indices the kernel eigenfunctions discussed in section 2.2. In the following, we limit our consideration to smooth enough functions $f(v) = f(v, \cos \theta)$ that are bound

\[
\begin{align*}
v \in D_v : \ |f(v)| < M_1
\end{align*}
\]
and integrable in absolute value over their domain of definition $D_v$ in the velocity space:

$$\int_{D_v} d^3v |f(v)| = 2\pi \int_{D_v} v^2 dv \sin \theta d\theta |f(v, \cos \theta)| < M_2. \tag{2.47}$$

In this section we want to list the properties of the eigenvectors that we use to construct the expansions.

### 2.3.1 Limiting values

Spherical Neumann functions (equations 2.18 and 2.19) can be used in eigenfunction solutions 2.28 instead of the Bessel function (see section 2.1). Spherical Bessel and Neumann functions have different limiting values as $x \to 0$. From their series form ([3], p.724)

$$j_n(x) = 2^n x^n \sum_{s=0}^{\infty} \frac{(-1)^s (s + n)!}{s!(2s + 2n + 1)!} x^{2s} \tag{2.48}$$

$$n_n(x) = \frac{(-1)^{n+1}}{2^n x^{n+1}} \sum_{s=0}^{\infty} \frac{(-1)^s (s - n)!}{s!(2s - 2n)!} x^{2s} \tag{2.49}$$

one can determine their behavior for $0 < x \ll 1$ ([3], p.726)

$$j_n(x) = \frac{x^n}{(2n + 1)!!} + O(x^{n+2}), \tag{2.50}$$

$$n_n(x) = -(2n - 1)!! x^{-n-1} + O(x^{-n+1}). \tag{2.51}$$
The asymptotic form of the spherical Bessel and Neumann functions for $\frac{n(n+1)}{2} \ll x$ ([3], p.727)

\begin{align*}
j_n(x) &= \frac{1}{x} \sin \left(x - \pi \frac{n}{2}\right) + O(x^{-2}) \quad (2.52) \\
n_n(x) &= -\frac{1}{x} \cos \left(x - \pi \frac{n}{2}\right) + O(x^{-2}) \quad (2.53)
\end{align*}

can be determined from the asymptotic form of the Bessel and Neumann functions ([3], p.718)

\begin{align*}
J_{n+1/2}(x) &= \left(\frac{2}{\pi x}\right)^{\frac{1}{2}} \sin \left(x - \pi \frac{n}{2}\right) + O(x^{-\frac{3}{2}}) \quad (2.54) \\
N_{n+1/2}(x) &= -\left(\frac{2}{\pi x}\right)^{\frac{1}{2}} \cos \left(x - \pi \frac{n}{2}\right) + O(x^{-\frac{3}{2}}). \quad (2.55)
\end{align*}

Hence, for $0 < v \ll 1$

\begin{align*}
\xi_{n,\ell}(x) &= iv^n \frac{x^n}{(2n+1)!!} \alpha_{n,i} + O(x^{n+2}) \quad (2.56) \\
\tilde{\xi}_{n,\ell}(x) &= (-iv)^n \frac{x^{n+2}}{(2n+1)!!} \tilde{\alpha}_{n,i} + O(x^{n+4}) \quad (2.57) \\
\eta_{n,\ell}(x) &= -iv^{n} (2n-1)!! x^{-n-1} \alpha_{n,i} + O(x^{-n+1}) \quad (2.58) \\
\tilde{\eta}_{n,\ell}(x) &= (-iv)^n (2n-1)!! x^{-n+1} \tilde{\alpha}_{n,i} + O(x^{-n+3}) \quad (2.59)
\end{align*}
while the asymptotic form for \( \frac{n(n+1)}{2} \ll x \) is

\[
\xi_{n,\ell}(x) = \frac{i^n}{x} \sin \left( x - \frac{n}{2} \right) \alpha_{n,i} + O(x^{-2}) \tag{2.60}
\]

\[
\tilde{\xi}_{n,\ell}(x) = -i^n x \sin \left( x + \frac{n}{2} \right) \tilde{\alpha}_{n,i} + O(1) \tag{2.61}
\]

\[
\eta_{n,\ell}(x) = -\frac{i^n}{x} \cos \left( x - \frac{n}{2} \right) \alpha_{n,i} + O(x^{-2}) \tag{2.62}
\]

\[
\tilde{\eta}_{n,\ell}(x) = -i^n x \cos \left( x + \frac{n}{2} \right) \tilde{\alpha}_{n,i} + O(1). \tag{2.63}
\]

\subsection{2.3.2 Parity}

Parity properties for the eigenfunctions

\[
\xi_{n,\ell}(x) = i^n j_n(x) \alpha_{n,\ell} = (-1)^n \xi_{n,\ell}(-x) = (-1)^n \xi_{n,-\ell}(x) = \xi_{n,-\ell}(-x) \tag{2.64}
\]

\[
\tilde{\xi}_{n,\ell}(x) = x^2 i^n j_n(-x) \tilde{\alpha}_{n,\ell} = (-1)^n \tilde{\xi}_{n,\ell}(-x) = (-1)^n \tilde{\xi}_{n,-\ell}(x) = \tilde{\xi}_{n,-\ell}(-x) \tag{2.65}
\]

\[
\eta_{n,\ell}(x) = i^n n_n(x) \alpha_{n,\ell} = (-1)^{n+1} \eta_{n,\ell}(-x) = (-1)^n \eta_{n,-\ell}(x) = -\eta_{n,-\ell}(-x) \tag{2.66}
\]

\[
\tilde{\eta}_{n,\ell}(x) = x^2 i^n n_n(-x) \tilde{\alpha}_{n,\ell} = (-1)^{n+1} \tilde{\eta}_{n,\ell}(-x) = (-1)^n \tilde{\eta}_{n,-\ell}(x) = -\tilde{\eta}_{n,-\ell}(-x) \tag{2.67}
\]

follow from the parity of

\[
j_n(-x) = (-1)^n j_n(x) \quad \text{and} \quad n_n(-x) = (-1)^{n+1} n_n(x), \tag{2.68}
\]

and the parity for the eigenvectors of matrix \( A \) (see formula D.27). Formula 2.68 is a consequence of the series expansions 2.48 and 2.49. Let’s also notice that all
eigenfunctions form their complex conjugates similarly

\[ (-1)^n \xi_{n,\ell}(x) = \xi_{n,\ell}(x), \quad (-1)^n \tilde{\xi}_{n,\ell}(x) = \tilde{\xi}_{n,\ell}(x), \tag{2.69} \]

\[ (-1)^n \eta_{n,\ell}(x) = \eta_{n,\ell}(x), \quad (-1)^n \tilde{\eta}_{n,\ell}(x) = \tilde{\eta}_{n,\ell}(x). \]

Parity of the eigenfunctions allows rearrangements in the sums as

\[ \sum_{q \neq 0, \ell \neq 0} f_{q,\ell} \xi_{\ell}(qv) = \sum_{0 < q, \ell \neq 0} \phi_{q,\ell} \xi_{\ell}(qv) = \sum_{q \neq 0, 0 < \ell} \phi_{q,\ell} \xi_{\ell}(qv) = \tag{2.70} \]

\[ \sum_{q < 0, \ell \neq 0} \phi_{q,\ell} \xi_{\ell}(qv) = \sum_{q \neq 0, \ell < 0} \phi_{q,\ell} \xi_{\ell}(qv), \]

where summation goes over a symmetric range of indices \(-q, +q\) and \(-\ell, +\ell\) and we introduce the auxiliary function

\[ \phi_{q,\ell} = f_{q,\ell} + f_{-q,-\ell}. \tag{2.71} \]

Next we want to determine the number of linearly independent eigenfunctions corresponding to a given eigenvalue

\[ i\lambda = iqa_\ell \quad \text{that is when} \quad q = \frac{\lambda}{a_\ell}. \tag{2.72} \]

Parity of the eigenvalues of matrix A: \(a_\ell = -a_{-\ell}\) (see formula D.11) combined with
parity properties given by formulas 2.64 - 2.67 yield

\[ \xi_{n,\ell}(\frac{\lambda}{a_{\ell}}) = \xi_{n,-\ell}(\frac{\lambda}{a_{-\ell}}) \]  
\[ \tilde{\xi}_{n,\ell}(\frac{\lambda}{a_{\ell}}) = \tilde{\xi}_{n,-\ell}(\frac{\lambda}{a_{-\ell}}) \]  
\[ \eta_{n,\ell}(\frac{\lambda}{a_{\ell}}) = -\eta_{n,-\ell}(\frac{\lambda}{a_{-\ell}}) \]  
\[ \tilde{\eta}_{n,\ell}(\frac{\lambda}{a_{\ell}}) = -\tilde{\eta}_{n,-\ell}(\frac{\lambda}{a_{-\ell}}). \]

Hence the full range of linearly independent eigenfunctions for \( \lambda \neq 0 \) can be obtained by choosing either \( 0 < \ell \) and \( q \neq 0 \) or \( \ell \neq 0 \) and \( 0 < q \).

### 2.3.3 Trigonometric form.

Spherical Bessel and Neumann functions can be expressed in a finite number of terms by means of algebraic and trigonometric functions (see reference [55], p.52), which is especially simple for a real argument \( x \):

\[ j_n(x) = \frac{1}{x}(e^{ix}p_n(x) + e^{-ix}\overline{p}_n(x)) \]  \hspace{1cm} \text{and}  
\[ n_n(x) = (-1)^{n+1}\frac{1}{x}(e^{ix}p_n(x) - e^{-ix}\overline{p}_n(x)), \]  
\[ p_n(x) = \rho_n(x) + i\sigma_n(x) = \sum_{r=0}^{n} \frac{i^{n-r-1}(n+r)!}{r!(n-r)!(2x)^r}. \]
is an \( n \)-th order polynomial of \( \frac{1}{x^2} \). Expressions

\[
e^{ix}p_n(x) + e^{-ix}\overline{p}_n(x) = 2[\rho_n(x) \cos x - \sigma_n(x) \sin x] \tag{2.80}
\]

\[
i[e^{ix}p_n(x) - e^{-ix}\overline{p}_n(x)] = -2[\sigma_n \cos x + \rho_n(x) \sin x] \tag{2.81}
\]

are combinations of trigonometric functions. Using formulas 2.77 and 2.78, the component forms of the eigenvectors 2.64 - 2.67 and parity property of the Bessel functions given by formulas 2.68, we obtain

\[
\xi_{n,\ell}(x) = i^n \frac{1}{x}(e^{ix}p_n(x) + e^{-ix}\overline{p}_n(x))\alpha_{n,\ell} \tag{2.82}
\]

\[
\tilde{\xi}_{n,\ell}(x) = (-i)^n x(e^{ix}p_n(x) + e^{-ix}\overline{p}_n(x))\tilde{\alpha}_{n,\ell} \tag{2.83}
\]

\[
\eta_{n,\ell}(x) = (-i)^{n+1} \frac{1}{x}(e^{ix}p_n(x) - e^{-ix}\overline{p}_n(x))\alpha_{n,\ell} \tag{2.84}
\]

\[
\tilde{\eta}_{n,\ell}(x) = i^{n+1} x(e^{ix}p_n(x) - e^{-ix}\overline{p}_n(x))\tilde{\alpha}_{n,\ell} . \tag{2.85}
\]

### 2.3.4 Expansion on a half-line \( 0 \leq v \)

To expand the smooth, bound and absolute value integrable functions \( f \) defined on a half-line \( 0 \leq v \), we have to exclude eigenfunctions \( \eta_{q,\ell}(v) \) and \( \chi_s(v) \) for \( s = 0, -1, -2, \ldots \) from the expression 2.45 because otherwise their singularity at \( v \to 0 \) violates property 2.46. We also have to exclude \( \chi_s(v) \) for \( s = 1, 2, \ldots \) because their growth at \( v \to \infty \) violates both properties 2.46 and 2.47. With the discussed limita-
tions, the expansion 2.45 is

\[ f_n(v) = \int_0^\infty dq \sum_\ell \phi_{q,\ell} \xi_{n,\ell}(qv), \] (2.86)

where we used summation over \(0 < q\) and full range of \(\ell\)-s (see formulas 2.70 and 2.71).

Using the closure relation for the Bessel functions (see [3], p.735)

\[ \int_0^\infty dv (pv)^2 j_n(pv) j_n(qv) = \frac{\pi}{2} \delta(p - q), \] (2.87)

we obtain closure for \(J(v)\)

\[ \int_0^\infty dv (pv)^2 J(-pv) J(qv) = \frac{\pi}{2} \delta(p - q), \] (2.88)

and the closure relation

\[ \int_0^\infty dv \tilde{\xi}_i(pv) \xi_j(qv) = \frac{\pi}{2} \delta_{i,j} \delta(p - q), \] (2.89)

which is an indication of completeness for the set of eigenfunctions \(\xi_\ell(qv)\).

The expansion coefficients in formula 2.86 can be found as

\[ \phi_{q,\ell} = \frac{2}{\pi} \int_0^\infty dv \tilde{\xi}_\ell(qv) f(v). \] (2.90)
The parity property for the expansion coefficients
\[ \phi_{q,-\ell} = \overline{\phi_{q,\ell}} \] (2.91)
directly follows from formulas 2.65 and 2.69.

2.4 Advection equation

Variables \( t \) and \( v \) in the \( P_N \) approximation of advection equation 2.8 separate. Looking for a time-dependent solution in the form
\[ f(t, v) = f_{q,\ell} e^{-i\omega t} \xi_{\ell}(qv) \] (2.92)
and substituting it into equation 2.8, we obtain
\[ i f_{q,\ell} e^{-i\omega t} \xi_{\ell}(qv) [\omega + a_z q a_{\ell}] = 0, \] (2.93)
and the “dispersion” relation
\[ \omega = a_z q a_{\ell}, \] (2.94)
where we made use of equations 2.28 and 2.29.

Hence, the general solution of advection equation 2.8 is
\[ f(t, v) = \sum_{\omega \neq 0, \ell \neq 0} f_{\omega,\ell} \xi_{\ell}(a_z v \omega) e^{-i\omega t} + \sum_{q} f_{q,0} \xi_{0}(qv) + \sum_{s} f_{s}^{0} \chi_{n,s}(v). \] (2.95)
The last two terms represent the stationary part of the general solution. The second term is present in the $P_N$ approximation for even $N$ and includes eigenfunctions of $L(v)$ corresponding to a zero eigenvalue of matrix $A$. The third term combines eigenfunctions of $L(v)$ not associated with a zero eigenvalue of matrix $A$.

2.4.1 Solution on a half-line $v \geq 0$

For $v \geq 0$, the general solution 2.95 takes the form

$$f(t, v) = \sum_{\omega \neq 0, i \neq 0} f_{\omega,i} e^{-i\omega t} \xi_{\ell} + \sum_{q} f_{q,0} \xi_{0}(qv) = \sum_{0<q,i} \phi_{q,\ell} e^{-ia_{\ell}vq\ell t} \xi_{\ell}(qv).$$  \hspace{1cm} (2.96)

The terms $\chi_{n,s}(v)$ are excluded from the general solution for the reasons discussed in 2.3.4. Summation over $q$ allows us to collect all the terms under one sum. Later, for continuous $\omega$ that is for $0 < q$, we use the following form of the general solution

$$f(t, v) = \int_{0}^{\infty} dq \sum_{\ell} \phi_{q,\ell} e^{-ia_{\ell}q\ell t} \xi_{\ell}(qv).$$  \hspace{1cm} (2.97)

The expansion coefficients in the above formula can be found using equation 2.90

$$\phi_{q,\ell} = \frac{2}{\pi} \int_{0}^{\infty} dv \tilde{\xi}_{\ell}(qv) f(0, v),$$  \hspace{1cm} (2.98)

where $f(0, v)$ are initial conditions at $t = 0$. 
To show that the solution 2.97 stays real it can be re-expressed as

\[ f(t, v) = \int_0^\infty dq \phi_{q,0} \xi_0(qv) + \int_0^\infty dq \sum_{0<\ell} \left( \phi_{q,\ell} e^{-iazqa_\ell t} \xi_\ell(qv) + \bar{\phi}_{q,\ell} e^{iazqa_\ell t} \bar{\xi}_\ell(qv) \right), \]  

(2.99)

where we used the parity property for the eigenfunctions 2.64 and 2.69, the expansion coefficients 2.91 and the eigenvalues of matrix \( A \) given by formula D.11.

The general solution 2.97 can be obtained in a different form, that may be computationally more convenient. The expansion coefficients 2.90, substituted into the component form of equation 2.97 yield

\[ f_n(t, v) = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \xi_{n,\ell}(qv)e^{-iazq_{\ell}t}\bar{\xi}_{k,\ell}(qv') \right) f_k(0, v') \]

(2.100)

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} (\alpha_{n,\ell}(qv)e^{-iazq_{\ell}t}\bar{\alpha}_{k,\ell}) \right) dv'(qv')^2 \]

\[ \times \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) (\alpha_{n,\ell}(qv)e^{-iazq_{\ell}t}\bar{\alpha}_{k,\ell}) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \right( \sum_{\ell} \left[ e^{-iazq_{\ell}A} \right]_{n,k} \right) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) \left( \sum_{\ell} \right) \right) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) \right) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) \right) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) \right) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) \right) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) \right) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) \right) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) \right) dv'(qv')^2 \]

\[ = \int_0^\infty dq \int_0^\infty dv' \frac{2}{\pi} \sum_k \left( \sum_{\ell} \right) \right) dv'(qv')^2 \]

The above derivation uses a component form of formula D.26 for \( e^{Ax} \). The result of the derivation can be conveniently summarized in matrix form

\[ f(t, v) = \int_0^\infty dq J(qv)e^{-iazqA} \varphi_q, \]

(2.101)

\[ \varphi_q = \frac{2}{\pi} \int_0^\infty dv(qv)^2 J(-qv)f(0, v). \]
2.4.2 Wave nature of the solution.

The eigenfunctions $\xi_{n,\ell}(x)$ can be reexpressed in their trigonometric form 2.82 in the component form of the general solution 2.97 to yield

$$f_n(t, v) = \frac{i^n}{v} \int_0^\infty \frac{dq}{q} \sum_\ell \phi_{q,\ell} e^{-iqa_r v t} [e^{iqv} p_n(qv) + e^{-iqv} \overline{p}_n(qv)] \alpha_{n,\ell} \quad (2.102)$$

$$= \frac{i^n}{v} \int_0^\infty \frac{dq}{q} \sum_\ell \phi_{q,\ell} [e^{iqv} p_n(qv) + e^{-iqv} \overline{p}_n(qv)] \alpha_{n,\ell}.$$

It has the form of multiple “waves” traveling in opposite directions along $v$ with “velocities” $\pm a_z a_\ell$. The next chapter provides a detailed discussion on the behavior of the amplitudes of these waves introduced there as the “characteristic variables.”

2.4.3 Examples.

Here we consider examples of the analytical solution for equation 2.2 and $a_z = 1$. The numerical values of the analytical solution have been obtained using formula 2.101 and initial conditions at $t = 0$ given by a Gaussian

$$f(t = 0, v, \theta) = e^{-\frac{v^2}{2\sigma^2}} \quad \text{with} \quad 2\sigma^2 = 0.01 \quad (2.103)$$

as displayed in figure 2-1. Since initial conditions are independent of $\theta$, only $f_0 = e^{-\frac{v^2}{2\sigma^2}}$ is different from zero while for the rest $f_{n>0} = 0$.

Behavior of the analytic solution for $P_{64}$ at different times is shown in figures 2-2 and 2-3 to illustrate the case of a sufficiently large $N$. Graphs of the expansion coefficients versus time are presented on the left. The expansion coefficients $f_0$-$f_7$
are represented by thick colored lines while the rest of the expansion coefficients $f_{n>7}$ are indicated by thin black lines. On the right are the graphs of the corresponding functions $f(v, \theta)$ (see appendix F for explanation). Two features can be immediately noticed. One is that the Gaussian moves with a constant rate in the direction of $v_z$ without visible distortion of its shape. This behavior for the solution of equation 2.2 is well predictable, because as $N \to \infty$ it has to approach the solution of equation 2.1. Intuitively we can say that for the given solution and $t \leq 1$, $N = 64$ is sufficiently large. The other feature is that the farther the Gaussian moves from the origin, the more of the expansion coefficients become different from zero. As time advances, the expansion coefficients $f_n$ grow and decline in order, according to their $n$ as seen in figures 2-2 and 2-3. They are clearly different from zero and visibly positive on a limited interval whose length remains constant while being close to zero everywhere else.

The examples of the solution for the same $t$ and initial conditions for $P_7$ and $P_8$, when $N$ clearly can not be considered sufficiently large, are given in figures 3-5 - 3-8.
of chapter 3. Analytical solutions are presented by colored curves. Note that after
\( t = 0.2 \), the expansion coefficients \( f_n \) for both \( P_7 \) and \( P_8 \) behave differently from those
in figures 2-2 and 2-3. In particular, \( f_0 \) becomes negative at certain \( v \).

Convergence of the analytic solution \( f(t, v, \theta) \) for even and odd \( N \) is displayed in
figure 2-4 for \( t = 0.5 \). An additional brown vertical reference line of unit length is
placed in the figure at the position of a maximum of \( f(t = 0.5, v, \theta) \) for \( P_\infty (v_x = 0 \)
and \( v_z = 0.5 \)). Different behavior of the solutions for even and odd \( N \) is clearly
noticeable.
Figure 2-2: Analytic solution for $P_{04}$ at $t=0.1$, 0.2, 0.3, 0.4.
Figure 2-3: Analytic solution for $P_{64}$ at $t=0.5, 0.6, 0.7, 0.8$. 
Figure 2-4: Convergence for odd and even $N$ at $t=0.5$
Chapter 3

Numerical solution of the $P_N$ approximation of the Boltzmann equation.

In this chapter we are going to consecutively apply operator-splitting (discussed in appendix G) to develop a numerical solution of the $P_N$ approximation of the Boltzmann equation

\[
\frac{\partial f}{\partial t} + a_z \left( A \frac{\partial f}{\partial v} + \frac{1}{v} B f \right) + v A \frac{\partial f}{\partial z} = S(f). \tag{3.1}
\]

First, we are interested in the numerical reproduction of the results obtained in the previous chapter for the advection equation in the velocity space. We are able to induce a proper behavior of the solution at the origin of the velocity coordinates by a proper choice of the boundary conditions at $v = 0$. Introducing boundary
conditions at \( v = V \) and a minor change in the splitting procedure, we will achieve exact numerical conservation of particles. After that we will include collision integrals and compare stationary solutions obtained through the \( P_N \) approximation and Monte-Carlo techniques. Finally, we will include the space dependence. Discussing stability requirements at each step, we will obtain constraints on the time increment.

We need to introduce the notations to be used in finite difference formulation of problem 3.1. In numerical description, the largest possible value of the absolute velocity will be limited to \( V \), so that the domain of definition for \( v \) is the interval \( v \in [0, V] \). We will use \( \nu = \frac{V}{N_v} \) for the length of the velocity mesh interval, where \( N_v \) is the number of velocity mesh intervals; \( v_i = i\nu \), with \( i = 0, N_v \), are values of the velocity at the edges of the velocity mesh intervals and \( v_{i+1/2} = (i + \frac{1}{2})\nu \), with \( i = 1, N_v \), are velocities at the centers of the velocity mesh intervals. In the same way, we define the domain of definition for \( z \) to be the interval \( z \in [0, L] \) where \( L \) defines the length of this space interval. The length of the space mesh interval is then given by \( h = \frac{L}{N_z} \), where \( N_z \) is the number of space mesh intervals in the region; \( z_j = jh \), with \( j = 0, N_z \), are the values of the space coordinate at the edges of the space mesh intervals; and \( z_{j+1/2} = (j + \frac{1}{2})h \), with \( j = 1, N_z \), are the values of the space coordinate at the centers of the space mesh intervals. To deal with time, we define the variable time interval as \( \tau_{s+1} = t_{s+1} - t_s \). We define the values of functions at the centers of the space \( z_{j+1/2} \) and velocity mesh intervals \( v_{i+1/2} \) at time \( t_s \) and will use component or matrix notations \( f_{j+1/2,i+1/2}^s = [f_{0,j+1/2,i+1/2}^s \ f_{1,j+1/2,i+1/2}^s \cdots \ f_{N,j+1/2,i+1/2}^s]^T \).

Values of the functions \( f_{j+1/2,i}^s \) and \( f_{j+1/2,i}^s \) at the edges of the space and velocity mesh intervals will be obtained through interpolation. Often, when formulas include
values of the function at adjacent moments of time we will shorten the notations to \( \tau = \tau_{s+1}, f = f^s \) and \( f^+ = f^{s+1} \). When equations do not include space or velocity we will drop the corresponding index in function notations.

Our ultimate goal will be to construct an evolution operator \( B(\tau) \) that will allow us to obtain the numerical solution of equation 3.1 at time \( t_{s+1} \) if the solution at \( t_s \) is known, that is ”update” or ”advance” the solution by the time step \( \tau_{s+1} \):

\[
F^{s+1} = B(\tau_{s+1})F^s, \quad \text{where} \quad B(\tau_{s+1}) = \prod_p e^{\Omega_p \tau_{s+1}}. 
\]

In the above formula \( F^s \) is a column matrix containing all of the values of \( f_{n,j-1/2,i-1/2}^s \) at time \( t_s \) with indices \( n, j, i \) going over the range \( n = 0, N, j = 1, N_z, i = 1, N_v \). When equations that we consider do not include a space or velocity dependence we will assume that the corresponding index, \( j \) or \( i \), is dropped in the construction of \( F^s \).

We will consecutively split the whole equation 3.1 into its elementary evolution equations for which the numerical solutions, or in other words the evolution operators, \( e^{\Omega_p \tau_{s+1}} \) can be easily constructed. The idea of representing a linear numerical method, obtained by the technique of operator splitting, by means of linear operators is adopted by the author from reference [30].

All the numerical solutions discussed in this dissertation were implemented in Fortran 95 using double precision for real numbers.
3.1 Advection in the velocity space.

The advection equation in the velocity space

\[
\frac{\partial f}{\partial t} + a_z \left( A \frac{\partial f}{\partial v} + \frac{1}{v} B f \right) = 0, \tag{3.3}
\]

splits (see appendix G) into

\[
\frac{\partial f}{\partial t} + a_z A \frac{\partial}{\partial v} f = 0 \tag{3.4}
\]

and

\[
\frac{df}{dt} + \frac{a_z}{v} B f = 0. \tag{3.5}
\]

In order to numerically solve 3.3 by operator splitting we need to construct the evolution operators \( T_{adv}^v(a_z \tau) \) and \( R_{adv}^v(a_z \tau) \) that solve the finite-difference analogs of equations 3.4 and 3.5 and construct the resultant operator that solves the finite-difference analog of equation 3.3 as their product:

\[
A_v(a_z \tau) = R_{adv}^v(a_z \tau) T_{adv}^v(a_z \tau). \tag{3.6}
\]

3.1.1 Solution of \( \frac{\partial f}{\partial t} + a_z A \frac{\partial f}{\partial v} = 0. \)

We start with obtaining an analytical solution of equation 3.4. Introduction of “characteristic variables” \( g \) (see reference [30], p.58)

\[
g = \begin{bmatrix} g_{-s} & g_{-s+1} & \cdots & g_t & \cdots & g_{s-1} & g_s \end{bmatrix}^T = P^{-1} f, \tag{3.7}
\]
(for definition of $P^{-1}$, see formula D.24) transforms equation 3.4 into

$$\left( \frac{\partial}{\partial t} + a_z P^{-1} A P \frac{\partial}{\partial v} \right) P^{-1} f = \left( \frac{\partial}{\partial t} + a_z \hat{A} \frac{\partial}{\partial v} \right) g = 0. \quad (3.8)$$

In the above construction, matrices $A$ and $B$ are defined by equations 2.5 and 2.6, and $P$ is the matrix that diagonalizes the matrix $A$ as $P^{-1} A P = \hat{A} = \text{diag}(a_\ell)$ (see formula D.25). In $g_\ell$, the index $\ell$ goes through the range given by expression D.12. We will sometimes refer to the $g_\ell$ as “waves” to reflect their tendency to propagate with definite speeds in both the velocity and spatial domains.

Both equations 3.4 and 3.8 can be classified as strictly hyperbolic (see [30], p.58) because the values of $a_\ell$ are real and distinct. Equation 3.8 is just $N + 1$ uncoupled advection equations

$$\frac{\partial g_\ell}{\partial t} + a_z a_\ell \frac{\partial g_\ell}{\partial v} = 0, \quad (3.9)$$

so that its general solution can be immediately written as

$$g(t, v) = \left[ w_{-s}(v - a_z a_{-s}t) \cdots w_\ell(v - a_z a_{\ell}t) \cdots w_s(v - a_z a_{s}t) \right]^T, \quad (3.10)$$

where the functions $w_\ell(v)$ are determined by the initial conditions at some moment of time $t_0$

$$g(t_0, v) = w(v). \quad (3.11)$$

With time, solutions $g_\ell = w_\ell(v - a_z a_\ell t)$ propagate toward $v = 0$ for $a_z a_\ell < 0$ and toward $v = V$ for $0 < a_z a_\ell$. For $N = \text{even}$, there is a solution $g_0(t, v) = w_0(v)$ with $a_z a_0 = 0$ that stands still.
To form a well defined initial-boundary-value problem (or Cauchy’s problem, see discussion for hyperbolic equations in reference [36], chapter 6), the boundary conditions

\[ g_\ell(t, 0) = b_\ell(t) \quad \text{for} \quad 0 < a_z a_\ell \]  
\[ g_\ell(t, V) = b_\ell(t) \quad \text{for} \quad a_z a_\ell < 0 \]  

have to be specified at \( v = 0 \) for solutions propagating toward \( v = V \) and at \( v = V \) for solutions propagating toward \( v = 0 \). No boundary conditions are needed for \( g_0(t, v) \).

We will determine the values of \( b_\ell(t) \) later in 3.1.3).

Solution 3.10 can be used to determine \( f \) by the linear transformation inverse to

\[ f = Pg. \]  

We write the finite-difference analog of equation 3.4 as

\[ \frac{f_{i+1/2}^+ - f_{i-1/2}}{\tau} + a_z A f_{i+1} - f_i \nu = 0. \]  

Solution of above equation together with a finite-difference equivalent of the boundary conditions 3.12 and 3.13, determines an approximation to the evolution operator that we further refer to as \( T_v^{\text{adv}}(a \tau) \).

We have to define \( f_{i}^s \) in order for equation 3.15 to make sense. Similar to the
analytical case, introduction of the characteristic variables

\[ g_{i+1/2} = P^{-1} f_{i+1/2} \]  

(3.16)
transforms 3.15 into

\[ \frac{g^+_{i+1/2} - g^{-1/2}_i}{\tau} + a_z \hat{A} \frac{g_{i+1} - g_i}{\nu} = 0 \]  

(3.17)
and yields \( N + 1 \) uncoupled scalar equations

\[ \frac{g^+_{\ell,i+1/2} - g^{-1/2}_{\ell,i+1}}{\tau} + a_\ell a_z \frac{g_{\ell,i+1} - g_{\ell,i}}{\nu} = 0. \]  

(3.18)

Each of the above equations can be solved separately with a desired accuracy that is determined by the way \( g^s_{\ell,i} \) is “recovered” from the surrounding \( g^s_{\ell,i+1/2} \). The simplest of them is “upwind” (see vol.1, p.280 of [14] and/or p.18 of [37]), that is when

\[ g^s_{\ell,i} = \begin{cases} 
  g^s_{\ell,i-1/2} & \text{for } 0 < a_z a_\ell \\
  g^s_{\ell,i+1/2} & \text{for } a_z a_n < 0 
\end{cases} \]  

(3.19)
Upwinding produces an explicit scheme that is accurate to first-order. The method is stable when the corresponding CFL (Courant-Friedrichs-Levy) numbers (see vol.1 p.280 of [14])

\[ c_n = \frac{\tau a_z a_n}{\nu} \]  

are so that \( |c_n| \leq 1 \),

(3.20)
and restricts the time step to

\[
\tau \leq \tau_v^a = \min_{\ell} \frac{\nu}{|a_\nu a_\ell|}.
\] (3.21)

We adopt the value of \( \tau_v^a \) as an estimation of the characteristic time of the operator \( T_v^{\text{adv}}(a_z\tau) \), based on formula G.15. More accurate methods that can be used to determine \( g_\ell \) (see references [25] and [26]) result in the same stability requirement (see [27] and [29]). After the \( g_\ell \) are recovered they can be used to determine \( bm f_i \) via the equation

\[
f_i = P g_i.
\] (3.22)

Substitution of these values into equation 3.15 allows us to solve for \( f_i^+ \). Definition of the operator \( T_v^{\text{adv}}(a_z\tau) \) is continued in 3.1.3 where the specific boundary conditions at \( v = 0 \) and \( v = V \) are introduced to replace the generic ones given by formulas 3.12 and 3.13.

**3.1.2 Solution of** \( \frac{df}{dt} + \frac{a_z}{v} B f = 0 \).**

Formal solution of the ordinary differential equation 3.5 can be written as

\[
f(t + \tau) = e^{-\frac{a_z}{v} B\tau} f(t),
\] (3.23)

where the matrix \( B \) is defined by equation 2.6. To be able to construct \( e^{-\frac{a_z}{v} B\tau} \) we need to know the Jordan canonical form of matrix \( B \) which can be obtained through
a similarity transformation
\[ \hat{B} = S^{-1}BS, \] (3.24)

where \( S \) is a regular matrix determined by \( B \) (see [15], p.132). The eigenvalues of matrix \( B \) are purely imaginary. We denote them as \( \mp ib_k \) and arrange their indexation so that \( b_k < b_{k+1} \). Their absolute values found numerically for \( N \leq 31 \) are given in figure 3-1. The line \( \max(b_k) \approx 0.82(N - 1) + 0.0024(N - 1)^2 \) shows the growth of the

![Figure 3-1: Absolute values of eigenvalues of matrix \( B \).](image)

largest absolute eigenvalue of matrix \( B \) for \( 1 \leq N \leq 31 \).

For even \( N \),
\[ \hat{B} = \text{diag}(0, -ib_1, ib_1, ..., -ib_{N/2}, ib_{N/2}) \] (3.25)
is diagonal with one zero eigenvalue. For odd \( N \)
\[ \hat{B} = \text{diag}(\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, -ib_1, ib_1, ..., -ib_{N-1}, ib_{N-1}). \] (3.26)
Its zero eigenvalue has multiplicity two, corresponding to a Jordan block \(
\begin{bmatrix}
0 & 1 \\
0 & 0
\end{bmatrix}
\). Using the two first terms in the Taylor series for an exponent (see equation G.4), we find that 
\[
\exp \begin{bmatrix}
0 & x \\
0 & 0
\end{bmatrix} = \begin{bmatrix}
1 & x \\
0 & 1
\end{bmatrix}.
\]

We can now calculate the exponents we need for equation 3.23. For even \(N\)

\[
e^{\tilde{B}x} = \text{diag}(1, e^{-i b_1 x}, e^{i b_1 x}, ..., e^{-i b_N x}, e^{i b_N x}),
\] (3.27)

and for odd \(N\)

\[
e^{\tilde{B}x} = \text{diag}\left(\begin{bmatrix}
1 & x \\
0 & 1
\end{bmatrix}, e^{-i b_1 x}, e^{i b_1 x}, ..., e^{-i b_{N-1} x}, e^{i b_{N-1} x}\right).
\] (3.28)

Formula 3.24 allows us to calculate

\[
e^{Bx} = S e^{\tilde{B}x} S^{-1}.
\] (3.29)

The finite-difference analog of equation 3.5 can be obtained using its analytic solution 3.23:

\[
f_{i+1/2}^+ = e^{-\frac{a_z}{\tau_{i+1/2}} B\tau} f_{i+1/2}.
\] (3.30)

The above formula defines the action of the operator further referred to as \(R_{\text{adv}}^\phi(a_z \tau)\). Since we used the exact solution 3.5 to define the evolution operator in finite-difference case we do not need to put any stability restrictions on the time step. Using formula
G.15, the characteristic time $\tau_v^r$ of the operator $\mathcal{R}_v^{\text{adv}}(a_z\tau)$ can be estimated as

$$
\tau_v^r = \min_{i,k} v_i^{+1/2} a_z b_k = \frac{v_{1/2}}{a_z} \min_k \frac{1}{b_k},
$$

where the $b_k$ are the absolute values of the eigenvalues of the matrix $B$.

### 3.1.3 Boundary conditions at $v = 0$ and $v = V$.

In subsection 3.1.1 we mentioned the boundary conditions at the ends of velocity interval 3.12 and 3.13 for the system of equations 3.9 and their finite-difference analogs 3.18. Here our goal is to specify the boundary conditions at $v = 0$ and $v = V$.

We can start by attempting to find a reasonable boundary condition for the equation

$$
\frac{\partial g}{\partial t} + a \frac{\partial g}{\partial x} = 0 \text{ for } 0 < a \text{ on the interval } 0 \leq x \leq X
$$

with “initial” conditions given by

$$
g(t = 0, x) = w(x)
$$

on the same interval. Consider a solution of the above equation given by

$$
g(t, x) = w(x - at)
$$

It is easy to see that for any $t : 0 < t < X/a$, the solution 3.34 is not defined for $x : 0 \leq x < at$. This issue can be resolved, if in addition to the initial condition 3.33,
we define a “boundary condition” on the left boundary

\[ g(t, x = 0) = b(t) \text{ for } 0 \leq t. \quad (3.35) \]

The corrected solution

\[
g(t, x) = \begin{cases} 
w(x - at) & \text{for } 0 \leq x - at \leq X \\ 
b(t - \frac{x}{a}) & \text{for } x - at < 0 \end{cases} \quad (3.36)
\]

takes into account the boundary condition 3.35.

In general, setting any boundary condition at the right boundary is not possible, since at least for \(0 \leq t \leq X/a\), the solution \(g(t, X)\) is determined by the initial conditions. Consider the example, when solution 3.34 describes the motion of particles with \(g(t, x)\) being the particle density. This example corresponds to a physical situation when the boundary condition on the left of the interval “injects” particles into it. The particles move with a constant velocity \(a\) to the right and disappear beyond the right boundary. Next, we can imagine a situation when particles are stopped at \(x = X\) and remain there afterwards. This situation can by described by the equations

\[
\frac{\partial g}{\partial t} + \frac{\partial J}{\partial x} = 0 \text{ with } J(t, x) = \begin{cases} 
a \ b(t) & \text{for } x = 0 \\ 
a \ g(t, x) & \text{for } 0 < x < X \\ 
0 & \text{for } x = X \end{cases} \quad (3.37)
\]
The solution can be written as

\[
g(t, x) = \begin{cases} 
  w(x - at) & \text{for } 0 \leq x - at \leq X \text{ and } x \neq X \\
  b(t - x/a) & \text{for } 0 < t - x/a \text{ and } x \neq X \\
  s(t)\delta(x - X) & \text{for } x = X 
\end{cases} 
\]  

(3.38)

and

\[
s(t) = a \int_0^{\max(0, t - X/a)} dt' b(t') + \int_{\max(0, X - at)}^X dx' w(x').
\]

It can be verified that all the particles that were initially present and later injected into the interval remain there afterwards. The described model can be implemented numerically by setting the flux \( J \) to zero at the right boundary. The particle density will then accumulate in the rightmost mash interval. We are ready now to discuss the boundary conditions we can impose on the solutions of equations 3.9 at \( v = 0 \) and \( v = V \).

The limiting values of the eigenfunctions 2.56 and equation 2.99 suggest that the behavior of the analytic solution close to the origin is given by

\[
f_n(t, v) = \varphi_n(t) \left[ v^n + O(v^{n+2}) \right],
\]

(3.39)

where \( \varphi_n(t) \) are some functions of \( t \). Transformed to the characteristic variables the above formula yields

\[
g_\ell(t, v) = \sum_{s=0}^N P_{\ell,s} \varphi_s(t) \left[ v^s + O(v^{s+2}) \right] = \alpha_{\ell,0} \varphi_0(t) + \alpha_{\ell,1} \varphi_1(t) v + O(t)O(v^2),
\]

(3.40)

where we used formula D.23 for \( P_{\ell,s} = \alpha_{\ell,s} \). Using the parity of the eigenvalues of
matrix $A$ given by formula D.27, we obtain

$$g_\ell(t, v) = \alpha_{\ell,0} \varphi_0(t) \mp \alpha_{\ell,1} \varphi_1(t) v + O(v^2).$$ (3.41)

The behavior of the characteristic variables given by the above formula is graphically illustrated in figure 3-2. The length of the arrows and their direction correspond to the absolute values and signs of the eigenvalues of matrix $A$. Arrows show the directions of motion of the corresponding $w_{e\ell l}$ functions given by formula 3.10. Functions $g_{\ell>0}(t, v)$ are continuations of $g_{\ell<0}(t, -v)$ and move to the right, while $g_0(t, v)$ stands still and is a continuation of itself: $g_0(t, -v)$. For $a_z < 0$ the situation reverses so that $g_{\ell<0}(t, v)$ become continuations of $g_{\ell>0}(t, -v)$ moving to the right.

![Figure 3-2: Behavior of the characteristic variables $g_\ell$ near zero for $P_4$ and $0 < a_z$.](image)
Formula 3.41 implies the boundary conditions to use in equation 3.4 at \( v = 0 \)

\[
g_{\ell>0}(t, v = 0) = g_{-\ell}(t, v = 0) \quad \text{for} \quad 0 < a_z
\]

\[
g_{\ell<0}(t, v = 0) = g_{-\ell}(t, v = 0) \quad \text{for} \quad a_z < 0
\]

which can be translated to finite-difference boundary conditions accurate to first-order

\[
g_{\ell>0,0} = g_{-\ell,1/2} \quad \text{for} \quad 0 < a_z
\]

\[
g_{\ell<0,0} = g_{-\ell,1/2} \quad \text{for} \quad a_z < 0.
\]

The smoothness of \( g_\ell(t, v) \) and their continuations \( g_{-\ell}(t, -v) \) allows construction of high order boundary conditions that require several points around \( g_{\ell,1/2} \) and \( g_{-\ell,1/2} \) to construct \( g_{\ell,0} \).

To determine the general form of the boundary conditions at \( v = V \), we consider the case of \( 0 < a_z \). In general, solutions \( g_{\ell>0}(t, v) \) that arrive to the point \( v = V \) from the left can be converted into \( g_{\ell<0}(t, v) \) that depart from the point \( v = V \) to the right in an arbitrary way. In reverse, when \( a_z < 0 \), \( g_{\ell<0}(t, v) \) can be converted into \( g_{\ell>0}(t, v) \) at \( v = V \). Both situations can be summarized as

\[
g_{\ell<0}(t, v = V) = \sum_{0<m} r_{\ell,m}(t) g_m(t, v = V) + s_{\ell}(t) \quad \text{for} \quad 0 < a_z
\]

\[
g_{\ell>0}(t, v = V) = \sum_{m<0} r_{\ell,m}(t) g_m(t, v = V) + s_{\ell}(t) \quad \text{for} \quad a_z < 0,
\]

where \( r_{\ell,m}(t) \) and \( s_{\ell}(t) \) are some arbitrary functions. The above translates into first-
order accurate finite-difference boundary conditions as

\[ g_{\ell < 0, N_v} = \sum_{0 \leq m} r_{\ell, m} g_{m, N_v - 1/2} + s_{\ell} \quad \text{for} \quad 0 < a_z \quad (3.45) \]

\[ g_{\ell > 0, N_v} = \sum_{m \leq 0} r_{\ell, m} g_{m, N_v - 1/2} + s_{\ell} \quad \text{for} \quad a_z < 0. \]

In the following we will be interested in the time-independent variant of the boundary conditions at \( v = V \), where \( r_{\ell, m} \) are constants and \( s_{\ell} = 0 \).

The boundary conditions 3.42 and 3.44 are based on a similar principle – “waves” \((g_\ell)\) emitted by the boundary are are determined by those arriving to the boundary.

If we do not want to inject \( g_\ell \) into the interval as well as not let \( g_\ell \) go outside of it, we can impose boundary conditions at \( v = V \), by simply setting boundary values of \( g_\ell \) to zero:

\[ g_{n \neq 0, N_v} = 0. \quad (3.46) \]

The justification of this idea for at least a finite-difference implementation is supported by our previous discussion for equation 3.37.

### 3.1.4 Characteristic variables.

Here we qualitatively explain the meaning of characteristic variables introduced by formula 3.7. The knowledge we gain about characteristic variables will help us later in subsections 3.3.2 and 3.3.3 to construct spatial boundary conditions.
Let’s re-express formula 3.7 in its component form as

\[ f_n = \sum_{\ell} P_{n,\ell} g_{\ell} = \sum_{\ell} \alpha_{n,\ell} g_{\ell} \quad \text{or in matrix notation as} \quad f = \sum_{\ell} \alpha_{\ell} g_{\ell}, \quad (3.47) \]

where we used formula D.23 for the elements of matrix \( P \). Consider the expansion

\[ f(\theta) = \sum_{n=0}^{N} f_n P_n(\cos \theta) = \sum_{\ell} g_{\ell} \alpha_{\ell}^N(\theta), \quad (3.48) \]

where we introduced

\[ \alpha_{\ell}^N(\theta) = \sum_{n=0}^{N} \alpha_{n,\ell} P_n(\cos \theta) = \sum_{n=0}^{N} (n + 1/2) P_n(a_{\ell}) P_n(\cos \theta), \quad (3.49) \]

and used formula D.14 for the components of \( \alpha_{n,\ell} = (n + 1/2) P_n(a_{\ell}) \). Using the orthogonality condition for Legendre polynomials (see reference [3], p.756)

\[ \int_{0}^{\pi} P_n(\cos \theta) P_m(\cos \theta) \sin \theta d\theta = \frac{\delta_{n,m}}{n + 1/2}, \quad (3.50) \]

one can easily find the expansion of the Dirac delta function into Legendre polynomials

\[ \delta(\cos \theta - \cos \theta') = \sum_{n=0}^{\infty} \delta_{n}(\cos \theta') P_n(\cos \theta) \quad \text{where} \quad \delta_{n}(\cos \theta') = (n + 1/2) P_n(\cos \theta'). \quad (3.51) \]
Comparing formulas 3.49 and 3.51 one can see that since

\[ \alpha_{n,\ell} = \delta_n(a_\ell), \]  
\[ \alpha^N_\ell(\theta) \to \alpha^\infty_\ell(\theta) = \delta(\cos \theta - \cos \theta_\ell) \text{ as } N \to \infty. \]

\( \alpha^N_\ell(\theta) \) has a maximum in the vicinity of \( \theta_\ell \) and is close to zero everywhere else. The estimates for \( \theta_\ell \), given by formulas D.30, suggest that they are distributed uniformly on the interval \([0, \pi]\). When \( N \to \infty \), \( \theta_\ell \) can be arbitrarily close to any given number in the interval \([0, \pi]\). We assume that \( \alpha^N_\ell(\theta) \) is different from zero on the interval \( \left[ \frac{\pi}{N+1}(\ell - 1/2) - \Delta \theta_\ell/2, \frac{\pi}{N+1}(\ell - 1/2) + \Delta \theta_\ell/2 \right] \), where \( \Delta \theta_\ell = \pi/(N+1) \). A conical region, “cut out” by the function \( \alpha^N_\ell(\theta) \) in the velocity space is illustrated by the left drawing in figure 3-3. The conical region defined by the function \( \alpha^N_\ell(\theta) \) in the velocity space

![Figure 3-3](image)
is shown on the left. The plane \( v_x0v_z \) is given in white. The conical region is light gray. Two sectors or “beams” defined by the intersection of the conical region with the plane \( v_x0v_z \) are dark gray. The beams are symmetric relative to the axis \( 0v_z \).

The beams defined by the functions \( \alpha_{-\ell}^N(\theta) \), \( \alpha_{0}^N(\theta) \) and \( \alpha_{\ell}^N(\theta) \) on the plane \( v_x0v_z \) are shown on the right in different shades of gray. Note that \( \theta_{-\ell} = \pi - \theta_{-\ell} \) and \( \theta_0 = \pi \).

To get an idea about what the characteristic variables are, let’s again consider expansion 3.48. On one hand

\[
f(\theta) = \sum_{\ell} \Delta \theta_{\ell} \left( \frac{g_{\ell}}{\Delta \theta_{\ell}} \right) \alpha_{\ell}^N(\theta) \xrightarrow{N \to \infty} \int_{0}^{\pi} d\theta_{\ell} \left( \frac{g_{\ell}}{\Delta \theta_{\ell}} \right) \Delta \theta_{\ell} \to 0 \alpha_{\ell}^\infty(\theta) \quad (3.54)
\]

On the other hand, using the identity

\[
f(\theta) = \int_{0}^{\pi} d\theta_{\ell} \sin \theta_{\ell} f(\theta_{\ell}) \delta(\cos \theta - \cos \theta_{\ell}). \quad (3.55)
\]

Comparing the above expressions, to be valid for an arbitrary \( f(\theta) \), we obtain

\[
f(\theta_{\ell}) = \frac{1}{\sin \theta_{\ell}} \left( \frac{g_{\ell}}{\Delta \theta_{\ell}} \right) \Delta \theta_{\ell} \to 0 \quad \text{or} \quad (3.56)
\]

\[
f(\theta_{\ell}) \Delta \omega_{\ell} = 2\pi g_{\ell} , \text{ where } \Delta \omega = 2\pi \sin \theta_{\ell} \Delta \theta_{\ell}. \quad (3.57)
\]

In the \( P_N \) approximation, \( \theta_{\ell} \) can be considered an equivalent of a discretization for the angular variable \( \theta \).
3.1.5  Action of operators $T^\text{adv}_v(a_z \tau)$ and $R^\text{adv}_v(a \tau)$.

To qualitatively explain what happens to the function

$$f_{i+1/2}(t, \theta) = \sum_n f_{n,i+1/2} P_n(\theta)$$

(3.58)

after its components $f_{n,i+1/2}$ are updated by means of the action of operators $T^\text{adv}_v(a_z \tau)$ and $R^\text{adv}_v(a \tau)$, consider $f_{i+1/2}(t, \theta) = g_{\ell,i+1/2}(v) \alpha^N_{\ell}(\theta)$. The function $f_{i+1/2}(t, \theta) \approx 0$ outside of the cone defined by $\theta_\ell$ (discussed in subsection 3.1.4), that is when $\theta < \frac{\pi}{N+1}(\ell - 1)$ or $\frac{\pi}{N+1}(\ell - 1) < \theta$. The construction of operator $T^\text{adv}_v(a_z \tau)$ given is subsection 3.1.1 suggests that its action is defined through the solution of equation 3.18. Equation 3.18 in turn is a finite-difference equivalent of equation 3.9 with a solution $g_{\ell}(t, v) = w_{\ell}(v - a_z a_{\ell} t)$ that describes translation along $v$ with the rate $a_z a_{\ell}$. Putting all of the above together, we can estimate that the approximate result of the action of $T^\text{adv}_v(a_z \tau)$ is a translation by distance $a_z a_{\ell} \tau$ in the velocity space along the direction defined by $\theta_\ell$. This description becomes exact when $N$ and $N_v$ tend to $\infty$ while $\tau$ approaches 0.

It is possible to develop the analogies even further. Let’s call two equations equivalent if they have the same solutions under a given condition. Under condition $N_v \to \infty$ and $\tau \to 0$, equation 3.18 that defines the action of operator $T^\text{adv}_v(a_z \tau)$ is equivalent to equation 3.8, which is equivalent to equation 3.4 under the transformation 3.7. Under condition $N \to \infty$ so that $\theta = \theta_\ell$, it’s possible to reverse the arguments of appendix C, and relate the equation 3.4 to the equation C.1 where the terms $\frac{\partial f}{\partial z}$, $\frac{\partial f}{\partial \zeta}$ and $S$ are removed. This description can be summarized in the following equivalence
where the arrows $\uparrow$ denote equivalence and the corresponding conditions for equivalence are stated beside the arrows. The last equation in the above chart,

$$\frac{\partial f(t, v, \theta)}{\partial t} + a_z \cos \theta \frac{\partial f(t, v, \theta)}{\partial v} = 0,$$

can be solved by the “method of characteristics” (see book [51] p.302). In this method, the characteristic line on the $(t, v)$ plane for the above equation has the form

$$\frac{dv}{dz} = a_z \cos \theta,$$

from which it follows that the solution of equation 3.60 can be written as

$$f(t, v, \theta) = w(v - ta_z \cos \theta, \theta),$$

where $w$ is a function matching initial conditions at a given time. The solution 3.62
describes translation along the surface of the cone defined by angle \( \theta \). Hence, we come to the same conclusion as before about the action of operator \( T_v^{\text{adv}}(a_z \tau) \).

The action of operator \( R_v^{\text{adv}}(a_z \tau) \) is defined by formula 3.30 which is a finite-difference analog of the analytical solution 3.23 of equation 3.5. Solutions 3.30 and 3.23 match when \( v = v_i \). Under the condition \( N \to \infty \) (so that \( \theta = \theta_e \)), equation 3.5 is equivalent to equation C.1 where the terms \( \frac{\partial f}{\partial \tau}, \frac{\partial f}{\partial v} \) and \( S \) are dropped. The above description can be organized in the equivalence chart

\[
R_v^{\text{adv}}(a_z \tau): \quad f^{+}_{i+1/2} = e^{-\frac{a_z}{v_i+1/2} B \tau} f_{i+1/2} \quad \text{formula 3.30}
\]

\[
\uparrow \quad v = v_{i+1/2}
\]

\[
f(t + \tau) = e^{-\frac{a_z}{v} B \tau} f(t) \quad \text{formula 3.23, the solution of equation 3.5}
\]

\[
\downarrow \quad N \to \infty
\]

\[
\frac{\partial f}{\partial t} + \frac{a_z}{v} B f + a_z v \frac{\partial f}{\partial \zeta} + a_z \frac{\partial f}{\partial \zeta} \frac{1-c^2}{v} \zeta - S = 0 \quad \text{equation C.1}
\]  

The last equation of the above chart

\[
\frac{\partial f(t, v, \theta)}{\partial t} - \frac{a_z}{v} \sin \theta \frac{\partial f(t, v, \theta)}{\partial \theta} = 0 \quad \text{(3.64)}
\]

approximately describes the action of \( R_v^{\text{adv}}(a_z \tau) \) and has the following equation for its characteristic curve on the \((t, \theta)\)-plane

\[
d\theta = -\frac{a_z}{v} \sin \theta dt. \quad \text{(3.65)}
\]
The solution of equation 3.64 is

\[ f(t, v, \theta) = u(v, e^{\frac{a_z}{v} \tan \frac{\theta}{2}}), \]  

(3.66)

where \( u \) is a function matching the initial conditions at a given time. Unfortunately, it is difficult to interpret. To find an interpretation, we can look at the equation for the characteristic curve 3.65 along which the solution 3.66 is a constant. As one can see, \( d\theta = -\frac{a_z}{v} \sin \theta dt \) describes an infinitesimal rotation in \( \theta \).

The infinitesimal motions of the point of constancy of solutions 3.62 and 3.66 and approximate actions of the operators \( T_{v}^{\text{adv}}(a_z \tau) \) and \( R_{v}^{\text{adv}}(a_z \tau) \). As one would expect, the result of the combined action of \( T_{v}^{\text{adv}}(a_z \tau) \) and \( R_{v}^{\text{adv}}(a_z \tau) \) is a translation by distance \( a_z \tau \) in the velocity space along the axis \( v_z \).

In brief, the statement of this subsection can be summarized in the following way: operators \( T_{v}^{\text{adv}}(a_z \tau) \) and \( R_{v}^{\text{adv}}(a_z \tau) \) are descendants of the operators \( e^{a_z \tau \cos \theta \frac{a_z}{v}} \) and

Figure 3-4: On the left, infinitesimal motions along the characteristic curves for solutions 3.62 and 3.66. On the right, action of operators \( T_{v}^{\text{adv}}(a_z \tau) \) and \( R_{v}^{\text{adv}}(a_z \tau) \).
$e^{\frac{a z r}{\nu} \sin \theta \frac{\partial}{\partial \theta}}$ and their action has to match for sufficiently large $N$ and $N_v$.

3.1.6 Particle conservation.

Acceleration in the advection equation 2.1 can be brought inside the velocity derivative in the same way it is done in appendix B (see formula B.1). Advection equation can be written in the form of a continuity equation

$$\frac{\partial f}{\partial t} + \frac{\partial J}{\partial v} = 0 \quad \text{where} \quad J = a z e v z f. \quad (3.67)$$

When $f$ is normalized to a number of particles as further given by formula 3.69, it is convenient to refer to $J$ as to the particle flux. Integrated over the region $D_v$ enclosed by the surface $S_v$ in the velocity space, the last equation yields

$$\frac{\partial n}{\partial t} + \int_{S_v} J \cdot d^2 s_v = 0, \quad \text{where} \quad n = \int_{D_v} d^3 v f \quad (3.68)$$

is the number of particles in $D_v$. In words, the change in the number of particles in volume $D_v$ equals the total flux of particles through its enclosing surface $S_v$.

We want to find if there exists a similar mechanism that ensures particle conservation in the $P_N$ approximation. Taking $D_v$ to be the region in the velocity space inside a sphere of radius $V$ with its center at the origin of velocity space, we can
calculate the number of particles inside $D_\nu$ with formula 3.69:

$$n = 4\pi \int_0^V dv \, v^2 f_0.$$  

(3.70)

Only $f_0$ remains under the above integral, all the rest of the expansion coefficients average to zero after integration over $\theta$. The time derivative of $f_0$ is given by the 0-th equation within the system of equations 3.3:

$$\frac{\partial f_0}{\partial t} + \frac{a_z}{3} \left( \frac{\partial f_1}{\partial v} + 2 \frac{f_1}{v} \right) = 0,$$  

(3.71)

and can be re-expressed as

$$\frac{\partial (v^2 f_0)}{\partial t} + \frac{\partial j_1}{\partial v} = 0 \quad \text{where} \quad j_1 = \frac{a_z}{3} v^2 f_1.$$  

(3.72)

Integrating over $v$, we obtain

$$\frac{\partial n}{\partial t} + a_z \frac{4\pi}{3} (v_2^2 f_1(v_2) - v_1^2 f_1(v_1)) = 0,$$  

(3.73)

the analog of particle conservation in the $P_N$ approximation. We write the finite-difference analog of equation 3.72 as

$$(v_2^2)_{i+1/2} \frac{f_{0,i+1/2}^+ - f_{0,i+1/2}}{\tau} + \frac{a_z}{3} \frac{v_1^2 f_{1,i+1} - v_2^2 f_{1,i}}{\nu} = 0.$$  

(3.74)

To evaluate the left side of this equation we need a representation for $(v^2)_{i+1/2}$. We
represent \((v^2)_{i+1/2}\) in a form so that the product \(4\pi(v^2)_{i+1/2}\nu\) is equal to the volume of the shell between the outer and inner spheres of radii \(v_{i+1}\) and \(v_i\) respectively. This leads to the formula

\[
(v^2)_{i+1/2} = \frac{v_{i+1}^3 - v_i^3}{3\nu}. \tag{3.75}
\]

Note that \((v^2)_{i+1/2} \neq (v_{i+1/2})^2\). The finite-difference analog of equation 3.70 for the number of particles can be introduced as

\[
n = 4\pi\nu \sum_{i=1}^{N_v} (v^2)_{i+1/2} f_{0,i+1/2}. \tag{3.76}
\]

Comparison of the above formula and formula 3.70 suggests that \(\int v^2 dv\) is replaced by \(\sum_i (v^2)_{i+1/2}\nu\) in the finite-difference equivalents of the integrals over a region in velocity space. It also determines the finite-difference analog of formula 3.73 for particle conservation

\[
\frac{n^+ - n}{\tau} + a_z \frac{4\pi}{3} (v_{i+2}^2 f_{i+2,i+1} - v_i^2 f_{i,i}) = 0. \tag{3.77}
\]

To later construct a finite-difference description of evolution equations supporting density conservation it will be convenient to introduce the conversion operator \(C_{v^2}\):

\[
(v^2 f)_{n,i+1/2} = (v^2)_{i+1/2} f_{n,i+1/2} \tag{3.78}
\]
and define its inverse $C_{v-2} = C_{v-2}^{-1}$:

$$f_{n,i+1/2} = \frac{(v^2 f)_{n,i+1/2}}{(v^2)_{i+1/2}}.$$  \hspace{1cm} (3.79)

### 3.1.7 Implementation of $A_v(a_z \tau)$ and comparison with the analytic solution.

One obvious implementation for the evolution operator advancing in time the solution of the finite-difference equivalent of equation 3.3 would be

$$A_v(a_z \tau) = R_{v}^{adv}(a_z \tau) T_{v}^{adv}(a_z \tau),$$  \hspace{1cm} (3.80)

where the finite-difference advection equation and the corresponding boundary conditions defining $T_{v}^{adv}(a_z \tau)$ are described in subsections 3.1.1 and 3.1.3 while the construction of $R_{v}^{adv}(a_z \tau)$ is given in subsection 3.1.2. Unfortunately, this implementation does not have the form of equation 3.74, and is not particle-conserving. In the following, we look for subtle modifications of the definitions of $R_{v}^{adv}(a_z \tau)$ and $T_{v}^{adv}(a_z \tau)$ to force their combined action to satisfy equation 3.74 and preserve the number of particles.

We can try to introduce conservation in the following way. The action of operator $T_{v}^{adv}(a_z \tau)$ is defined through the solution of the system of equations 3.15 where the
n-th equation is given by

\[
\frac{f_{n,i+1/2}^+ - f_{n,i-1/2}^-}{\tau} + a_z \sum_{n=0}^{N} A_{n,m} \frac{f_{m,i+1} - f_{m,i}}{\nu} = 0,
\]

and the 0-th equation defines the change in \( f_0 \) during each time-step. The definition of operator \( T_v^{\text{adv}}(a_z \tau) \) can be altered by means of substituting equation 3.74 for the 0-th equation of system 3.81 and keeping the rest of the equations (from equation one to equation \( N + 1 \)) unchanged. The values \( f_{m,i} \) of the function at the edges of the velocity mesh are still calculated according to the description of subsection 3.1.1 with boundary conditions described in subsection 3.1.3. Equation 3.74 contains the components that are also modified by the subsequent action of operator \( R_v^{\text{adv}}(a_z \tau) \). In order to not modify them twice, the definition of operator \( R_v^{\text{adv}}(a_z \tau) \), given by formula 3.30, has to be altered so that its subsequent action does not change \( f_0 \).

The definition of \( R_v^{\text{adv}}(a_z \tau) \) can be adjusted in the following way: after calculating the matrix \( e^{-\frac{a_z}{\nu+1/2} B \tau} \), the components of its 0-th row has to be replaced by the row 1 0 . . . 0. The adjusted operator \( R_v^{\text{adv}}(a_z \tau) \) does not modify \( f_0 \) as required. We refer to the modified operators as \( T_v^{\text{cadv}}(a_z \tau) \) and \( R_v^{\text{cadv}}(a_z \tau) \). The finite-difference equivalent of equation 3.3 can be solved as before through their combined action

\[
\mathcal{A}_v^{\text{cadv}}(a_z \tau) = T_v^{\text{cadv}}(a_z \tau)R_v^{\text{cadv}}(a_z \tau),
\]

Numerical experiments conducted by the author show that the discussed evolution
operators $A_{adv}^a(a_z \tau)$ and $A_{adv}^c(a_z \tau)$ are stable for a time-step

$$\tau \leq \min(\tau^a_v, \tau^c_v), \tag{3.83}$$

where $\tau^a_v$ and $\tau^c_v$ are given by formulas 3.21 and 3.31.

Figures 3-5 and 3-6 compare the numerical solutions obtained with formula 3.82 to the analytic solution given by formula 2.101 for $P_7$. Figures 3-7 and 3-8 provide the comparison for $P_8$. For both the analytical and numerical solutions $a = 1$ and initial conditions at $t = 0$ are given by a Gaussian 2.103. The numerical solutions shown in the figures for both $P_7$ and $P_8$ have the following parameters: the number of velocity points $N_v = 80$, the largest value of the absolute velocity $V = 1$, the time step $\tau = 0.01$, resulting in the corresponding characteristic times $\tau^a_v/\tau = 0.0768$, $\tau^c_v/\tau = 0.793$ for $N = 7$ and $\tau^a_v/\tau = 0.0774$, $\tau^c_v/\tau = 0.929$ for $N = 8$. In both cases, $\tau^c_v/\tau$ is close to one. The values of the characteristic variables at the edges of the velocity mesh $g_{\ell,i}$ in equation 3.18 are determined through 7-th order flux-limited polynomial interpolation as described in article [26]. In the plots on the left, the analytical solutions are given by the continuous colored lines and the numerical solutions $f_{n,i+1/2}^a$ are presented by the circles of the same color. One can see that the numerical solution closely matches the analytical one. The number of particles determined by formula 3.76 is displayed below the time label to demonstrate a 15-digit accurate particle conservation achieved by the operator $A_{adv}^c(a_z \tau)$. 
On the right side, the plots show the functions

$$f(t^s, v_i, \theta) = \sum_{n=0}^{N} f_{n,v_i}^s P_n(\cos \theta), \quad (3.84)$$

on the plane $(v, \theta)$, determined by the found numerical values of $f_{n,i+1/2}^s$. The values of the coefficients $f_{n,v_i}^s$ at the edges of the velocity intervals have been determined by simple averaging $f = (f_{n,i-1/2}^s + f_{n,i+1/2}^s)/2$ in the middle points $i = 1, N_v - 1$ of the velocity interval $[0, V]$ and by the boundary conditions 3.43 and 3.46 at its ends for $i = 0$ and $i = v_{N_v}$.

### 3.2 Discretization of collision integrals.

In this section we construct finite-difference analogs of the $P_N$ approximation of collision integrals and their evolution operators (see appendix G) to solve the finite-difference analog of equation

$$\frac{\partial f}{\partial t} + a_z \left( A \frac{\partial f}{\partial v} + \frac{1}{v} B f \right) + v A \frac{\partial f}{\partial z} = S(f). \quad (3.85)$$

To do so we will have to re-examine the collision integrals discussed in appendix H, to take into account particle conservation.

For later use, we introduce the loss rate

$$r_n(v)_{pr} = N_s v Q_{npr}^v (v), \quad (3.86)$$
the average loss rate on the interval \([v_i, v_{i+1}]\):

\[
\rho_{n,i+1/2}^{pr} = e^{-\tau r_n^{pr}(v_i, v_{i+1})},
\]

(3.88)

where the index \(pr = el, ex, io\) denotes the type of the scattering process: elastic, excitation and ionization.

### 3.2.1 Elastic collision integral.

The \(P_N\) approximation of elastic collision integral is given by equation H.20. The corresponding evolution equation is

\[
\frac{\partial f_n}{\partial t} = S_n^el = N_s v \left( (Q_{n}^{el}(v) - Q_0^{el}(v)) f_n - \frac{\eta}{v^3} \frac{\partial}{\partial v} \left[ v^4 K_n^{el}(v) f_n \right] \right).
\]

(3.89)

It will be convenient to further split it into the two evolution equations

\[
\frac{\partial f_n}{\partial t} = -N_s \frac{\eta}{v^2} \frac{\partial}{\partial v} \left[ v^2 K_n^{el}(v) f_n \right]
\]

(3.90)

and

\[
\frac{df_n}{dt} = (r_n^{el}(v) - r_0^{el}(v)) f_n
\]

(3.91)
and to consider them separately.

Equation 3.90 can be further written in the form of a continuity equation

$$\frac{\partial (v^2 f_n)}{\partial t} + \frac{\partial J}{\partial v} = 0 \quad \text{where} \quad J = q(v) v^2 f_n \quad \text{and} \quad q(v) = N_s \eta v^2 K_{n}^{\text{col}}(v). \quad (3.92)$$

The finite-difference analog of the above equation is

$$\frac{(v^2 f)^{+}_{n,i+1/2} - (v^2 f)_{n,i+1/2}}{\tau} + \frac{j_{n,i+1} - j_{n,i}}{\nu} = 0, \quad (3.93)$$

with the first-order accurate flux

$$j_{n,i} = \begin{cases} q_{n,i}(v^2 f)_{n,i-1/2} & \text{for} \quad 0 \leq q_{n,i} \\ q_{n,i}(v^2 f)_{n,i+1/2} & \text{for} \quad q_{n,i} < 0 \end{cases} \quad \text{and} \quad q_{n,i} = q_n(v_i). \quad (3.94)$$

The boundary conditions

$$j_{n,0} = j_{n,N_v} = 0 \quad (3.95)$$

“stop the density leaks” at the ends of the interval. Equations 3.93, 3.94 and 3.95 define the action of the evolution operator later referred to as $T^{\text{col}}_v(\tau)$.

Limitations on the size of the time-step can be found by requiring that the CFL numbers

$$c^{\text{col}}_{n,i} = \tau^{\text{ael}} \frac{q_{n,i}}{\nu} \quad \text{are such that} \quad |c^{\text{col}}_{n,i}| \leq 1. \quad (3.96)$$
Keeping the solution positive in addition requires

\[ \tau_{\text{cel}} \left| \frac{q_{n,i+1} - q_{n,i}}{\nu} \right| \leq 1. \]  \hspace{1cm} (3.97)

Both requirements provide estimation of the characteristic time \( \tau_{v}^{\text{cel}} \) for the operator \( \mathcal{T}_{v_n^2}(\tau) \) and restrict the time step to

\[ \tau \leq \tau_{v}^{\text{cel}} = \min(\tau_{v}^{\text{ael}}, \tau_{v}^{\text{cel}}) \quad \text{where} \quad \tau_{v}^{\text{ael}} = \min_{n,i} \frac{\nu}{|q_{n,i}|} \quad \text{and} \quad \tau_{v}^{\text{cel}} = \min_{n,i} \frac{\nu}{|q_{n,i+1} - q_{n,i}|}. \]  \hspace{1cm} (3.98)

The analytical solution of equation 3.91 is

\[ f_{n}(t + \tau, v) = e^{\tau(r_{n}^{\text{el}}(v) - r_{0}^{\text{el}}(v))} f_{n}(t, v). \]  \hspace{1cm} (3.99)

The finite-difference analog of the above solution can be constructed as

\[ (v^2 f)^+_{n,i+1/2} = \frac{\rho_{0,i+1/2}^{\text{el}}}{\rho_{n,i+1/2}^{\text{el}}} (v^2 f)_{n,i+1/2}. \]  \hspace{1cm} (3.100)

It defines the action of the evolution operator later referred to as \( \mathcal{Q}_{v_n^2}(\tau) \). The operator \( \mathcal{Q}_{v_n^2}(\tau) \) does not have any restrictions on the time-step, due to its construction through the analytic solution. Using formula G.15, its characteristic time can be estimated as

\[ \tau_{v}^{\text{qel}} = \min_{n,i} \frac{1}{|r_{n}^{\text{el}}(v_i, v_{i+1}) - r_{0}^{\text{el}}(v_i, v_{i+1})|}. \]  \hspace{1cm} (3.101)

Operator \( \mathcal{Q}_{v_n^2}(\tau) \) describes isotropization of the density function \( f \), eliminating
\( f_{n>0} \), due to \( r_n^{\text{el}}(v) - r_0^{\text{el}}(v) < 0 \). Operator \( T_{\alpha 2}(\tau) \) brings the density function \( f \) closer to the origin of the velocity space because \( q_{n=0}(v) < 0 \). Their combined action causes growth of \( f_0 \) at the origin of the velocity space while \( f_{n>0} \) decreases everywhere. Particle conservation by \( T_{\alpha 2}^{\text{el}}(\tau) \) is supported by the continuity form of equation 3.93 and because operator \( Q_{\alpha 2}^{\text{el}}(\tau) \) does not alter \( f_0 \).

### 3.2.2 Excitation collision integral.

The \( P_N \) approximation of the excitation collision integral is given by equation H.26. The corresponding evolution equation is

\[
\frac{df_n(t, v)}{dt} = S_n^{\text{ex}} = N_s v \left( \left( \frac{v'}{v} \right)^2 Q_n^{\text{ex}}(v') f_n(t, v') - Q_0^{\text{ex}}(v) f_n(t, v) \right),
\]

(3.102)

where

\[
v'^2 = v^2 + v_{ex}^2
\]

(3.103)

describes energy conservation. It can be re-written as

\[
\frac{d[v^2 f_n(t, v)]}{dt} dv = r_n^{\text{ex}}(v') [v^2 f_n(t, v')] dv' - r_0^{\text{ex}}(v) [v^2 f_n(t, v)] dv
\]

(3.104)

and re-expressed in the integral form as

\[
\frac{d}{dt} \int_{v_1}^{v_2} dv [v^2 f_n(t, v)] = \int_{v_1}^{v_2} dv r_n^{\text{ex}}(v) [v^2 f_n(t, v)] - \int_{v_1}^{v_2} dv r_0^{\text{ex}}(v) [v^2 f_n(t, v)].
\]

(3.105)
With use of the integral form, the finite-difference evolution operator $Q^e_n(\tau)$ can be constructed as

$$(v^2f)^+_{n,i+1/2} = q_{0,i+1/2}(v^2f)_{n,i+1/2} + \sum_{i'=1}^{N_n} k^e_{n; i+1/2,i'+1/2}(1 - q_{n,i'+1/2})(v^2f)_{n,i'+1/2}. \quad (3.106)$$

Matrix $k^e_{n; i+1/2,i'+1/2}$ in the second term redistributes the losses on the interval $[v_i, v_{i+1}]$ into the gains on the other intervals.

To construct $k_{i,i'}$, we need to know how the gains are distributed. Figure 3-9 shows where particles scattered at a particular velocity interval arrive in the velocity space obeying energy conservation given by formula 3.103. The solid curve shows the energy conservation $v'^2 = v^2 + v^2_{ex}$, $v_i = \nu i$ denotes the ends of the velocity intervals and $v'^2_i = v^2_i + v^2_{ex}$. The excitation threshold $v_{ex}$ falls into the velocity interval $[v_s, v_{s+1}]$. It is convenient to divide each interval $[v_i, v_{i+1}]$ into subintervals $[\nu_j, \nu_{j+1}]$ according to the rule

$$[\nu_1', \nu_2'] \text{ so that } |\nu_2 - \nu_1| = \max_{[\nu_1', \nu_2'] \subset [\nu_i, \nu_{i+1}]} |\nu_2 - \nu_1|, \quad (3.107)$$

illustrated in figure 3-9. We are looking at the largest interval within $[v_i, v_{i+1}]$ whose image, projected with the conservation law 3.103 fits into $[\nu_1', \nu_{i+1}']$. For example, for $i = 0$ and $i' < s$: $\nu_1'$ and $\nu_2'$ do not exist, for $i = 0$ and $i' = s$: $\nu_1' = v_{ex}$ and $\nu_2' = v_1'$, for $i = 1$ and $j = s$: $\nu_1' = v_1'$ and $\nu_2' = v_2'$, for $i = 2$ and $j = s$: $\nu_1' = v_2'$ and $\nu_2' = v_{s+1}$.
and so on. Based on the above consideration, we find

\[
\begin{align*}
    k_{n; i+1/2, i'+1/2}^{\text{ex}} &= \begin{cases} 
        0, & \text{if } \nu_1'(i, i') \text{ and } \nu_2'(i, i') \text{ do not exist or } r_n^{\text{ex}}(v_{i'}, v_{i'+1}) = 0 \\
        r_n^{\text{ex}}(\nu_1'(i, i'), \nu_2'(i, i'))/r_n^{\text{ex}}(v_{i'}, v_{i'+1}), & \text{otherwise}
    \end{cases}.
\end{align*}
\]

(3.108)

Particle conservation is supported because for any \(i'\)

\[
\sum_{i=1}^{N_v} k_{n; i+1/2, i'+1/2}^{\text{ex}} = 1.
\]

(3.109)

Using formula G.15, the characteristic time of the operator \(Q^{\text{ex}}_{v_2}(\tau)\) can be estimated as:

\[
\tau^{\text{ex}}_v = \min_{n,i} \frac{1}{|r_n^{\text{ex}}(v_i, v_{i+1}) - r_0^{\text{ex}}(v_i, v_{i+1})|}.
\]

(3.110)

### 3.2.3 Ionization collision integral.

The \(P_N\) approximation of the ionization collision integral is given by equation H.51. We write the corresponding evolution equation on the velocity interval \([0, V]\) as

\[
\frac{df_n(t, v)}{dt} = S_n^{\text{io}} = N_s \left( \delta_{0,n} 8\pi \int_0^V dv' \ v'^3 g(v^2, v'^2 - v_0^2) Q_0^{\text{io}}(v') f_0(t, v') - v Q_0^{\text{io}}(v) f_n(t, v) \right),
\]

(3.111)

where \(g(v^2, v'^2)\) describes the distribution of the scattered electrons and additional free electrons created in ionizing collisions. As we mention in section H.3, the above equation supports energy conservation for the scattered electrons and the electrons.
produced in the ionizing collisions in the form

\[ \nu^2 = 8\pi \int_0^\nu dv \, v^4 \rho(v^2, \nu^2) = \nu^2 - \nu_{io}^2. \] (3.112)

Equation 3.111 can be written as

\[ \frac{d}{dt} \int_{v_1}^{v_2} [v^2 f_n(t, v)] = \delta_{0,n} 8\pi \int_0^V d\nu' \rho(v^2, \nu^2 - \nu_{io}^2) r_0^{in}(\nu') [v^2 f_n(t, \nu')] \] (3.113)

and re-expressed in integral form

\[ \frac{d}{dt} \int_{v_1}^{v_2} [v^2 f_n(t, v)] = \sum_{i=1}^{N_u} \delta_{0,n} 8\pi \int_{u_{i-1}}^{u_i} d\nu' r_0^{in}(\nu') [v^2 f_n(t, \nu')] \int_{v_1}^{v_2} d\nu \rho(v^2, \nu^2 - \nu_{io}^2) - \int_{v_1}^{v_2} d\nu \ r_0^{in}(\nu) [v^2 f_n(t, v)], \]

where \(0 = u_0 < u_1 < u_2 < ... u_{N_u-1} < u_{N_u} = V\) are arbitrary and \(N_u > 0\) is an arbitrary integer number.

Using the integral form, the finite-difference evolution operator \(Q_{io}^{kn}(\tau)\) can be constructed as:

\[ (v^2 f)^{+}_{n,i+1/2} = \rho_{0,i+1/2}^{io}(v^2 f)_{n,i+1/2} + \sum_{i'=1}^{N_u} k_{n,i+1/2,i'+1/2}^{io} (1 - \rho_{n,i'+1/2})(v^2 f)_{n,i'+1/2}; \] (3.115)

where matrix \(k_{n,i+1/2,i'+1/2}^{io}\) in the second term redistributes the losses on the interval.
To construct $k_{n; i+1/2, i'+1/2}$, we need to know how the gains are distributed. Redistribution of the scattered and produced electrons is illustrated in figure 3-10. The solid curve shows energy conservation $\nu^2 = \nu'^2 - v_{ioi}^2$, $\nu = \nu\iota$ denotes the ends of the velocity intervals and $\nu_i^2 = v_{i'}^2 - v_{ioi}^2$. Ionization threshold $v_{in}$ falls into the velocity interval $[v_s, v_{s+1}]$. The electrons scattered and produced in ionizing collisions by electrons with impact velocity $v'$ are redistributed in the velocity interval $[0, \nu]$ as displayed in the figure by the dotted lines. For example, the impact electrons with their initial velocities in the interval $[v_{io}, v_{s+1}]$ are scattered and produce new electrons in the interval $[0, \nu_{s+1}]$ that include intervals $[0, v_1]$, $[v_1, v_2]$ and $[v_2, v_{s+1}] \subset [v_2, v_3]$; electrons with the impact velocity in the interval $[v_{s+1}, v_{s+2}]$ are scattered and create new electrons in the interval $[0, \nu_{s+2}]$ that include intervals $[0, v_1]$, $[v_1, v_2]$, $[v_2, v_3]$ and $[v_3, v_{s+2}] \subset [v_3, v_4]$; and so on.

Based on the above consideration, we find

$$k_{n; i+1/2, i'+1/2} = \frac{8\pi \delta_{0,n}}{r_0^*(v', v_i)} \frac{3}{v_{i'+1}^3 - v_{i+1}^3} \int_{v_i}^{v_{i'+1}} dv' r_0^*(v') \int_{v_i}^{v_{i+1}} dv g(v^2, v'^2 - v_{ioi}^2).$$

(3.116)

Particle conservation is supported because for any $i'$

$$\sum_{i=1}^{N_{\nu}} k_{n; i+1/2, i'+1/2} = 2$$

(3.117)

Using formula G.15, the characteristic time of the operator $Q_{\nu, 2}^*(\tau)$ can be estimated
\[ \tau_{v}^{qio} = \min_{n,i} \frac{1}{|r_{n}^{io}(v_{i}, v_{i+1}) - r_{0}^{io}(v_{i}, v_{i+1})|}. \]  

(3.118)

### 3.2.4 Addition of collisions. Comparison with the Monte-Carlo stationary solution.

The results obtained to this point allow us to advance the numerical solution of the finite-difference analog of equation 3.85 by means of the particle-conserving operator

\[ B_{v}(\tau) = C_{v,2}^{-1} Q_{v,2}^{io}(\tau) Q_{v,2}^{ex}(\tau) Q_{v,2}^{el}(\tau) T_{v,2}^{cel}(\tau) C_{v,2} A_{v}^{2}(a_{z} \tau). \]  

(3.119)

The operators \( C_{v,2} \) and \( C_{v,2}^{-1} \) are present in the construction because the application of the particle conserving operators \( Q_{v,2}^{io}(\tau), Q_{v,2}^{ex}(\tau), Q_{v,2}^{el}(\tau), T_{v,2}^{cel}(\tau) \) requires prior conversion to the variables \( (v^{2}f)_{n,i+1/2} \). Numerical experiments conducted by the author show that the operator 3.119 provides an adequate time resolution of the advection and collision processes for a time step

\[ \tau \leq \tau_{v}^{b} = \min(\tau_{v}^{a}, \tau_{v}^{r}, \tau_{v}^{ael}, \tau_{v}^{cel} / 10, \tau_{v}^{qex} / 4, \tau_{v}^{qel} / 4, \tau_{v}^{qio} / 4). \]  

(3.120)

The numerical method defined by the operator \( B_{v} \) in equation 3.119 has been evaluated for \( P_{15} \) and the following parameters: the number of velocity points \( N_{v} = 40 \), the largest value of the absolute velocity \( V = 8.39 \times 10^{8} \text{ cm/s} \) corresponding to the electron kinetic energy of 200 eV, and the electron accelerations \( a_{z} = 2.9 \times 10^{20} \text{ cm/s}^{2} \) and \( 2.9 \times 10^{19} \text{ cm/s}^{2} \) corresponding to the electric fields of 100 Td and 1000 Td.
The collision operators included in the formula 3.119 have been constructed using the numerical values for the argon collision cross-sections from the BOLSIG database (see reference [1]). The argon cross-sections $Q_{0}^{\text{el}}(v)$, $Q_{0}^{\text{ex}}(v)$, $Q_{0}^{\text{io}}(v)$ used in the calculation are displayed in the figure 3-11. The excitation and ionization threshold energies of the argon atom are 11.6 eV and 15.7 eV, they correspond to the electron velocities of $2.02 \times 10^8$ cm/s and $2.35 \times 10^8$ cm/s respectively. The chosen argon pressure of 500 Torr and temperature of 20 °C corresponds to the density of the background argon atoms of $N_s = 1.65 \times 10^{19}$ 1/cm$^3$. The time step of the calculation has been set equal to $\tau_v^b$.

The numerical solution was analyzed for the two cases. In one, the ionization process was treated as excitation so that the two excitation-collision operators $Q_{0}^{\text{ex}}(v)$ corresponding to the excitation and ionization cross-sections were included in $B_v$ and no ionization-collision operator. In the other, the ionization was treated appropriately. Irrespective of the initial conditions, the numerical solution has visibly converged to a stationary solution for the first case and to the solution exponentially growing in $t$, but stationary in $v$, for the second case. The determined times of the sure convergence are $t = 5 \times 10^{-9}$ s and $t = 5 \times 10^{-11}$ s for electric fields of 100 Td and 1000 Td.

The solution of the same stationary problems have been obtained using a Monte-Carlo solver (developed by A. Shvidky and V. N. Khudik and used in the simulations of article [49]). To collect statistics, values of $\theta$ have been accumulated on 180 intervals in the range from 0 to $\pi$ and values of $v$ in the range from 0 to $V$ on 100 intervals. The electrons with velocities greater then $V$ have been put in the sampling intervals corresponding to $V$ and a correct $\theta$. The statistics of the electron velocities have
been accumulated starting at the convergence times, until visibly smooth distribution
functions are obtained and expansion coefficients $f_n$ for the obtained distribution
functions have been calculated after the distribution function was normalized to the
same number of particles as in the solution obtained for $P_{15}$.

The obtained solutions for the first case (ionization treated as excitation) and for
an applied electric field of 1000 Td are compared in figure 3-12. For the second case
(true ionization) and the applied electric field of 1000 Td and 100 Td, the solutions
are compared in the figures 3-13 and 3-14. For all figures, on the the top-left chart,
the coefficients $f_n$ for the Monte-Carlo solution are displayed by continuous colored
lines. The coefficients $f_n$ obtained in the numerical solution for $P_{15}$ are presented by
black dots connected by colored lines. The top-right figure shows the same solutions
multiplied by $v^4$ to resolve behavior of the tails of the distribution functions. The left
and right bottom shapes display the corresponding distribution functions obtained
by the Monte-Carlo method and the numerical solution of the $P_{15}$ method. The
difference in the solutions is displayed by the red frame. The blue and brown curves
on the surfaces, representing the electron distribution functions, mark velocities of
$2.02 \times 10^8$ cm/s and $2.35 \times 10^8$ cm/s corresponding to the 11.6 eV excitation and
15.7 eV ionization thresholds of the argon atom respectively. To make comparison
possible, the distribution functions are normalized to a unit density $n = 1$ for both
the Monte-Carlo and $P_{15}$ solutions. The electron drift velocity is found as

$$
\langle v_z \rangle = \frac{1}{n} \int_{D_v} d^3v f v_z = \frac{4\pi}{3n} \int_0^V dv v^3 f_1
$$

(3.121)
analytically, or as
\[
\langle v_z \rangle = \frac{4\pi}{3n} \nu \sum_{i=1}^{N_v} \left( v^2 \right)_{i+1/2} v_{i+1/2} f_{i+1/2}
\]  
(3.122)

numerically. The mean electron energy is found as
\[
\langle \varepsilon \rangle = m_e \frac{\langle v^2 \rangle}{2},
\]  
(3.123)

where \( m_e \) is the electron mass and \( \langle v^2 \rangle \) is the mean square electron velocity. The mean square electron velocity can be obtained as
\[
\langle v^2 \rangle = \frac{1}{n} \int_{D_v} d^3v f v^2 = 4\pi \int_0^V dv v^4 f_0,
\]  
(3.124)

analytically, or as
\[
\langle v^2 \rangle = 4\pi \nu \sum_{i=1}^{N_v} \left( v^2 \right)_{i+1/2} v_{i+1/2} f_{0,i+1/2}
\]  
(3.125)

numerically. (When the distribution function is not normalized to a unit density, the density \( n \) in the above equations can be found using formulas 3.70 or 3.76).

For both cases the pictures show an excellent match except for a few points in the vicinity of \( v = 0 \) for the case of true ionization. The difference in the solutions for true ionization can be explained by recalling that the collision integral for the ionization process defined by the formula H.51 is singular at \( v = 0 \). The singularity of order \( 1/v^2 \) is introduced by the distribution of the electrons scattered and produced in the ionization collisions (see formula H.52). The numerical method defined by \( B_v \) is not expected to resolve the singularity, but to treat it smoothly, according to the
boundary conditions 3.43.

3.3 Spatial dependence.

The following section finalizes the description of the computational method by including spatial dependence and boundary conditions and discusses the effective way of parallel implementation. With the knowledge gained during the construction of the numerical solution of $P_N$ approximation of advection equation, including space becomes a surprisingly easy task. We will see that the evolution equations that we have to consider are similar to the equations of neutron transport (see reference [5]) and so the spatial boundary conditions for the absorbing boundary, developed in neutron transport theory, are directly applicable to the $P_N$ approximation of Boltzmann equation.

3.3.1 Solution of $\frac{\partial f}{\partial t} + vA \frac{\partial f}{\partial z} = 0$ and the spatial flux.

To add spatial dependence to the solution 3.119, we have to construct the the evolution operator $T_{z}^{adv}(v_i \pm 1/2 \tau)$ defined by the finite-difference analog of the evolution equation

$$\frac{\partial f}{\partial t} + vA \frac{\partial f}{\partial z} = 0.$$  \hspace{1cm} (3.126)

We can notice that interchanges

$$a_z \rightleftharpoons v \quad \text{and} \quad \partial v \rightleftharpoons \partial z \hspace{1cm} (3.127)$$
allow transformation of the equation 3.4: \( \frac{\partial f}{\partial t} + a_z A \frac{\partial}{\partial v} f = 0 \) into equation 3.126 as well as the reverse transformation. The construction of the evolution operator for equation 3.4 is presented in full detail in subsection 3.1. The finite-difference analog of equation 3.126 can be written as

\[
\frac{f_{j+1/2}^+ - f_{j-1/2}^-}{\tau} + v_{j+1/2} A \frac{f_{j+1} - f_j}{h} = 0.
\]

(3.128)

One can notice that the above equation is the same as equation 3.15:

\[
\frac{f_{i+1/2}^+ - f_{i-1/2}^-}{\tau} + a_z A \frac{f_{i+1} - f_i}{h} = 0,
\]

where the following interchanges occur

\[
a_z \leftrightarrow v_{j+1/2}, \quad \nu \leftrightarrow h \quad \text{and} \quad f_i, f_{i+1/2} \leftrightarrow f_j, f_{j+1/2}.
\]

(3.129)

With the interchanges given by expressions 3.127 and 3.129, the construction of the evolution operator \( T_{z \text{adv}}(v_{i+1/2} \tau) \) is the same as that of \( T_{v \text{adv}}(a_z \tau) \). Boundary conditions required for the construction are presented in subsections 3.3.2 and 3.3.3.

The numerical method defining the constructed evolution operator \( T_{z \text{adv}}(v_{i+1/2} \tau) \) is stable when the corresponding CFL numbers

\[
c_n = \frac{\tau v_{i+1/2} a_n}{h} \quad \text{are so that} \quad |c_n| \leq 1,
\]

(3.130)

which restricts the time step to

\[
\tau \leq \tau^a_z = \min_{i, \ell} \frac{\nu}{|v_{i+1/2} a_\ell|}.
\]

(3.131)
We adopt the value of $\tau_z^a$ as an estimation of the characteristic time of the operator $T_z^{\text{adv}}(a_z \tau)$ based on formula G.15.

Equation 3.126 remains valid under the interchange $f \rightleftharpoons (v^2 f)$ and equation 3.128 allows interchanging $f_{i+1/2} \rightleftharpoons (v^2)_{i+1/2} f_{i+1/2}$. This suggests that the change of the total number of particles calculated for equations 3.126 and 3.128 is determined by only spatial boundary fluxes.

The spatial fluxes can be found in the following way. Notice that with the introduction of space, formulas 3.70 and 3.76 determine the particle density and its finite-difference equivalent. The 0-th equation in the system 3.126

$$\frac{\partial f_0}{\partial t} + \frac{v}{3} \frac{\partial f_1}{\partial z} = 0 \quad (3.132)$$

multiplied by $4\pi v^2 dv$ and integrated over the velocity interval becomes

$$\frac{\partial n}{\partial t} + \frac{\partial J}{\partial z} = 0, \quad (3.133)$$

where

$$J = \frac{4\pi}{3} \int_0^V dv \, v^3 f_1 \quad (3.134)$$

determines the spatial (density) flux and

$$n(t, z) = 4\pi \int_0^V dv \, v^2 f_0(t, z) \quad (3.135)$$

is the particle density (see also formula 3.70). To obtain the finite-difference analog
of the above equations, the 0-th equation of system 3.128

\[ \frac{f_{0,j+1/2}^+ - f_{0,j+1/2}}{\tau} + \frac{v_{j+1/2} f_{1,j+1} - f_{1,j}}{3} = 0 \] (3.136)

is multiplied by \( 4\pi(v^2)_{i+1/2} \nu \) and after summation over the velocity mesh intervals yields

\[ \frac{n_{j+1/2}^+ - n_{j+1/2}}{\tau} + \frac{J_{j+1} - J_j}{h} = 0, \] (3.137)

where

\[ J_j = \frac{4\pi}{3} \nu \sum_{i=1}^{N_v} (v^2)_{i+1/2} v_{i+1/2} f_{1,j,i+1/2} \] (3.138)

and

\[ n_{j+1/2}^s = 4\pi \nu \sum_{i=1}^{N_v} (v^2)_{i+1/2} f_{0,j+1/2,i+1/2} \] (3.139)

(see also formula 3.76) are the finite-difference equivalents of the spatial flux and particle density. Note that formula 3.138 defines the spatial flux \( J_j \) at the edge of the spatial mesh \( z_j \), while formula 3.139 defines the number of particles \( n_{j+1/2}^s \) at the center of the spatial mesh \( z_{j+1/2} \). The continuity form of equations 3.132 and 3.136 suggests particle conservation where the number of particles on the spatial interval \([z_1, z_2]\) is determined by

\[ \mathcal{N}(t) = \int_0^L n \, dz = 4\pi \int_0^L d z \int_0^V d v \, v^2 f_0 \] (3.140)
in the continuous case of equations 3.126, 3.133, and by

\[ N^s = h \sum_{j=1}^{N_z} \nu_n n^{s}_{i+1/2} = 4\pi h \sum_{j=1}^{N_z} \nu \sum_{i=1}^{N_v} (v^2)_{i+1/2} f_{0,i+1/2}^s \]  

(3.141)

on the spatial interval \([0, L]\) for the finite-difference case given by equations 3.128, 3.136.

### 3.3.2 Semi-reflecting boundary.

The discussion of the meaning of the characteristic variables given in subsection 3.1.4 greatly facilitates the conversion of the spatial boundary conditions from their formulation in Cartesian coordinates into the \(P_N\) approximation.

As an example, let's consider a semi-reflecting boundary on the left where particles have a probability \(p\) to be reflected and \(1 - p\) to be absorbed in collisions with the boundary. When the particle is reflected the angle characterizing the direction of its velocity is changing from \(\theta \in (\pi/2, \pi]\) to \(\pi - \theta\) as shown in figure 3-15. Correspondingly, the distribution function at the left semi-reflecting boundary can be written as

\[ f(\pi - \theta) = pf(\theta), \text{ where } \theta \in (\pi/2, \pi]. \]  

(3.142)

From the discussion of subsection 3.1.4 we know that when \(N \to \infty\): \(g_\ell = f(\theta_\ell) \sin \theta_\ell \Delta \theta_\ell\) (see formula 3.56), \(\theta_\ell = \pi - \theta_{-\ell}\) (see figure 3-3) and that \(\Delta \theta_\ell = \Delta \theta_{-\ell}\). Combining the above formulas and formula 3.142, we obtain boundary conditions for the left
semi-reflecting boundary

\[ g_{\ell>0} = p \ g_{-\ell}. \]  

(3.143)

The boundary conditions for the right boundary:

\[ g_{\ell<0} = p \ g_{-\ell} \]  

(3.144)

are obtained by the interchange \( \ell > 0 \leftrightarrow \ell < 0 \). The boundary conditions 3.143 and 3.144 have a simple intuitive interpretation. If the impact velocity of the particle is within the cone defined by \( g_\ell \) (see figure 3-3) the velocity of the reflected particle lies in the cone defined by \( g_{-\ell} \). Here, again, as in subsection 3.1.3 - “waves” that leave the boundary \( (g_{\ell>0} \text{ for the left boundary and } g_{\ell<0} \text{ for the right boundary}) \) are determined by those arriving at the boundary \( (g_{\ell<0} \text{ and } g_{\ell>0} \text{ correspondingly}) \).

The \( P_N \) approximation of the Boltzmann equation used in Neutron Transport Theory (see books [34], [9] and [5]):

\[ \frac{\partial f}{\partial t} + a_z \left( A \frac{\partial f}{\partial v} + \frac{1}{v} B f \right) + v A \frac{\partial f}{\partial z} = S(f). \]  

(3.145)

has the same spatial terms as equation 3.1 that we study. It would be plausible to expect that similar boundary conditions had to exist for the above equation. And indeed, it is possible to show that in the case of the purely absorbing boundary \( (p = 0) \), the derived boundary conditions exactly match Mark boundary conditions of Neutron Transport Theory (for a discussion of Mark’s boundary conditions see books [9], p.129 and [5], p.97). A clear advantage of the derived boundary conditions
3.143 and 3.144 is their clear interpretation in terms of the characteristic variables. In practice, for a choice of small \( N \) (few terms in the \( P_N \) expansion), Marshak, Federighi or Pomraning boundary conditions may provide better accuracy (see article [24] and references therein).

For further use we will need an equation for the boundary current determined by the boundary conditions 3.143 and 3.144. To find it, coefficients \( g_\ell \) can be converted into \( f_n \) with formula 3.47 and the boundary currents can be calculated using expression 3.134:

\[
J_{\text{left}} = \frac{4\pi}{3} \int_0^V dv \, v^3 \sum_{\ell < 0} (1 - p) \alpha_{1,\ell} g_\ell(v) 
\]

\[
J_{\text{right}} = \frac{4\pi}{3} \int_0^V dv \, v^3 \sum_{0 < \ell} (1 - p) \alpha_{1,\ell} g_\ell(v). 
\]

Here we used the parity property for the eigenvectors of matrix \( A \) given by formula D.27: \( \alpha_{1,-i} = -\alpha_{1,i} \) and excluded \( \ell = 0 \) from the summation since \( \alpha_{1,0} = 0 \).

Boundary conditions 3.143 and 3.144 can be easily translated into their finite-difference equivalents

\[
g_{\ell > 0,j=0,j+1/2} = p \ g_{-\ell,j=0,j+1/2} 
\]

\[
g_{\ell < 0,j=N_z,j+1/2} = p \ g_{-\ell,j=N_z,j+1/2}. 
\]
The finite-difference equivalent of formulas 3.146 and 3.147 for the boundary currents

\[
J_{j=0} = \frac{4\pi}{3} \nu \sum_{i=1}^{N_v} (v^2)_{i+1/2} v_{i+1/2} \sum_{\ell<0} (1-p) \alpha_{1,\ell} g_{\ell,j=0,i+1/2} \\
J_{j=N_z} = \frac{4\pi}{3} \nu \sum_{i=1}^{N_v} (v^2)_{i+1/2} v_{i+1/2} \sum_{0<\ell} (1-p) \alpha_{1,\ell} g_{\ell,j=N_z,i+1/2}
\]  

(3.150)  

(3.151)

can be obtained by use of equations 3.138 and 3.47.

### 3.3.3 Secondary emission.

The effective secondary emission coefficient \( \gamma \), describing production of electrons by ion impact on the electrodes, can be introduced by the formula

\[
J^e = -\gamma J^i.
\]  

(3.152)

where \( J^e \) is electron current and \( J^i \) is the ion current directed toward the boundary (for more details see references [39], [53] and [11]). We want to append the secondary emission to the boundary conditions 3.143 and 3.144. We discuss the continuous case first and then obtain its finite-difference equivalent.

Let’s consider the left spatial boundary with the distribution of the secondary electrons in the velocity space given by \( \varphi^{left}(v, \theta) \):

\[
0 \leq \varphi^{left}(v, \theta) \text{ for } 0 < \theta < \pi/2 \\
\varphi^{left}(v, \theta) = 0 \text{ for } \pi/2 < \theta < \pi.
\]  

(3.153)
Suppose that $\varphi_{\text{left}}(v, \theta)$ can be approximated by means of characteristic variables $\mu_{\ell}^{\text{left}}$:

$$
\varphi_{\text{left}}(v, \theta) \approx \sum_{\ell} \mu_{\ell}^{\text{left}}(v) \alpha_{\ell}^N(\theta),
$$

(3.154)

where $\alpha_{\ell}^N(\theta) = \sum_{n=0}^{N} \alpha_{n,\ell} P_n(\cos \theta)$ is given by formula 3.49. As it follows from the discussion of subsection 3.1.4

$$
\mu_{\ell<0} \approx 0
$$

(3.155)

for considerably large $N$. Secondary emission can be included into the boundary conditions on the left semi-reflecting boundary given by equation 3.143 as

$$
g_{\ell>0} = p_{\ell} g_{-\ell} + c_{\ell}^{\text{left}} \mu_{\ell}^{\text{left}}.
$$

(3.156)

To determine the value of $c_{\ell}^{\text{left}}$ in the above formula, coefficients $g_{\ell}$ can be converted into $f_n$ using formula 3.47 and the boundary electron current $J^e$ can be calculated using equation 3.134:

$$
J^e = J_{\text{left}}^{\text{left}} + c_{\ell}^{\text{left}} \kappa_{\phi}^{\text{left}}.
$$

(3.157)

The current $J_{\phi}^{\text{left}}$ determined by the boundary conditions at the semi-reflecting boundary is given by formula 3.146 and

$$
J_{\phi}^{\text{left}} = 4\pi \int_{0}^{V} dv \, v^3 \varphi_{1}^{\text{left}}(v) = 4\pi \int_{0}^{V} dv \, v^3 \sum_{\ell} \alpha_{1,\ell} \mu_{\ell}^{\text{left}}(v)
$$

(3.158)

is the current corresponding to the distribution 3.154. After substitution of $J^e$ given...
by formula 3.157 into equation 3.152 we find

\[ c_{\text{left}} = -\frac{\gamma J_i + J_{\text{left}}}{J_{\phi}^{\text{left}}}. \] 

Right boundary conditions can be constructed similarly:

\[ g_{\ell < 0} = p g_{\ell} - \gamma J_i + J_{\text{right}} \phi_{\text{right}}. \]  

where

\[ \varphi_{\text{right}}(v, \theta) \approx \sum_{\ell} \mu_{\ell}^{\text{right}}(v) \alpha_{\ell}^{N}(\theta) \]  

with \[ \mu_{\ell > 0} \approx 0 \] is the distribution of the secondary electrons on the right spatial boundary and

\[ c_{\text{right}} = -\frac{\gamma J_i + J_{\text{right}}}{J_{\phi}^{\text{right}}}. \] 

Above, \( J_{\phi}^{\text{right}} \) is given by formula 3.147 and

\[ J_{\phi}^{\text{right}} = 4\pi \int_{0}^{V} dv \, v^3 \varphi_{1}^{\text{right}}(v) = 4\pi \int_{0}^{V} dv \, v^3 \sum_{\ell} \alpha_{1,\ell} \mu_{\ell}^{\text{right}}(v). \]  

Note that the values of the constants \( c_{\text{left}} \) and \( c_{\text{right}} \) have to be positive for the flux of the secondary electrons to be directed from the boundary.

To complete the construction we need to determine \( \mu_{\ell}^{\text{left}}(v) \) and \( \mu_{\ell}^{\text{right}}(v) \). Intro-
ducing

\[ \tilde{\alpha}^N_{\ell}(\theta) = \sum_{m=0}^{N} (m + 1/2) \tilde{\alpha}_{m,\ell} P_m(\cos \theta), \]  

(3.165)

and using the orthogonality relation for Legendre polynomials 3.50 combined with the component form of formula D.20: \[ \sum_{n=0}^{N} \tilde{\alpha}_{n,i} \alpha_{n,j} = \delta_{i,j} \] one can prove an orthogonality property for \( \tilde{\alpha}^N_i(\theta) \) and \( \alpha^N_j(\theta) \)

\[ \int_{0}^{\pi} d\theta \cos \theta \, \tilde{\alpha}^N_j(\theta) \alpha^N_i(\theta) = \delta_{j,i}. \]  

(3.166)

Using the above orthogonality relation, the expansion coefficients can be constructed as

\[ \mu_{\ell}^{left}(v) = \begin{cases} 0 & \text{for } \ell \leq 0 \\ \int_{0}^{\pi} d\theta \cos \theta \, \tilde{\alpha}^N_{\ell}(\theta) \varphi^{left}(v, \theta) & \text{for } 0 < \ell \end{cases} \]  

(3.167)

and

\[ \mu_{\ell}^{right}(v) = \begin{cases} 0 & \text{for } \ell \leq 0 \\ \int_{0}^{\pi} d\theta \cos \theta \, \tilde{\alpha}^N_{\ell}(\theta) \varphi^{right}(v, \theta) & \text{for } 0 < \ell \end{cases} \]  

(3.168)

Two important features have to be noted. First, though the secondary electron distribution functions \( \varphi^{left}(v, \theta) \) and \( \varphi^{left}(v, \theta) \) are given approximately by equations 3.154 and 3.161, equation 3.152 is satisfied exactly at the left and right boundaries by construction of \( c^{left} \) and \( c^{right} \) given by formulas 3.159 and 3.163. Second, as before the “waves” leaving the boundary are determined by the “waves” and the ion current arriving at the boundary.

The same is true for the finite-difference equivalents of the boundary conditions
3.156 and 3.160 that can be written as

\begin{align}
g_{\ell>0,j=0,i+1/2} &= p \ g_{\ell,j=0,i+1/2} + c^{left} \ \mu_{\ell,j=0,i+1/2} \\
g_{\ell<0,j=N_z,i+1/2} &= p \ g_{\ell,j=N_z,i+1/2} + c^{right} \ \mu_{\ell,j=N_z,i+1/2}
\end{align}

(3.169) (3.170)

where

\begin{align}
c^{left} &= -\frac{\gamma J_j + J_j=0}{J^{left}_\phi} \\
c^{right} &= -\frac{\gamma J_j + J_j=N_z}{J^{left}_\phi}.
\end{align}

(3.171) (3.172)

Above, \(J_j=0\) and \(J_j=N_z\) are given by formulas 3.150 and 3.151,

\[ J^{left/right}_\phi = \frac{4\pi}{3} \nu \sum_{i=1}^{N_v} (v^2)_{i+1/2} v_{i+1/2} \sum_{\ell} \alpha_{1,\ell} \ \mu^{left/right}_{\ell,j=0,i+1/2} \]

(3.173)

is obtained by use of equations 3.138 and 3.47, and

\[ \mu^{left/right}_{\ell,i+1/2} = \mu^{left/right}_{\ell}(v_i+1/2) \]

(3.174)

where \(\mu^{left/right}\) are given by formulas 3.167 and 3.168.

### 3.3.4 Parallel implementation.

By this point we obtained the set of the evolution operators needed for the construction of the numerical method to solve the \(P_N\) approximation of Boltzmann equa-
tion. The finite-difference equivalent of equation 3.1 can be solved by the operator

\[ \mathcal{B}(\tau) = \prod_{i=1}^{N_v} T_{z}^{\text{adv}}(v_{i-1/2}\tau) \prod_{j=1}^{N_z} \mathcal{B}_{v,j-1/2}(\tau). \]  

(3.175)

where

\[ \mathcal{B}_{v,j+1/2}(\tau) = C_{v,2}^{-1} Q_{v,2}^{\text{lo}}(\tau) Q_{v,j}^{\text{ex}}(\tau) Q_{v,j}^{\text{el}}(\tau) T_{v,2}^{\text{cel}}(\tau) C_{v,2} A_{v}^{c}(a_{z,j+1/2}\tau) \]  

(3.176)

is the operator \( \mathcal{B}_v(\tau) \) defined by formula 3.119 whose acceleration \( a_z = a_{z,j+1/2} \) depends on the spatial index \( j + 1/2 \). The value of acceleration \( a_{z,j+1/2} \) is defined in the middle point \( z_{j+1/2} \) of the mesh interval \([z_j, z_{j+1}]\).

The array of accelerations \( a_{z,1/2}, a_{z,3/2}, \ldots, a_{z,N_z-1/2} \) is input data for the algorithm 3.175. Often, the input array of accelerations \( a_{z,0}, a_{z,1}, \ldots, a_{z,N_z} \) is defined at the edge points \( z_j \) of the mesh interval (see discussion on coupling of the Poisson and Boltzmann equations in the subsection 4.1). In this situation the input array \( a_{z,j} \) has to be interpolated to provide the required input of \( a_{z,j+1/2} \). The author has used simple averaging

\[ a_{z,j+1/2} = (a_{z,j} + a_{z,j+1})/2. \]  

(3.177)

Better stability and suppression of spurious oscillations by the algorithm 3.175 could probably be achieved if the values \( a_\ell a_{z,j+1/2} \) in equations 3.18 are interpolated relative to the signs of \( a_\ell a_{z,j} \) (see discussion on the appropriate transverse velocities in the article [28]).

Equation 3.175 combines action of the two operators \( T_{z}^{\text{adv}}(v_{i-1/2}\tau) \) and \( T_{v}^{\text{adv}}(a_{z,j-1/2}\tau) \),
describing translations in the directions of the $z$ and $v$ axes on the $(z, v)$ plane. The possibility and limitations of a combination of two finite-difference operators describing translations in the perpendicular directions are discussed in the article [28].

Numerical experiments conducted by the author show that operator 3.175 provides time resolution of all the included processes for a time step

$$\tau \leq \tau^b = \min(\tau^b_v, \tau^a_z).$$

(3.178)

Construction of the operator $B(\tau)$ given by formula 3.175 suggests a straightforward parallel implementation. The operator $T^{\text{adv}}_z(v_{i+1/2})$ modifies only $f^s_{i+1/2,j+1/2}$ with fixed $i + 1/2$ that is along the line $v_{i+1/2}$ while the operator $B_s(a_{z,j+1/2}\tau)$ modifies only $f^s_{i+1/2,j+1/2}$ with fixed $i + 1/2$ or along the line $z_{i+1/2}$ as displayed in the left picture in figure 3-16. Calculation of $B(\tau)$ can be implemented in two steps. In the first step, the array of data $f^s_{i+1/2,j+1/2}$, collected initially on one node is split into the data sets in the spatial index $j$ and broadcast to several computational nodes. On each node the data is updated by the corresponding operators $B_{v,j+1/2}$ and broadcast again to be collected on one node. In the second step, the data array is split into the sets in the velocity index $i$ and broadcast to several computational nodes. On each node the data is updated by the corresponding operators $T^{\text{adv}}_z(v_{i-1/2})$ and is broadcast to be collected on one node again. The described process, schematically illustrated by the right chart in figure 3-16, can be repeated for the required number of time steps.
Figure 3-5: Analytical and numerical solutions for $P_7$ at $t=0.1, 0.2, 0.3, 0.4$. 
Figure 3-6: Analytical and numerical solutions for $P_7$ at $t=0.5, 0.6, 0.7, 0.8$. 
Figure 3-7: Analytical and numerical solutions for $P_8$ at $t=0.1, 0.2, 0.3, 0.4$. 

$t=0.1$
$n = 5.58288850990126$

$t=0.2$
$n = 5.58288850990122$

$t=0.3$
$n = 5.58288850990122$

$t=0.4$
$n = 5.58288850990122$
Figure 3-8: Analytical and numerical solutions for $P_8$ at $t=0.5, 0.6, 0.7, 0.8$. 
Figure 3-9: Distribution of scattered electrons in the excitation collisions.

Figure 3-10: Distribution of scattered and produced electrons in the ionization collisions.
Figure 3-11: Cross-sections of elastic, excitation and ionization collision processes for argon.

Figure 3-12: Stationary solution for $E = 1000$ Td and $P_{15}$, ionization as excitation.
Figure 3-13: Stationary solution for $E = 1000$ Td and $P_{15}$, realistic ionization.

Figure 3-14: Stationary solution for $E = 100$ Td and $P_{15}$, realistic ionization.
Figure 3-15: Left semi-reflecting boundary.

Figure 3-16: Parallel implementation of $B(\tau)$. 
Chapter 4

Electrical discharge in Argon.

In this chapter we demonstrate that the developed method can be successfully used to numerically solve the time-dependent electron Boltzmann equation within a framework of a typical self-consistent model of a gaseous discharge. The discharge is modeled in a gap between two plane bare-metal electrodes displayed in figure 4-1. The transverse size of the electrodes is assumed to be much larger than the electrode separation $L$. The two parallel-plate electrode geometry is commonly used in theoretical models and experimental studies of gaseous plasmas [40].

When a potential difference $U$ is applied across the electrodes it creates an electric field $E = U/L$. The free electrons, present in the gas due to the ionization of the gas atoms by natural background radiation and thermal or field electron emission from the electrode surfaces, are accelerated toward the anode. They collide with neutral gas atoms and cause their excitation and ionization. The additional electrons, released through ionization continue the described process, producing an electron avalanche. The spatial growth of the electron density $n^e$ and electron flux $J^e$ in a constant electric
field is approximately described by

$$\frac{\partial n_e}{\partial t} + \frac{\partial J^e}{\partial z} = \alpha J^e,$$  \hspace{1cm} (4.1)

where $\alpha$ is Townsend’s ionization coefficient (see article [44]).

The electrons are much lighter than the gas atoms and lose little energy in elastic collisions with the gas atoms (see formula H.9). Reaching the anode, the electrons are absorbed at the electrode surface. Ions, produced in ionizing collisions with the free electrons, move toward the cathode. Being much heavier than the electrons, the ions obtain much less acceleration from the electric field and effectively exchange the accumulated kinetic energy in the collisions with the surrounding neutral gas atoms. These factors cause the much higher drift electron velocities compared to the ion drift velocities in an electric field of the same magnitude. Under conditions of a typical
low temperature plasma discharge, the ions move toward the cathode not producing ionization. Hitting the cathode surface, the ions are absorbed, producing secondary electrons that join the discharge process. The electron flux at the electrode surface is characterized by formula 3.152: $J^e = -\gamma J^i$, where $\gamma$ is the effective secondary emission coefficient and $J^i$ is the ion flux.

Development of the discharge can be divided into three stages (see article [50] and dissertation [48]):

*Linear stage.* For high enough values of the applied voltage $U$, creation of the secondary electrons at the cathode not only sustains the electron flux but allows for its temporal growth. Because the electrons move through the gap much faster than the ions, their concentration in the gap is negligible compared to the ion concentration at the initial stage of the discharge. The number of ions grows approximately exponentially with time. The positive charge, growing in the gap, screens the electric field. The electric field decreases at the anode and increases at the cathode.

*Breakdown stage.* Weak electric fields provide for slow electron drift velocities at the anode. At some moment the electric field is screened to the extent that the electron density starts growing, neutralizing the positive charge at the cathode. The electric field vanishes at the anode and from that moment on there coexist two regions in the gap: One, the *plasma trail region*, filled with neutral plasma where the electric field is comparatively low, begins at the anode. The other, the *cathode fall region*, where the electric field is strong and the electron density is negligible, is adjacent to the cathode. With time, the cathode fall region contracts while the discharge current continues to grow rapidly.
**DC cathode fall stage.** The shrinking of the cathode fall region and the growth of the discharge current slows down and eventually stops completely. At this moment the production the electrons in the gap gets neutralized by the process of electron-ions recombination and the discharge becomes stationary.

In the parallel-plate electrode geometry, the electron distribution function is expected to be azimuthally symmetric so that the electron kinetics can be modeled by the $P_N$ approximation of the Boltzmann equation (see the discussion in appendix A). Used in numerous theoretical and computational models, the two parallel-plate electrode geometry is also a common experimental setup to study the physical characteristics of gaseous plasma [40]. We start with a description of the model parameters and continue with a brief discussion of the physical results.

### 4.1 Model and parameters.

The discharge in argon gas is modeled at 500 Torr pressure for a parallel-plate two-electrode geometry with an electrode separation of $L = 25 \, \mu m$ and a range of applied voltages $U = 100 - 1000 \, V$.

The argon ions and neutrals are described by the continuity equations and fluid approximation for the corresponding fluxes (as in works [35], [44] and [46]):

\[
\frac{\partial n^s}{\partial t} + \frac{\partial J^s}{\partial z} = S^s, \tag{4.2}
\]

\[
J^s = K^s En^s - D^s \frac{\partial n^s}{\partial z}, \tag{4.3}
\]
where the index \( s = i, x \) for the argon ions and the excited species respectively. The spatial excitation and ionization sources are found using the corresponding out-scattering collision terms integrated over \( d^3v = 4\pi v^2 d\theta \sin \theta \):

\[
S^x(z, t) = \int_0^V d^3v \, S^{\text{out,ex}}(t, z, v) = 4\pi \int_0^V dv \, v^2 S^{\text{out,ex}}_0(t, z, v) \tag{4.4}
\]

and

\[
S^i(z, t) = \int_0^V d^3v \, S^{\text{out,io}}(t, z, v) = 4\pi \int_0^V dv \, v^2 S^{\text{out,io}}_0(t, z, v), \tag{4.5}
\]

where \( S^{\text{out,ex}}_0 \) and \( S^{\text{out,io}}_0 \) are obtained from formulas H.25 and H.50. The dependence of the ion mobility \( K^i \) and diffusion \( D^i \) on the electric field have been found from data tables [12]. The boundary fluxes used in the boundary conditions for equations 4.2 assume zero density of the species on the electrode surface. For the excited argon species \( K^x = 0 \) and their diffusion coefficient is assumed to be the same as the coefficient of self-diffusion of neutral argon atoms (calculated using the method of book [16] p.580). The equation for the chemical kinetics of argon ion and excited species is neglected since their characteristic times are much longer than the time length considered by the model (< 200 ns).

The electron kinetics is described by the \( P_N \) approximation of the Boltzmann equation

\[
\frac{\partial f_n}{\partial t} + \left\{ v \frac{\partial f_{n+1}}{\partial z} + a_z \left( \frac{\partial f_{n+1}}{\partial v} + f_{n+1} \frac{(n + 2)}{v} \right) \right\} \frac{n + 1}{2n + 3} + \left\{ v \frac{\partial f_{n-1}}{\partial z} + a_z \left( \frac{\partial f_{n-1}}{\partial v} - f_{n-1} \frac{(n - 1)}{v} \right) \right\} \frac{n}{2n - 1} = S_n, \tag{4.6}
\]
where
\[ a_z = \frac{eE_z}{m_e} \] (4.7)
is the electron acceleration along the z axis. The equation uses the \( P_N \) approximation of the collision integrals discussed in appendix H and the set of electron-argon collision cross sections used in subsection 3.2.4. Attachment processes and electron-electron collisions are not included. Because of the omission of the attachment process the stationary stage of the discharge cannot be reached within this model. The above equation is solved with the spatial boundary conditions 3.156 and 3.160 discussed in subsection 3.3.3. The value of the effective secondary emission coefficient is taken to be \( \gamma = 0.05 \). The distribution of the secondary electrons produced through secondary emission at the electrode surfaces (see formula 3.153) is assumed to be Maxwellian (see formula 1.3) corresponding to a mean electron energy of 2 eV.

The strength of the electric field is found from the solution of the Poisson equation
\[ \frac{\partial E}{\partial z} = \frac{q}{\epsilon_0}, \] (4.8)
where the charge density
\[ q = e(n_i - n_e) \] (4.9)
is determined by the ion and electron densities. The electron density is found from the electron distribution function as
\[ n_e = 4\pi \int_0^V dv v^2 f_0 \] (see expressions 3.70 and 3.76). The electron drift velocity and mean energy, displayed in the figures below, are obtained using formulas 3.121, 3.122 and formula 3.123 respectively.
The numerical model uses the same number of discretization points \( N_v = 40 \) and \( N_z = 40 \) for the absolute value of the electron velocity \( v \) and the spatial coordinate \( z \). The maximum absolute value of the electron velocity \( V = 8.388 \times 10^8 \) cm/s corresponds to an electron energy of 200 eV. The maximum value of the spatial coordinate is equal to the gap length \( L = 0.025 \) µm. A short length of the gap has been chosen to allow about 10 spatial points for resolution of the cathode fall region.

The drift-diffusion equations 4.2 and 4.3 are solved using a high-order extension of the method considered in article [38]. The \( P_N \) approximation of the electron Boltzmann equation 4.6 is solved by the method described in chapter 3, where the values of the characteristic variables \( g_{i,j,d}^s \) at the edges of the mesh boundaries (see subsections 3.1.1 and 3.3.1) are determined by a high-order flux-limited polynomial interpolation discussed in article [26] and report [25]. To minimize numerical diffusion, the numerical methods for solution of the drift-diffusion equations 4.2 and calculation of the values of the characteristic variables at the edges of the mesh boundaries in the \( P_N \) approximation of electron Boltzmann equation 4.6 use a 7-th order polynomial interpolation as recommended in article [28] for two dimensional advection problems. The expansion of the distribution function into the Legendre polynomials 1.4 is truncated to contain 16 expansion coefficients \( f_0 - f_{15} \) (\( P_{15} \) approximation of the electron distribution function). The electric field \( E_{z,j} \) at the edges of the spatial mesh intervals is found from the numerical solution of the Poisson equation 4.8, using the numerical method described in the dissertation [48]. The accelerations at the edges of the spatial mesh intervals \( a_{z,j} = \frac{e}{m_e} E_{z,j} \) are interpolated to obtain the accelerations at the middle points of the intervals by use of formula 3.177.
At the start of the simulation, the electron distribution function is assumed to be zero everywhere except in one spatial mesh closest to the cathode (24.375 µm < z < 25 µm) where the electron density is set to $10^{11}/\text{cm}^3$ with the velocity distribution corresponding to 4 eV.

### 4.2 The results

Following is a short discussion of the results obtained in the simulation.

For any number of polynomials in the expansion of the distribution function, the electron density $n^e$ given by formula 3.139 become and stay positive at all of the spatial points shortly after the beginning of the simulation. The total number of particles is conserved within at least 12 digits accuracy throughout the simulation.

The values of the ionization coefficient $\alpha/p$ found in the computational experiment, displayed by the circles, are compared in figure 4-2 with the experimental values from article [22], displayed by the continuous curve. The computed values of the ionization coefficient were determined from the regions of exponential spatial growth of the electron current at positive values of the electric field by a least-squares fit. The secondary emission electron current at the surface of the right electrode was kept constant in time and low enough to maintain constancy of the electric field in the gap within 1% accuracy. Under the described conditions, the spatial growth of the electron current is given by the stationary variant of equation 4.1: $\frac{\partial J^e}{\partial z} = \alpha J^e$ (see book [45], p.53).

From a number of performed simulations, we consider the one carried out for an
applied voltage of \( U = 200 \) V. The dependence of the discharge current on time found in this simulation is given in figure 4-3. The three stages of the discharge are clearly noticeable. The linear stage lasts approximately for 120 ns. The breakdown stage lasts about 20 ns, and then follows the DC cathode fall stage. A large value of the electric current density \( \sim 300 \) mA/cm\(^2\), reached at the 200 ns point in the simulation of the DC cathode fall stage, is expected for a comparatively high applied voltage and a short gap space.

The electric field, species density, electron drift velocity and mean electron energy at \( t = 60 \) ns is displayed in figure 4-4. The exponential growth of the electron density in the direction from the cathode to the anode is determined by the electron avalanches. The electric field of about \( E = 730 \) Td is weakly distorted by the positive charge accumulated in the gap. The distribution functions at the same time and at selected spatial points are displayed in figures 4-5 and 4-6. The order of the pictures
Figure 4-3: Dependence of the discharge current on time.

of the distribution functions in the figures follows the order of the points selected by the circles in figure 4-4. The maximum absolute velocity $V = 8.388 \times 10^8$ cm/s, marked on the horizontal axis, corresponds to the electron energy of 200 eV. The distribution functions are normalized to the spatial electron densities. The mark on the vertical axis gives the maximum value reached by the distribution function. The blue and brown curves on the surfaces, representing the electron distribution functions, mark velocities of $2.02 \times 10^8$ cm/s and $2.35 \times 10^8$ cm/s corresponding to the 11.6 eV excitation and 15.7 eV ionization thresholds of the argon atom respectively. The first picture in figure 4-5 shows the distribution function at the left electrode and the last picture in figure 4-6 shows the one at the right electrode. Note the absence of electrons going in the direction away from the surface of the left electrode (the anode). The shape of the distribution function at the right electrode (the cathode) is mainly determined by secondary emission electrons leaving its surface. The roundly
shaped base of the distribution function at the spatial point closest to the cathode indicates the presence of back-scattered electrons. The influence of the boundaries disappears at distances of approximately 2 \( \mu \text{m} \) from the anode and 3 \( \mu \text{m} \) from the cathode. Farther from the electrodes the shape of the distribution function remains the same.

Expulsion of the electric field by the neutral plasma during the breakdown stage is shown in figure 4-7. Electron and ion densities and the strength of the electric field are presented at \( t = 117, 125, 130, 140 \) ns. We consider the initiation of the breakdown at \( t = 117 \) ns in more detail. The electric field, species density, electron drift velocity and mean electron energy at \( t = 117 \) ns are displayed in figure 4-8. The electron distribution functions at the same time are given in figures 4-9 and 4-10. The influence of the boundaries vanishes at the same distances from the electrodes as in the previous example. Gradual cooling of the electrons by inelastic collisions follows the decrease in the electric field. Close to the anode the electrons are rapidly cooled by the excitation collisions.

Finally, we consider an example from the DC cathode stage. The electric field, species density, electron drift velocity and mean electron energy at \( t = 200 \) ns are given in figure 4-11. The gap space is clearly divided between the cathode fall region and the plasma trail region. The cathode fall region spans a distance of \( \sim 5 \mu \text{m} \) from the cathode. The electron distribution functions at the same time are given in figures 4-12 and 4-13. Within the distance of \( \sim 1 \mu \text{m} \) from the cathode, the electrons gain energy and their velocities are mostly directed toward the anode. In the next \( \sim 3 \mu \text{m} \) the average electron energy decreases, while their distribution function becomes more
isotropic. Mixing of the hot electrons coming from the cathode fall region with the cold electrons diffusing from the plasma trail region that occurs at a distance of $\sim 4 \ \mu m$ from the cathode is shown in the first picture in figure 4-13. In the plasma trail region, the electrons are comparatively cold and the shapes of the distribution functions are almost spherically symmetric due to the low value of the electric field.
Figure 4-4: Electric field, densities of electrons and ions, electron drift velocity and mean electron energy at 60 ns.
Figure 4-5: Electron distribution function at 60 ns.
Figure 4-6: Electron distribution function at 60 ns (continued).
Figure 4-7: Electric field and species densities during the breakdown.
Figure 4-8: Electric field, densities of electrons and ions, electron drift velocity and mean electron energy at 117 ns.
Figure 4-9: Electron distribution function at 117 ns.
Figure 4-10: Electron distribution function at 117 ns (continued).
Figure 4-11: Electric field, densities of electrons and ions, electron drift velocity and mean electron energy at 200 ns.
Figure 4-12: Electron distribution function at 200 ns.
Figure 4-13: Electron distribution function at 200 ns (continued).
Chapter 5

Conclusions.

Throughout the present dissertation the main effort has been to develop a method for numerical solution of the system of partial differential equations for the coefficients in the N-term expansion of the solution of the Boltzmann equation in Legendre polynomials, also known as the $P_N$ approximation of the Boltzmann equation. About two years ago, when the author became interested in this problem there was no satisfactory method for the general case of an arbitrary number of expansion coefficients.

The key to construction of the present method has been development of a numerical algorithm for the accurate solution of the $P_N$ approximation of the Boltzmann equation without collisions and space dependence, that is, the $P_N$ approximation of the advection equation. After a thorough consideration of the advection equation in the velocity space both analytically and numerically, addition of collisions and space dependence became an easy task.

The method has been successfully used to describe the electron kinetics in a model electrical discharge in argon in a two plain-electrode geometry. The model includes
the $P_N$ approximation of the electron Boltzmann equation, drift-diffusion equations for ions and neutrals and the Poisson equation.

Following is the summary of the obtained results:

1. In appendices A and B, I considered the necessary conditions for applicability of the $P_N$ approximation of the Boltzmann equation.

2. In Chapter 2, I analytically developed the general solution of the $P_N$ approximation of the advection equation on the half-line $v \geq 0$. The system of eigenfunctions constructed in this chapter can also be used for solution of the same equation on the interval $0 \leq v \leq V$ and for various problems involving the space-independent Boltzmann equation. The $P_N$ approximation of the advection equation is nonselfadjoint, as is the Boltzmann equation. Matching the initial conditions with the general solution requires knowledge of the associated eigenfunctions. The set of associated eigenfunctions is constructed in appendix E. The end of chapter 2 reveals the wave nature of the general solution, which intrinsically contains multiple waves moving in opposite directions.

3. Chapter 3 is directed toward the development of a new numerical method for solution of the $P_N$ approximation of the Boltzmann equation using operator splitting. The development starts with numerical solution of the $P_N$ approximation of the advection equation on the interval $0 \leq v \leq V$ through introduction of characteristic variables. Employing the wave nature of the general solution of the $P_N$ approximation of the advection equation I constructed the boundary conditions at $v = 0$ and $v = V$ that lead to a smooth behavior of the distribution function at the origin of the velocity space. I found an intuitive interpretation of the characteristic variables, representing
the waves of given velocity in the numerical solution that facilitate construction of spatial boundary conditions. Later on I considered addition of collisions and spatial dependence to the developed method for numerical solution of the \( P_N \) approximation of the advection equation. Notable features of the new method are numerically exact particle conservation and the possibility of an efficient parallel implementation. I have verified the accuracy of the numerical solution for the obtained method in the stationary case by comparing it with the Monte-Carlo solution.

4. In Chapter 4, I demonstrated that the numerical routine employing the obtained method can be successfully coupled with a solver for the Poisson equation as in self-consistent modeling of plasma discharges.

Lastly, I would like to discuss issues related to this dissertation.

1. The extension of the developed method to the general case of spherical harmonics seems to be straightforward. The characteristic variables in the general case will represent beams in the velocity space. In the case of operator splitting, the numerical implementation will include operators representing translations along the beams, two rotation operators corresponding to the polar and azimuthal angles, and collision operators.

2. The set of eigenfunctions developed for the general solution of the \( P_N \) approximation of the advection equation can be immediately used in analytical solution of the space-independent Boltzmann equation containing an elastic collision term when the collision cross sections are proportional to \( 1/v \).

3. Chapter 2 shows that the requirement of boundedness for the general solution of the \( P_N \) approximation of the advection equation immediately induces a smooth
behavior of the solution at the origin $v = 0$. In this sense, the analytic solution does not need any boundary conditions at $v = 0$. It is the author’s belief that the only function of the boundary conditions at $v = 0$ in the developed numerical method is the provision for an uninterrupted flow of numerical errors through the point $v = 0$.

4. The Behavior of the solution of the time-dependent Boltzmann equation and its $P_N$ approximation at $v = 0$ in the case that the source behaves as $1/v^2$, as in the model of the ionization collisions introduced in appendix H.3, are of continued interest. The numerical solution obtained with a Monte Carlo technique in chapter 3 seems to suggest the existence of a singularity in $f_0$ at $v = 0$, while the rest of the expansion coefficients seem to be bound. It seems likely though that singularities do exist in all the expansion coefficients, but were not resolved numerically by the technique used here.

5. The author’s current opinion is that the expediency of using many terms in the numerical solution of the space-dependent $P_N$ approximation of the Boltzmann equation generally depends on the desired angular resolution of the distribution function in velocity space.
Appendix A

Geometry that allows $P_N$ approximation

We discuss conditions for the solution of the Boltzmann equation to be independent of the angle $\phi$ in the velocity space (azimuthally symmetric around the $v_z$-axis) so that the $P_N$ approximation of the distribution function can be used. Consider the Boltzmann equation for the distribution function $f(t, r, v)$:

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + a \frac{\partial f}{\partial v} = S,$$  \hspace{1cm} (A.1)

$$S(t, r, v) = \int \gamma(r, v; v') f(t, r, v'),$$  \hspace{1cm} (A.2)

where $\gamma(r, v; v')$ is the scattering kernel, $v_x = v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} + v_z \frac{\partial f}{\partial z}$ and $a = a_x \frac{\partial f}{\partial v_x} + a_y \frac{\partial f}{\partial v_y} + a_z \frac{\partial f}{\partial v_z}$. The required conditions can be determined by identifying and eliminating the terms that introduce dependence on $\phi$ into the equation A.1.

Spherical coordinates in the velocity space (see figure A-1) are given by formulas:
Figure A-1: Spherical coordinates in the velocity space.

\[ v_x = v \sin \theta \cos \phi \]  
(A.3)

\[ v_y = v \sin \theta \sin \phi \]  
(A.4)

\[ v_z = v \cos \theta \]  
(A.5)

\[ \frac{\partial f}{\partial v_x} = \sin \theta \cos \phi \frac{\partial f}{\partial v} + \frac{\cos \theta \cos \phi}{v} \frac{\partial f}{\partial \theta} - \frac{\sin \phi}{v \sin \theta} \frac{\partial f}{\partial \phi} \]  
(A.6)

\[ \frac{\partial f}{\partial v_y} = \sin \theta \sin \phi \frac{\partial f}{\partial v} + \frac{\cos \theta \sin \phi}{v} \frac{\partial f}{\partial \theta} + \frac{\cos \phi}{v \sin \theta} \frac{\partial f}{\partial \phi} \]  
(A.7)

\[ \frac{\partial f}{\partial v_z} = \cos \theta \frac{\partial f}{\partial v} - \frac{\sin \theta}{v} \frac{\partial f}{\partial \theta}. \]  
(A.8)

Above, \( \phi \) is the azimuthal angle and \( \theta \) is the polar angle.

We can immediately see that the components of acceleration in \( x \) and \( y \) directions are associated with the terms dependent on \( \phi \) so that \( x \) and \( y \) components of acceleration has to be forbidden:

\[ a_x = a_y = 0. \]  
(A.9)
Transforming equations A.1 and A.2 to spherical coordinates in the velocity space yields:

$$\frac{\partial f}{\partial t} + v \sin(\theta) \cos \phi \frac{\partial f}{\partial x} + v \sin \theta \cos \phi \frac{\partial f}{\partial y} + v \cos \theta \frac{\partial f}{\partial z} + a_z(x, y, z) \left( \cos \theta \frac{\partial f}{\partial v} - \frac{\sin \theta \partial f}{v \theta} \right) = S(t, x, y, z, v, \theta, \phi). \quad (A.10)$$

Now we see that the dependence on $\phi$ may still enter the equation through the variation of the distribution in $x$ and $y$ coordinates, introduced by the terms associated with $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$. Hence, we need further restrictions to eliminate this dependence.

We have to forbid the dependence of $a_z$ on $x$ and $y$ and also forbid the dependence of $S$ on $x$, $y$ and $\phi$

$$a_z(x, y, z) = a_z(z) \quad (A.11)$$

$$S(t, x, y, z, v, \theta, \phi) = S(t, z, v, \theta). \quad (A.12)$$

The last formula implies that the scattering kernel $\gamma$ has to be independent of $x,y,\phi$ so than $S$ does not depend on $x,y,\phi$ as well

$$S(t, z, v, \theta) = \int d^3\mathbf{v}' \gamma(z, v, \theta; v', \theta', \phi') f(t, z, v', \theta', \phi'). \quad (A.13)$$
Subject to the introduced restrictions, equation A.10 becomes

$$
\frac{\partial f}{\partial t} + v \sin(\theta) \cos \phi \frac{\partial f}{\partial x} + v \sin \theta \cos \phi \frac{\partial f}{\partial y} + v \cos \theta \frac{\partial f}{\partial z} + a_z(z) \left( \cos \theta \frac{\partial f}{\partial v} - \frac{\sin \theta \partial f}{\partial \theta} \right) = S(t, z, v, \theta). \quad (A.14)
$$

The terms \(v \sin(\theta) \cos \phi \frac{\partial f}{\partial x}\) and \(v \sin \theta \cos \phi \frac{\partial f}{\partial y}\) are still present in the above equation, and there is no way to get rid of them, but it is possible to force them to stay zero. To do that we need to eliminate possibility for \(\phi\) dependence to enter the problem through its boundary conditions at the ends of the spatial interval. We assume that kernels \(\alpha_i\) and values of the boundary sources \(\omega_i\) in the boundary conditions do not depend on \(x, y, \phi\) so that the boundary conditions in \(z\) can be satisfied by a distribution function \(f\) that does not depend on \(x, y, \phi\)

$$
\int v d^3 v' \alpha_i(v, \theta; v', \theta', \phi') f(t, z_i, v', \theta') = \omega_i(t, v, \theta). \quad (A.15)
$$

In the boundary conditions A.15, \(i\) can be equal to \(l\) or \(r\), for left or right boundary, kernel \(\alpha_i\) accounts for reflection from the surface, and \(\omega_i\) is a surface source.

The following statement can now be formulated. If restrictions A.9, A.11, A.13 are satisfied, it is possible to find a solution of equation

$$
\frac{\partial \psi}{\partial t} + v \cos \theta \frac{\partial \psi}{\partial z} + a_z(z) \left( \cos \theta \frac{\partial \psi}{\partial v} - \frac{\sin \theta \partial \psi}{\partial \theta} \right) = S(t, z, v, \theta) \quad (A.16)
$$

satisfying boundary conditions A.15 and initial conditions that do not depend on \(x\),
then the found solution will satisfy equation A.1, subject to the same restrictions, boundary and initial conditions. This statement can be easily validated through the following consideration. Suppose, \( \psi(t, z, v, \theta) \), a solution of the equation A.16 is found. Setting \( f(t, x, y, z, v, \theta, \phi) = \psi(t, z, v, \theta) \) and substituting \( f \) into the equation A.10 will satisfy equation A.10 subject to restrictions A.11, A.13. The solution \( f \), transformed to cartesian coordinates with formulas A.3-A.5 will also satisfy equation A.1 because of the restriction A.9.

Proving the above statement validates the following practical recipe. Whenever equation A.1 has to be solved under conditions A.9, A.11, A.13, A.15 and A.17, solve A.16 instead. A simple idea lies behind the statement and the recipe. If at some initial time the solution does not depend on \( x, y, \phi \), and acceleration, the boundary conditions as well as the scattering term \( S \) do not introduce this dependence at later times, then the solution will stay independent of \( x, y, \phi \).

The statement however does not provide any means to find out whether solutions different from the one found with the recipe are possible for equation A.1. To be sure, one would need a uniqueness theorem for equation A.1.

Somewhat interesting is the fact that the dependence of the initial conditions for \( f \) on \( x \) or \( y \) breaks the symmetry in \( \phi \) at later times. Let’s consider an example where it happens. Suppose at the origin of the coordinate space, \( x=y=z=0 \) and at \( t = 0 \) there are \( N \) particles with their velocities distributed uniformly over the surface of a sphere.
in velocity space with a radius equal to \( v_0 \). There is no acceleration, and there are no collisions. This physical system can be described by equation A.1 where \( \mathbf{a} \) and \( S \) are set to zero. The solution, \( f = \frac{N}{4\pi v^3_0} \delta(v_x t - x) \delta(v_y t - y) \delta(v_z t - z) \delta(v^2_x + v^2_y + v^2_z - v^2_0) \), can be interpreted in the following way. At any time, the distribution function is different from zero only for \( \mathbf{v} = (v_x, v_y, v_z) \), satisfying \( v^2_x + v^2_y + v^2_z = v^2_0 \) and for \( \mathbf{r} = (v_x t, v_y t, v_z t) \). The distribution function will not be independent of \( \phi \) except at \( t = 0 \). To see the contrary, one may consider another situation, when at \( t = 0 \), particles with the same initial velocity distribution as in the previous example are uniformly spread over the surface of the plane \( z = 0 \) with their surface density being equal to \( N \). The solution, \( f = \frac{N}{4\pi v^3_0} \delta(v_z t - z) \delta(v^2_x + v^2_y + v^2_z - v^2_0) \), remains independent of \( \phi \) for any \( t \). Here uniformity in \( x \) and \( y \) eliminate dependence on \( \phi \).
Appendix B

Uniqueness of the solution of the Boltzmann equation

Considering the question of uniqueness of the solution of equation A.1 for a given initial and boundary value problem, we will give a proof for the case of a linear collision integral and an arbitrary spatial geometry following the framework established in [8] p.172. We assume that initial conditions are given and boundary conditions of the form A.15 are to be satisfied at the stationary boundary surface. Let’s suppose that the problem has two possible solutions \( h_1 \) and \( h_2 \) and let \( h = h_1 - h_2 \) be their difference. Since both \( h_1 \) and \( h_2 \) take the same initial values, \( h = 0 \) at the initial time \( t_0 \), the solution difference \( h \) will satisfy equation A.1, where \( v \) and \( a \) can be brought inside the derivatives

\[
\frac{\partial h}{\partial t} + \frac{\partial (vh)}{\partial x} + \frac{\partial (ah)}{\partial v} = S. \quad (B.1)
\]
The collision integral,

\[ S = \int_{D_r} d^3v' \gamma(r, v, v') h(t, r, v'), \quad (B.2) \]

we consider, is linear in \( h \): \( S(\alpha h) = \alpha S(h) \). Here, \( \gamma(r, v, v') \) is the scattering kernel.

It is possible for the velocity coordinate \( v \) because it is an independent coordinate in the phase space. Acceleration \( \mathbf{a} \) caused by the electromagnetic field can be brought inside the derivatives because in this case \( a_x = \frac{q}{m_e} (E_x(x, y, z) + v_y B_z(x, y, z) - v_z B_y(x, y, z)) \) does not depend on \( v_x \) (see reference [45], p.79). Multiplying equation B.1 by \( h \), integrating over domains of definition of \( r : D_r \) and domain of definition of \( v : D_v \), and introducing the norm of \( h \) as

\[ \| h \|^2 = \int_{D_r} d^3r \int_{D_v} d^3v h^2(t, r, v), \quad (B.3) \]

we obtain an equation for the square of the norm:

\[
\frac{1}{2} \frac{\partial \| h \|^2}{\partial t} + \int_{D_r} d^3r \int_{D_v} d^3v \frac{\partial (a_x^2)}{\partial v_x} + \int_{D_v} d^3v \int_{D_r} d^3r \frac{\partial (v_x^2)}{\partial r_x} = \\
\int_{D_r} d^3r \int_{D_v, D_v'} d^3v d^3v' h(t, r, v) \gamma(r, v, v') h(t, r, v'). \quad (B.4)
\]

The first and the second integrals on the right hand side can be transformed into
surface integrals by the divergence theorem

\[
\int_{D_r} d^3r \int_{D_v} d^3v \frac{\partial (a_\varepsilon^2)}{\partial \varepsilon} = \int_{D_r} d^3r \int_{D_{sv}} d^2s_v \cdot a_\varepsilon \frac{h^2}{2}, \quad (B.5)
\]

\[
\int_{D_v} d^3v \int_{D_r} d^3r \frac{\partial (v_\varepsilon^2)}{\partial \varepsilon} = \int_{D_v} d^3v \int_{D_{sr}} d^2s_r \cdot v_\varepsilon \frac{h^2}{2}, \quad (B.6)
\]

where integration in the surface integrals goes over the boundary regions: \(D_{sr}\) and \(D_{sv}\) of the domains of definition \(D_r\) and \(D_v\).

For later we assume that extension of the integration region in the velocity space to infinity leads to

\[
\int_{D_{sv}} d^2s_v \cdot a_\varepsilon \frac{h^2}{2} \to 0 \quad (B.7)
\]

when the points on the surface \(s_v\) tend to infinity.

The boundary conditions for \(h\) are the same as for \(f\) (equation A.15) except that the surface source terms \(\omega_i\) cancel out and \(i\) denotes the position of the point on the boundary

\[
\int_{D_v} d^3v' \alpha_i(r, v', v) f(t, r, v') = 0. \quad (B.8)
\]

Suppose the reflection kernels \(\alpha_i\) are such that

\[
\int_{D_v} d^3v \, n_i \cdot v_\varepsilon \frac{h^2}{2} \geq 0 \quad (B.9)
\]

for any point \(i\) on the space boundary with \(n_i\) pointing to the outside of the space region.

To estimate the integral on the right hand side of equation B.1, let’s decompose
the scattering kernel $\gamma$ into its symmetric and antisymmetric parts

$$\gamma = \gamma_s + \gamma_a$$

(B.10)

$$\gamma_s(r, v, v') = \frac{1}{2}(\gamma(r, v, v') + \gamma(r, v', v))$$

(B.11)

$$\gamma_a(r, v, v') = \frac{1}{2}(\gamma(r, v, v') - \gamma(r, v', v)),$$

(B.12)

and suppose that for the symmetric part

$$\int_{all v'} d^3v' \gamma_s(r, v, v') \leq c. \quad \text{(B.13)}$$

The integration over $v$ and $v'$ for the antisymmetric part yields zero for any $h$. Using the Schwartz inequality

$$\int d^n x f(x) g(x) \leq \left[ \int d^n x f^2(x) \right]^{\frac{1}{2}} \left[ \int d^n x g^2(x) \right]^{\frac{1}{2}}, \quad \text{(B.14)}$$
the symmetric part can be estimated

\[
\int d^3r \int d^3v d^3v' h(t, r, v) \gamma_s(r, v, v') h(t, r, v') =
\]

\[
\int d^3r \int d^3v d^3v' h(t, r, v) \gamma_s^{1/2}(r, v, v') h(t, r, v') \gamma_s^{1/2}(r, v, v') \leq
\]

\[
\int d^3r \left[ \int d^3v d^3v' h^2(t, r, v) \gamma_s(r, v, v') \int d^3v d^3v' h^2(t, r, v') \gamma_s(r, v, v') \right]^{1/2} =
\]

\[
\int d^3r \int d^3v h^2(t, r, v) \int d^3v' \gamma_s(r, v, v') \leq c \int d^3r \int d^3v h^2(t, r, v) = c \|h\|^2.
\]

(B.15)

Combining equations B.4, B.7, B.9, B.15, we obtain

\[
\frac{1}{2} \frac{d\|h\|^2}{dt} \leq c \|h\|^2,
\]

(B.16)

so that

\[
\frac{d}{dt} (\|h\|e^{-ct}) \leq 0.
\]

(B.17)

From equation B.17 it follows that a non-negative \(\|h\|e^{-ct}\) cannot increase with time starting from its zero value at \(t_0\). The conclusion is that \(\|h\| = 0\) for \(t_0 < t\), or that \(h_1 = h_2\) (almost everywhere).
Appendix C

Derivation of $P_N$ approximation for the Boltzmann equation

Using the substitution $\zeta = \cos \theta = \frac{v_z}{v}$, equation A.16 can be rewritten as

$$
\frac{\partial f}{\partial t} + \frac{\partial f}{\partial z} v\zeta + a_z \left( \frac{\partial f}{\partial v} \zeta + \frac{\partial f}{\partial \zeta} \frac{1 - \zeta^2}{v} \right) = S. \quad (C.1)
$$

Formally expanding $f$ and $S$ into spherical harmonic series (the possibility of expansion implies that $f$ and $S$ are smooth enough functions of $\theta$, for the discussion of required smoothness see reference [3] p.893)

$$
f(t, z, v, \theta) = \sum_{n=0}^{\infty} f_n(t, z, v) P_n(\zeta), \quad (C.2)
$$

$$
S(t, z, v, \theta) = \sum_{n=0}^{\infty} S_n(t, z, v) P_n(\zeta), \quad (C.3)
$$
and further using $P_n$ for $P_n(\zeta)$, yields

$$\sum_{n=0}^{\infty} \left\{ \frac{\partial f_n}{\partial t} P_n + \left( v \frac{\partial f_n}{\partial z} + a_z \frac{\partial f_n}{\partial v} \right) \zeta P_n + a_z f_n \frac{\partial P_n}{\partial \zeta} \frac{1 - \zeta^2}{v} - S_n P_n \right\} = 0. \quad (C.4)$$

Utilizing the recurrence relations for Legendre polynomials [3] p.748-750, terms with $\zeta P_n(\zeta)$ and $(\zeta^2 - 1) \frac{dP_n(\zeta)}{d\zeta}$ can be re-expressed as linear combinations of Legendre polynomials of order $n - 1$ and $n + 1$

$$\zeta P_n = \frac{n}{2n+1} P_{n-1} + \frac{n+1}{2n+1} P_{n+1}, \quad (C.5)$$

$$(\zeta^2 - 1) \frac{dP_n}{d\zeta} = \frac{n(n+1)}{2n+1} (-P_{n-1} + P_{n+1}). \quad (C.6)$$

Substituting relations C.5 and C.6 into C.4 and collecting terms involving Legendre polynomials of the same order, we obtain

$$\sum_{n=0}^{\infty} \left\{ v \frac{\partial f_n}{\partial z} + a_z \left( \frac{\partial f_n}{\partial v} + \frac{f_n}{v} (n + 1) \right) \right\} \frac{n}{2n+1} P_{n-1} + \sum_{n=0}^{\infty} \left\{ \frac{\partial f_n}{\partial t} - S_n \right\} P_n$$

$$+ \sum_{n=0}^{\infty} \left\{ v \frac{\partial f_n}{\partial z} + a_z \left( \frac{\partial f_n}{\partial v} - \frac{f_n}{v} n \right) \right\} \frac{n+1}{2n+1} P_{n+1} = 0. \quad (C.7)$$

Noticing that the term corresponding to $n = 0$ in the first sum and the term corresponding to $n = -1$ in the last sum are equal to zero, we can change the indexation in the first and the last sums such that $n \to n + 1$ and $n \to n - 1$ respectively. Collecting
of all the terms involving Legendre polynomials of the same order, we obtain

\[
\sum_{n=0}^{\infty} \left\{ \frac{\partial f_n}{\partial t} + \left\{ v \frac{\partial f_{n+1}}{\partial z} + a_z \left( \frac{\partial f_{n+1}}{\partial v} + \frac{f_{n+1}}{v} (n + 2) \right) \right\} \frac{n + 1}{2n + 3} \\
+ \left\{ v \frac{\partial f_{n-1}}{\partial z} + a_z \left( \frac{\partial f_{n-1}}{\partial v} - \frac{f_{n-1}}{v} (n - 1) \right) \right\} \frac{n}{2n - 1} - S_n \right\} P_n = 0. \tag{C.8}
\]

Closure for a particular approximation order \( N \) is achieved by dropping all of the terms containing Legendre polynomials of the order higher that \( N + 1 \), which is equivalent to setting

\[ f_n = 0 \quad \text{for} \quad N < n. \tag{C.9} \]
Appendix D

Properties of matrix $A$

Let’s look for the solution of the eigenvalue problem

$$A\alpha(a) = a\alpha(a),$$  \hspace{1cm} (D.1)

where matrix $A$ is defined by formula 2.5. Rewriting the previous equation for the components of $\alpha(a)$ yields

$$\frac{n}{2n-1} \alpha_{n-1}(a) - a \alpha_n(a) + \frac{n+1}{2n+3} \alpha_{n+1}(a) = 0.$$  \hspace{1cm} (D.2)

Substituting

$$\alpha_n(a) = (2n+1)\varsigma_n(a)$$  \hspace{1cm} (D.3)

into D.2, we obtain

$$n \varsigma_{n-1}(a) - a (2n+1) \varsigma_n(a) + (1+n) \varsigma_{n+1}(a) = 0.$$  \hspace{1cm} (D.4)
Comparing with the recurrence relation for Legendre polynomials C.5

\[ n P_{n-1}(x) - x (2n + 1) P_n(x) + (1 + n) P_{n+1}(x) = 0, \]  
(D.5)

we can see that for real \( a \)

\[ \zeta_n(a) = c(a) P_n(a) \]  
(D.6)

where \( c(a) \) is an arbitrary (normalization) constant. The closure relation for the \( P_N \) approximation (see C.9) requires that

\[ \zeta_{N+1}(a) = c(a) P_{N+1}(a) = 0 \]  
(D.7)

and defines \( N + 1 \) distinct eigenvalues \( a \) as roots of

\[ P_{N+1}(a) = 0. \]  
(D.8)

Because of the parity property of the Legendre polynomials (see [3], p.752)

\[ P_n(-a) = (-1)^n P_n(a), \]  
(D.9)

for every positive root of equation D.8, there is also a negative root of the same absolute value. When \( N \) is even, equation D.8 has a root \( a = 0 \). In the following we
introduce indexation for the roots of equation D.8 so that

\[ a_\ell < a_{\ell+1}, \text{ and } a_1 = \min_{0<a_\ell}(a_\ell) \quad (D.10) \]

Indexed this way

\[ a_\ell = -a_{-\ell} \text{ and } a_0 = 0 \quad (D.11) \]

when \( a_0 \) appears for even \( N \). Index \( \ell \) can take the following integer values

\[ \ell = \begin{cases} 
-\frac{N+1}{2}, & \text{for } N = \text{odd} \\
-\frac{N}{2}, & \text{for } N = \text{even} 
\end{cases} \quad (D.12) \]

where

\[ s = \begin{cases} 
\frac{N+1}{2}, & \text{for } N = \text{odd} \\
\frac{N}{2}, & \text{for } N = \text{even} 
\end{cases} \quad (D.13) \]

Combining equations D.3 and D.6, for the components of \( \alpha(a) \), we obtain:

\[ \alpha_n(a_\ell) = c(a_\ell)(2n+1)P_n(a_\ell), \text{ where we can set } c(a_\ell) = \frac{1}{2}, \quad (D.14) \]

for the purpose of convenience that becomes evident in subsection 3.1.4.

We also need to know the solutions of the equation adjoint to D.1, that is

\[ \tilde{\alpha}(a)A = \tilde{\alpha}(a)a, \quad (D.15) \]

or in the component form

\[ n\tilde{\alpha}_{n-1}(a) - a(2n+1)\tilde{\alpha}_n(a) + (n+1)\tilde{\alpha}_{n+1}(a) = 0. \quad (D.16) \]
We already solved the above equation (see formulas D.6 and D.7) and know the solutions
\[ \tilde{\alpha}_n(a) = \tilde{c}(a) P_n(a) \] (D.17)

where \( c(a) \) is an arbitrary constant. The values of \( a \) are determined from the equation D.8 as required by closure relation for \( P_N \) approximation (see equation C.9) and so are the same for equations D.15 and D.1. We will adopt the same indexation D.10 for the found solutions.

Eigenvectors \( \alpha(a_i) \) and \( \tilde{\alpha}(a_j) \) have the following property
\[ \tilde{\alpha}(a_i) \alpha(a_j) = \delta_{i,j} \tilde{c}(a_i) \sum_{n=0}^{N} (n + 1/2) P_n(a_i)^2, \] (D.18)

that comes from the fact that for \( i \neq j \): \( \tilde{\alpha}(a_i) A \alpha(a_j) = a_i \tilde{\alpha}(a_i) \alpha(a_j) = a_j \tilde{\alpha}(a_i) \alpha(a_j) \), and hence \( (a_i - a_j) \tilde{\alpha}(a_i) \alpha(a_j) = 0 \). It is convenient to set
\[ \tilde{c}(a_i) = \left( \sum_{n=0}^{N} (n + 1/2) P_n(a_i)^2 \right)^{-1}, \] (D.19)
so that \( \tilde{\alpha}_i(a_i) \alpha_j(a_j) = \delta_{i,j} \). (D.20)

To simplify notation, we will assign indices to the eigenvectors of matrix \( A \): \( \alpha(a) \) according to the indexing of their eigenvalues:
\[ \alpha_j = \alpha(a_j) \quad \text{and} \quad \tilde{\alpha}_i = \tilde{\alpha}(a_i). \] (D.21)

Let \( P \) be the matrix with \( \alpha_i \) being its columns.
\[ P = \left[ \begin{array}{ccc} \ldots & \alpha_{0,-i} & \alpha_{0,i} & \ldots \\ \ldots & \alpha_{1,-i} & \alpha_{1,i} & \ldots \\ \vdots & \vdots & \vdots & \vdots \\ \ldots & \alpha_{N,-i} & \alpha_{N,i} & \ldots \end{array} \right] \quad \text{and} \quad P' = \left[ \begin{array}{ccc} \ldots & \cdots & \cdots \\ \cdots & \tilde{\alpha}_{0,-i} & \tilde{\alpha}_{1,-i} & \cdots \\ \cdots & \vdots & \vdots & \vdots \\ \cdots & \tilde{\alpha}_{0,i} & \tilde{\alpha}_{1,i} & \cdots \end{array} \right] \] (D.22)

having \( \tilde{\alpha}_i \) as its rows; or for the components

\[ P_{n,i} = \alpha_{n,i} \quad \text{and} \quad P'_{i,n} = \tilde{\alpha}_{n,i}. \quad \text{(D.23)} \]

Formula D.20 implies that

\[ P'P = E \quad \text{and so} \quad P' = P^{-1}, \quad \text{(D.24)} \]

where \( E \) is the identity matrix. The above equalities suggest that \( P \) and \( P' \) are regular matrices and hence \( \alpha_\ell \) are linearly independent as well as \( \tilde{\alpha}_i \).

Using \( P \) and \( P^{-1} \), matrix \( A \) can be diagonalized

\[ \hat{A} = P^{-1}AP = diag(\alpha_\ell), \quad \text{(D.25)} \]

and its exponent can be calculated

\[ e^{Ax} = Pe^{P^{-1}APx}P^{-1} = Pe^{diag(\alpha_\ell)x}P^{-1} = P\text{diag}(e^{\alpha_\ell x})P^{-1}. \quad \text{(D.26)} \]
The parity property for the eigenvectors of matrix $A$

$$\alpha_{n,-i} = (-1)^n \alpha_{n,i} \quad \text{and} \quad \tilde{\alpha}_{n,-i} = (-1)^n \tilde{\alpha}_{n,i} \quad (D.27)$$

follows from that of the Legendre polynomials (see formula D.9). In particular, let’s notice that for the eigenvectors of matrix $A$, corresponding to a zero eigenvalue:

$$\alpha_{n=\text{odd},0} = \tilde{\alpha}_{n=\text{odd},0} = 0.$$  

Using the transformed Legendre equation (see reference [54], p.75) satisfying the conditions of the Sturm theorem (see reference [54], p.107), it is possible to show that the angles $\theta_\ell$ determined by the roots of equation D.8,

$$\cos \theta_\ell = a_\ell, \quad (D.28)$$

are uniformly distributed on the interval $0 < \theta_\ell < \pi$:

$$\frac{\pi}{2} + \pi \frac{\ell}{N+1} < \theta_\ell < \frac{\pi}{2} + \pi \frac{\ell + 1}{N+1} \quad \text{for} \quad N = \text{odd} \quad \text{and} \quad (D.29)$$

$$\frac{\pi}{2} + \pi \frac{\ell - 1/2}{N+1} < \theta_\ell < \frac{\pi}{2} + \pi \frac{\ell + 1/2}{N+1} \quad \text{for} \quad N = \text{even} .$$

The above relations provide the following estimates

$$\theta_\ell = \frac{\pi}{2} + \pi \frac{\ell + 1/2}{N+1} + O\left(\frac{1}{N+1}\right) \quad \text{for} \quad N = \text{odd} \quad \text{and} \quad (D.30)$$

$$\theta_\ell = \frac{\pi}{2} + \pi \frac{\ell}{N+1} + O\left(\frac{1}{N+1}\right) \quad \text{for} \quad N = \text{even} .$$
Appendix E

Eigensystem of $L^*(v)$

An operator adjoint to $L(v)$ can be found by integration by parts

$$
\int_0^V \tilde{f}(L(v)f)dv = \int_0^V \tilde{f}(A\frac{df}{dv} + \frac{1}{v}Bf))dv = 
$$

$$
\tilde{f}(Af)|_0^V + \int_0^V (-\frac{d\tilde{f}}{dv}A + \tilde{f}B\frac{1}{v})f dv = \tilde{f}(Af)|_0^V + \int_0^V (\tilde{f}L^*(v))f dv.
$$

The integrals on the right and left hand sides are equal to each other providing that

$$
\tilde{f}(Af)|_0^V = 0. \quad (E.2)
$$

When boundary conditions for $f$ are given, the above formula allows us to determine the boundary conditions for $\tilde{f}$. It follows from equation $E.1$ that action of $L^*(v)$ on an associated function $\tilde{f}$ is given by

$$
\tilde{f}L^*(v) = -\frac{d\tilde{f}}{dv}A + \tilde{f}B\frac{1}{v}. \quad (E.3)
$$
Assuming that the eigenvalues of $L^*(v)$ are pure imaginary numbers $i\lambda$

$$\tilde{f} L^*(v) = \tilde{f} i\lambda,$$ (E.4)

the eigensystem of the operator $L^*(v)$ can be found following the line of reasoning used in sections 2.1 and 2.2 to find eigensystem of the operator $L(v)$.

The component form of the above equation

$$\left( \frac{\partial \tilde{f}_{n+1}}{\partial v} + \frac{\tilde{f}_{n+1}}{v} n \right) \frac{n + 1}{2n + 1} + \left( \frac{\partial \tilde{f}_{n-1}}{\partial v} - \frac{\tilde{f}_{n-1}}{v} (n + 1) \right) \frac{n}{2n + 1} = -i\lambda \tilde{f}_n \quad (E.5)$$

can be easily obtained by changing the indexing in the definition of matrices $A$ and $B$ given by equations 2.5 and 2.6

$$A_{k,s} = (s\delta_{k+1,s} + (s + 1)\delta_{k-1,s}) \frac{1}{2s + 1}, \quad (E.6)$$

$$B_{k,s} = (\delta_{k+1,s} - \delta_{k-1,s}) \frac{s(s + 1)}{2s + 1}. \quad (E.7)$$

Equation E.5 can be reexpressed as

$$v^{-n} \frac{\partial (v^n \tilde{f}_{n+1})}{\partial v} \frac{n + 1}{2n + 1} + v^{n+1} \frac{\partial (v^{-(n+1)} \tilde{f}_{n-1})}{\partial v} \frac{n}{2n + 1} = -i\lambda \tilde{f}_n. \quad (E.8)$$

We will follow the arguments of chapter 2.1 and use the substitution

$$\tilde{f}_n(v) = i^n v^n J_{\nu_n}(v) \varphi_n, \quad (E.9)$$
where $\varphi_n$ are some coefficients, undetermined at this point. To match the recurrence relations for the Bessel functions 2.13, we have to satisfy equations

\[ n + s_{n+1} = \nu_{n+1} \quad \text{and} \quad n + 1 - s_{n-1} = \nu_{n-1}, \]  

(E.10)

with the solutions

\[ \nu_n = n + \frac{1}{2} \quad \text{and} \quad s_n = \frac{3}{2}, \]  

(E.11)

that determine the form of the associated functions:

\[ \tilde{f}_n(v) = i^n v^2 j_n(v)\varphi_n \text{ or } i^n v^2 n_n(v)\varphi_n. \]  

(E.12)

Substituting $\tilde{f}_n$ into equation E.5 (or E.8) and simplifying, we obtain

\[ i^{n+1} v^2 j_n(v) \left( \frac{n + 1}{2n + 1} \varphi_{n+1} + \frac{n}{2n + 1} \varphi_{n-1} \right) = -\lambda i^{n+1} v^2 j_n(v)\varphi_n, \]  

(E.13)

or, in matrix form,

\[ \tilde{f} L^*(v) = \varphi J(v) v^2 L^*(v) = \varphi AJ(v) v^2 i = -\varphi J(v) v^2 i\lambda = -\tilde{f} i\lambda. \]  

(E.14)

The second equality in the above formula suggests that for $L^*(v)$

\[ J(v) v^2 L^*(v) = iAJ(v) v^2. \]  

(E.15)
$L^*(v)$ and $L(v)$ share the same scaling property

$$\tilde{f}L^*(v) = -\frac{d\tilde{f}}{dv}A + \tilde{f}B\frac{1}{v} = q(-\frac{d\tilde{f}}{d(qv)}A + \tilde{f}B\frac{1}{qv}) = \tilde{f}qL^*(qv), \text{ for } q \neq 0. \quad \text{(E.16)}$$

Introducing the adjoint eigensystem of matrix $A$ (discussed in Appendix D), that is $\tilde{\alpha}_i$ and $a_\ell$ satisfying $\tilde{\alpha}_iA = \tilde{\alpha}_ia_\ell$, and using the properties of the operator $L^*(v)$ given by formulas E.15 and E.16, we obtain

$$\tilde{\alpha}_iJ(qv)(qv)^2 L^*(v) = \tilde{\alpha}_iJ(qv)(qv)^2 qL^*(qv) = iq\tilde{\alpha}_iAJ(qv)(qv)^2 = iqa_\ell\tilde{\alpha}_iJ(qv)(qv)^2. \quad \text{(E.17)}$$

Replacing $q$ by $-q$ in the above derivation results in

$$\tilde{\alpha}_iJ(-qv)(qv)^2 L^*(v) = -ia_\ell\tilde{\alpha}_iJ(-qv)(qv)^2. \quad \text{(E.18)}$$

Comparing with equation E.14, we conclude that

$$\tilde{f} = \tilde{\xi}_i(qv) = \tilde{\alpha}_iJ(-qv)(qv)^2 = \tilde{\alpha}_{-i}J(qv)(qv)^2 \quad \text{or} \quad \text{(E.19)}$$

$$\tilde{f} = \tilde{\eta}_i(qv) = \tilde{\alpha}_iN(-qv)(qv)^2 = -\tilde{\alpha}_{-i}N(qv)(qv)^2,$$

and $\lambda = qa_\ell \quad \text{(E.20)}$

are eigenfunctions and the corresponding eigenvalues of the operator $L^*(v)$. To make the arguments of the spherical Bessel functions positive, the expressions that follow the second equality signs are transformed into the expressions following the third equality signs by using the parity properties of the spherical Bessel functions (see
Next, we want to consider the case of $\lambda = 0$, that is to solve

$$
\tilde{f}L^*(v) = -\frac{d\tilde{f}}{dv}A + \tilde{f}B\frac{1}{v} = 0,
$$

(E.21)

or, in the component form for the $n$-th equation,

$$
\left(\frac{\partial \tilde{f}_{n+1}}{\partial v} + \frac{\tilde{f}_{n+1}}{v} n\right) \frac{n + 1}{2n + 1} + \left(\frac{\partial \tilde{f}_{n-1}}{\partial v} - \frac{\tilde{f}_{n-1}}{v} (n + 1)\right) \frac{n}{2n + 1} = 0,
$$

(E.22)

where $0 \leq n \leq N$ and $f_{N+1} = 0$ to satisfy the closure requirement for the $P_N$ approximation (see formula C.9).

First, we consider the case of an odd $N$ or $N + 1 = l_{even}$ number of equation. Looking for a solution in the form

$$
\tilde{f}_n(v) = c_n v^s \text{ for } s = 0, 1, 2...
$$

(E.23)

and substituting it to the above equation, we obtain the $n$-th relation for the coefficients $c_{n+1}$ and $c_{n-1}$

$$
(s + n) \frac{n + 1}{2n + 1} c_{n+1} + (s - n - 1) \frac{n}{2n + 1} c_{n-1} = 0.
$$

(E.24)

In the above equation and further in equation E.28 $c_1 = c_{N+1} = 0$. 

formula 2.68) and of the eigenvectors of matrix $A$ (see formula D.27).
For \( n = s - 1 \), equation E.24 becomes

\[
(2s - 1) \frac{s}{2s - 1} c_s + 0 \cdot c_{s-2} = 0,
\]

(E.25)

meaning that \( c_{s-2} \) is arbitrary. Relations E.24 further make \( c_{s-2}, c_{s-4}, \ldots \) proportional to \( c_{s-2} \), set \( c_s = c_{s+2} = c_{s+4} = 0 \), and make \( \ldots, c_{s-1}, c_{s+1}, \ldots \) proportional to each other.

If \( s - 2 \) is even, the odd relations E.24 define the sequence of coefficients with even indices \( c_0, c_2, \ldots, c_{s-2} \), while \( c_s = c_{s+2} = \ldots = c_{N+1} = 0 \) and \( c_1 = c_3 = \ldots = c_N = 0 \). If \( s - 2 \) is odd, the even relations determine the sequence of coefficients with odd indices \( c_1 = c_3 = \ldots = c_{s-2} = 0 \), while \( c_s = c_{s+2} = \ldots = c_N = 0 \) and \( c_0 = c_2 = \ldots = c_{N+1} = 0 \).

This way, we construct \( l_{\text{even}}/2 \) solutions of the form

\[
\tilde{f} = \tilde{\chi}'_{k/2+1} = [c_0 \quad 0 \quad c_2 \quad 0 \quad \cdots \quad 0 \quad c_k \quad 0 \quad \cdots \quad 0] v^{k+2} \quad \text{for} \quad k = 0, 2, \ldots, N - 1;
\]

(E.26)

where non-zero coefficients have even indices and are related by formula E.24.

Let’s further consider a solution in the form

\[
\tilde{f}_n(v) = c_n v^{-s}.
\]

(E.27)

The \( n \)-th relation for the coefficients \( c_{n+1} \) and \( c_{n-1} \) becomes

\[
(s - n) \frac{n + 1}{2n + 1} c_{n+1} + (s + n + 1) \frac{n}{2n + 1} c_{n-1} = 0.
\]

(E.28)
For \( n = s \), E.28 gives
\[
0 \cdot c_{s+1} + (2s + 1) \frac{s}{2s + 1} c_{s-1} = 0, \tag{E.29}
\]
leaving \( c_{s+1} \) arbitrary. Relations E.28 further make \( c_{s+3}, c_{s+5}, \ldots \) proportional to \( c_{s+1} \), set \( c_{s-1} = c_{s-3} = \ldots = 0 \), and make \( \ldots, c_{s}, c_{s+2}, \ldots \) proportional to each other.

If \( s \) is odd, the even relations E.28 will define the sequence of coefficients with odd indices: \( c_{s+1}, c_{s+3}, \ldots, c_{N} \), while \( c_{1} = c_{3} = \ldots = c_{s-1} = 0 \) and \( c_{0} = c_{2} = \ldots = c_{N+1} = 0 \). If \( s \) is even, the odd relations will determine the sequence of coefficients with even indices \( c_{s+1} = c_{s+3} = \ldots = c_{N+1} = 0 \), while \( c_{0} = c_{2} = \ldots = c_{s-1} = 0 \) and \( c_{1} = c_{3} = \ldots = c_{N} = 0 \). This way we find \( l_{\text{even}}/2 \) additional solutions of the form

\[
\tilde{f} = \chi'_{\frac{k}{2}} = \begin{bmatrix} 0 & \cdots & 0 & c_k & \cdots & 0 & c_{N-1} & c_N \end{bmatrix} v^{-k+1} \text{ for } k = 1, 3, \ldots, N; \tag{E.30}
\]

where non-zero coefficients have odd indices and are related by formula E.28.

The constructed \( l_{\text{even}} \) solutions E.26 and E.30 are linearly independent, so they are the only solutions of system 2.32. E.26 solves the odd equations and E.30 solves the even equations.

For \( l_{\text{odd}} = N + 2 \) number of equations, the solution is obtained following the same arguments as those of section 2.2. The system of even equations has only a trivial solution. The general solution for the system of odd equations is a linear combination of the \( (l_{\text{odd}} - 1)/2 \) solutions of the form E.26, the solution of equation

\[
\frac{\partial \tilde{f}_{N+1}}{\partial v} + \tilde{f}_{N+1} N = 0, \text{ obtained when the rest of } \tilde{f}_{n<N+1} = 0, \text{ given by }
\]

\[
\tilde{f} = \bar{\chi}_0 = \begin{bmatrix} 0 & \cdots & 0 & c_{N+1} \end{bmatrix} v^{-N}. \tag{E.31}
\]
and a solution

\[ \tilde{f} = (qv)^2 \sum_q \varphi(q) \left[ j_0(qv) \rho_0 \ 0 \ -j_2(qv) \rho_2 \ 0 \ \cdots \ 0 \ i^{N+1}j_{N+1}(qv) \rho_{N+1} \right], \tag{E.32} \]

where

\[ \frac{n+1}{2n+1} \rho_{n+1} + \frac{n}{2n+1} \rho_{n-1} = 0, \tag{E.33} \]

\( \varphi(q) \) is an arbitrary function of \( q \). In formula E.32, \( j_n(qv) \) can be replaced by \( n_n(qv) \).

Solution E.32 is identical to the eigenfunction of \( L^*(v) \) corresponding to a zero eigenvalue of matrix \( A \).
Appendix F

Graphs of azimuthally symmetric functions

For a given point \( v \) in the velocity space, azimuthally symmetric points are produced through rotation by angle \( \phi \). Azimuthally symmetric points (Fig. F-1) form a circle with its center positioned on axis \( 0v_z \) at the point corresponding to coordi-

Figure F-1: The solid circle displays azimuthally symmetric points.
nate $v_z$ and the plane of the circle being perpendicular to axis $0v_z$. An azimuthally symmetric function takes the same value for any point of the circle. It is completely defined by its values on any half-plane with the edge on axis $0v_z$.

The distribution functions obtained through the $P_N$ approximation are independent of azimuthal angle $\phi$, that is, azimuthally symmetric. The values of the distribution function can be displayed on the $v_xOv_z$ plane as in Fig. F-2.

Figure F-2: Azimuthally symmetric density function on the left and particles distributed in the velocity space according to this density function on the right.
Appendix G

Operator splitting

This technique is applied throughout chapter 3 to obtain numerical procedures for the solution of the Boltzmann equation. The following discussion is adopted from the book [30], p.202, and is extended here to the arbitrary (matrix) evolution equations.

Let $\Omega = [\Omega_{i,j}]$ be a $m \times m$ matrix that does not depend on $t$,

$$\left[ \frac{\partial}{\partial t}, \Omega \right] = 0, \quad \text{(G.1)}$$

acting on a column matrix $F(t) = (f_1(t), ..., f_m(t))^T$. For an evolution equation

$$\left( \frac{\partial}{\partial t} + \Omega \right) F = 0, \quad \text{(G.2)}$$
the formal solution is

\[ F(t + \tau) = e^{-\Omega \tau} F(t), \quad \text{where} \]

\[ e^{\Omega \tau} = \sum_{n=0}^{r} \frac{\tau^n}{n!} \Omega^n \quad \text{and} \quad r \to \infty. \]  

For the purpose of numerical representation of \( e^{\Omega \tau} \), the series G.4 must be truncated, that is \( r \) must be made finite. We further call

\[ U(\tau) = e^{-\Omega \tau} \quad \text{(G.5)} \]

the evolution operator for equation G.2 and the matrix \( \Omega \). If we can provide some approximate way to solve equation G.2,

\[ F(t + \tau) = \left( T(\tau) + O(\tau^r) \right) F(t), \]  

for an arbitrary \( F(t) \), then \( T(\tau) \) gives a representation of \( e^{\Omega \tau} \) to some accuracy

\[ U(\tau) = T(\tau) + O(\tau^r) \quad \text{or} \quad T(\tau) = e^{-\Omega \tau} + O(\tau^r). \]  

which can be used for the numerical representation of \( e^{\Omega \tau} \). In other words, any linear method that approximately solves equation G.2 simultaneously provides also for an approximation to the evolution operator G.5. This is the main idea behind the construction of all of the evolution operators of chapter 3.
We can consider the evolution equation with more than one matrix,

\[
\left( \frac{\partial}{\partial t} + \Omega_1 + \Omega_2 \right) F = 0. \tag{G.8}
\]

If we know the approximation of the evolution operators

\[
T_1(\tau) = e^{-\Omega_1 \tau} + O(\tau^{r_1}) \quad \text{and} \quad T_2(\tau) = e^{-\Omega_2 \tau} + O(\tau^{r_2}), \tag{G.9}
\]

an approximation of the resultant evolution operator \( U(\tau) \) for equation G.8 can be obtained as a product of the evolution operators G.9

\[
U(\tau) = e^{-(\Omega_1 + \Omega_2) \tau} \approx T_1(\tau)T_2(\tau). \tag{G.10}
\]

Replacement of the resultant evolution operator for the sum of matrices by the product of their corresponding evolution operators is referred to below as operator splitting.

In the case of commuting matrices

\[
[\Omega_1, \Omega_2] = 0, \quad U(\tau) = T_1(\tau)T_2(\tau) + O(\tau^r) \quad \text{and} \quad r = \min(r_1, r_2), \tag{G.11}
\]

that is, the order of approximation for the resultant evolution operator is limited by that of the operator with the lower order of approximation. But if the operators do not commute

\[
[\Omega_1, \Omega_2] \neq 0, \quad U(\tau) = T_1(\tau)T_2(\tau) - [\Omega_1, \Omega_2] \frac{\tau^2}{2} + O(\tau^r) \quad \text{and} \quad r = 3, \tag{G.12}
\]
the resultant evolution operator is at most accurate to first order and the second order splitting error is determined by $[\Omega_1, \Omega_2] \frac{t^2}{2}$. Introducing the norm of the operator $\Omega$:

$$||\Omega|| = \max_{||F||=1} ||\Omega F|| = \max_{i,j} |\Omega_{i,j}|,$$

based on the following simple norm for the column matrix $F$ (see book [20], p.139)

$$||F|| = \max_i |f_i|,$$

and the characteristic time $\tau_{\text{char}}$ of the evolution operator $e^{-\Omega t}$:

$$||\Omega|| \tau_{\text{char}} = 1,$$

the splitting error can be estimated as

$$||[\Omega_1, \Omega_2] \frac{t^2}{2} + O(t^3)|| \leq ||\Omega_2|| ||\Omega_1|| \frac{t^2}{2} + O(t^3) = \frac{t^2}{2\tau_1 \tau_2} + O(t^3),$$

where $\tau_1$ and $\tau_2$ are the characteristic times of $\Omega_1$ and $\Omega_2$. In the special case when the characteristic times are of different orders of magnitude $\tau_1 < \tau \ll \tau_2$, the approximation of the evolution operator $U(\tau) = T_1(\tau) T_2(\tau)$ will be mostly determined by $T_1(\tau)$:

$$U(\tau) = T_1(\tau) \left(1 + O\left(\frac{\tau}{\tau_2}\right)\right).$$
Appendix H

$P_N$ approximation of collision integrals

We will start with two expressions for the in-scattering and out-scattering collision integrals obtained in [17]. They apply to scattering processes that do not change the number of scattering particles. During a scattering collision a particle changes its position in the velocity space within a collision time, not changing its position in the coordinate space.

The number of particles scattered in time $dt$ out of $d^3v$ (see Fig. H-1) in all directions (through all angles $\psi'$) is

$$
dt\, d^3r\, d^3v\, S^{\text{out}}(t, r, v) = dt\, d^3r\, d^3v N_s(r) v f(t, r, v) \int d\omega' q(v, \psi').
$$

Later on, we call $S^{\text{out}}$ the out-scattering collision integral. Here $N_s$ is the density of scatterers, $q(v, \psi')$ is the scattering differential cross-section that does not depend
on azimuthal angle. The scattering angle $\psi'$ is the one between $v$ and $v'$. In this chapter, integration over $d\omega'$ is done over the range of the variables $0 \leq \theta' \leq \pi$ and $0 \leq \phi' \leq 2\pi$ that define the direction of the vector $v'$ in the velocity space. For convenience, we also often refer to $v^2$ as the electron kinetic energy.

The number of particles scattered in time $dt$ into $d^3v$ from all $d^3v'$ is

$$dt \ d^3r \ d^3v \ S^{\text{in}}(t, r, v) = dt \ d^3r \ d^3v N_s(r) v \int d\omega' f(t, r, v') \left( \frac{v'}{v} \right)^3 \frac{\partial v'}{\partial v} q(v', \psi'). \quad (H.2)$$

The velocity $v'(v, \psi')$ before the collision, in formula H.2, is determined by energy conservation in the scattering process and is a function of $v$ and $\psi'$. In what follows, we call $S^{\text{in}}$ the in-scattering collision integral.

We need to find expansion coefficients for collision integrals as suggested by formula C.3. Substituting $f(t, r, v) = f(t, z, v)$ given by formula C.2 into expression H.1,
we immediately find the expansion coefficients of the out-scattering collision integral

\[ S_{n}^{\text{out}}(t, z, v) = N(z) v f_n(t, z, v) Q_0(v). \]  \hspace{1cm} (H.3)

Formula H.3 remains unchanged for all of the scattering processes we discuss in this chapter.

In the above formula and below, partial integral cross-sections \( Q_n(v) \) are given by expression

\[ Q_n(v) = 2\pi \int_0^{\pi} d\phi \sin \phi P_n(\cos \phi) q(v, \phi). \]  \hspace{1cm} (H.4)

To find \( S_{n}^{\text{in}}(t, z, v) \), let’s substitute \( f(t, r, v') = f(t, z, v') \) given by formula C.2 into expression H.2 to obtain

\[ S_{n}^{\text{in}}(t, z, v) = N(z) v \sum_{n=0}^{N} \int d\omega' \left( \frac{v'}{v} \right)^3 \frac{\partial v'}{\partial v} q(v', \psi') f_n(t, z, v') P_n(\cos \theta'). \]  \hspace{1cm} (H.5)

Introducing angle \( \phi_{v, v'} \) (see Fig. H-2), we can utilize the addition theorem for associ-

![Figure H-2: Angle \( \phi_{v, v'} \) is measured from a projection of axes 0v_z to a projection of vector \( v' \) on a plane perpendicular to vector \( v \).]
ated Legendre polynomials (see reference [3], p.796)

\[ P_n(\cos \theta) = P_n(\cos \psi) + 2 \sum_{m=1}^{n} \frac{(n-m)!}{(n+m)!} P_n(\cos \theta) P_n(\cos \psi) \cos m\phi_{vz,v'}. \]  

(H.6)

If we substitute \( P_n(\cos \theta) \) into H.5, and integrate over \( 0 \leq \phi_{vz,v'} \leq 2\pi \), the terms containing \( \cos m\phi_{vz,v'} \) average to zero. Keeping the rest of the terms we obtain the expansion coefficients of the in-scattering collision integral

\[ S_n^{\text{in}}(t, z, v) = N_s(r) v \int d\omega' \left( \frac{v'}{v} \right)^3 \frac{\partial v'}{\partial v} P_n(\cos \psi) q(\psi', \psi') f_n(t, z, v'). \]  

(H.7)

Our further goal is to calculate the expansion coefficients of the complete collision integral

\[ S_n(t, z, v) = S_n^{\text{in}}(t, z, v) - S_n^{\text{out}}(t, z, v), \]  

(H.8)

where expressions \( S_n^{\text{in}}(t, z, v) \) and \( S_n^{\text{out}}(t, z, v) \) are given by formulas H.7 and H.3, for some of the most important electron-atom collision processes that take place in low temperature plasmas: elastic, excitation and ionization collisions.

### H.1 Elastic collisions

When a lighter particle of a mass \( m \) and an initial velocity \( v' \) collides into a heavier particle of a mass \( M \), initially at rest, the final velocity \( v \) and the scattering angle \( \psi' \) (between the directions of initial and final velocities) of the lighter particle are related
by formula (see reference [23], p.47)

$$\frac{v}{v'} = \frac{\eta}{1 + \eta} \cos \psi' + \left[ \left( \frac{1}{1 + \eta} \right)^2 - \left( \frac{\eta}{1 + \eta} \right)^2 \sin^2 \psi' \right]^{\frac{1}{2}} \text{ for } \eta = \frac{m}{M} < 1, \quad (H.9)$$

so that the energy loss $\left( \frac{v}{v'} \right)^2 \leq 0$ depends on the scattering angle $\psi'$. Expansion of the above formula into the powers of $\eta$ yields:

$$\left( \frac{v}{v'} \right)^2 = 1 - 2\eta(1 - \cos \psi') + 8\eta^2 \sin^4 \frac{\psi'}{2} + \ldots. \quad (H.10)$$

For electrons colliding with atoms $\eta$ is of the order of $10^{-5}$ to $10^{-3}$ and it is reasonable to only consider the first order of $\eta$:

$$v \approx v'(1 - \delta(\psi')) \text{ and } v' \approx v(1 + \delta(\psi')) \text{ where } \delta(\psi') = \eta(1 - \cos \psi'). \quad (H.11)$$

Formula H.7 requires calculation of several expressions, and so we obtain:

$$\frac{\partial v'}{\partial v} \approx 1 + \delta \approx \frac{v'}{v} \quad (H.12)$$

$$\left( \frac{v'}{v} \right)^3 \left( \frac{\partial v'}{\partial v} \right) \approx \left( \frac{\partial v'}{\partial v} \right)^4 \approx 1 + \delta(\psi')^4, \quad (H.13)$$

$$q^{el}(v', \psi') \approx q^{el}(v(1 + \delta(\psi'))), \psi') \approx q^{el}(v, \psi') + v\delta(\psi') \frac{\partial q^{el}(v, \psi')}{\partial v}, \quad (H.14)$$

and in the same way

$$f_n(t, z, v') \approx f_n(t, z, v) + v\delta(\psi') \frac{\partial f_n(t, z, v)}{\partial v}, \quad (H.15)$$
so that
\[
\left(\frac{v'}{v}\right)^3 \frac{\partial v'}{\partial v} q^\text{el}(v', \psi') f_n(t, z, v') \approx (H.16)
\]
\[
(1 + 4\delta(\psi')) q^\text{el}(v, \psi') f_n(t, z, v) + v\delta(\psi') \left( q^\text{el}(v, \psi') \frac{\partial f_n(t, z, v)}{\partial v} + \frac{\partial q^\text{el}(v, \psi')}{\partial v} f_n(t, z, v) \right) = q^\text{el}(v, \psi') f_n(t, z, v) + \frac{1}{v^3} \frac{\partial}{\partial v} \left( v^3 \delta(\psi') q^\text{el}(v, \psi') f_n(t, z, v) \right).
\]

Substitution of the above results into the formula H.7 yields
\[
S_{\text{el,in}}^n(t, z, v) = N_s(z) v \left( Q_n^\text{el}(v) f_n(t, z, v) - \frac{\eta}{v^3} \frac{\partial}{\partial v} [v^4 K_n^\text{el}(v) f_n(t, z, v)] \right) \quad (H.17)
\]
for the expansion coefficients of the in-scattering collision integral, where \( K_n(v) \) can be written in terms of the partial integral cross-sections \( Q_n(v) \) as
\[
K_n^\text{el}(v) = \int d\omega' (1 - \cos(\psi')) P_n(\cos \psi') q^\text{el}(v, \psi') \quad (H.18)
\]
\[
= - \frac{n + 1}{2n + 1} Q_{n+1}^\text{el}(v) + Q_n^\text{el}(v) - \frac{n}{2n + 1} Q_{n-1}^\text{el}(v).
\]
The above equation uses formula C.5 to re-express \( \cos \psi' P_n(\cos \psi') \).

The expansion coefficients of the out-scattering collision integral are given by equation H.3:
\[
S_{\text{el, out}}^n(t, z, v) = N_s(z) v Q_0^\text{el}(v) f_n(t, z, v). \quad (H.19)
\]

For the expansion coefficients of an elastic collision integral, characterized by energy conservation H.9 and the differential cross-section \( q^\text{el}(v, \psi') \), substitution of
the above results into formula H.8 yields

\[ S_n^{el}(t, z, v) = N_s(z)v\left((Q_n^{el}(v) - Q_0^{el}(v))f_n(t, z, v) - \frac{\eta}{v^3} \left[v^4 K_n^{el}(v)f_n(t, z, v)\right]\right). \]  \( \text{(H.20)} \)

### H.2 Excitation collisions

When an electron-atom collision results in excitation of the atom’s electron the impact electron loses the energy that we denote by \( \varepsilon_{ex} = \frac{mv^2}{2} \). We assume a simple formula relating the initial \( v' \) and final \( v \) velocities of the electron

\[ v^2 = v'^2 - \varepsilon_{ex}^2 \]  \( \text{(H.21)} \)

For the components of formula H.7, we obtain

\[ \frac{\partial v'}{\partial v} = \frac{\partial(v^2 + \varepsilon_{ex}^2)}{\partial v} \frac{1}{2} = \frac{v}{v'} \]  \( \text{(H.22)} \)

\[ \left( \frac{v'}{v} \right)^3 \left( \frac{\partial v'}{\partial v} \right) = \left( \frac{\partial v'}{\partial v} \right)^2. \]  \( \text{(H.23)} \)

The equation for the expansion coefficients of the in-scattering collision integral, given by equation H.7,

\[ S_n^{ex, \text{in}}(t, z, v) = N_s(z)v\left(\frac{v'}{v}\right)^2 Q_n^{ex}(v')f_n(t, z, v'), \]  \( \text{(H.24)} \)
and the equation for the expansion coefficients of the out-scattering collision integral, given by equation H.3,

\[ S_n^{\text{exc,out}}(t, z, v) = N_s(z)vQ_0^{\text{ex}}(v)f_n(t, z, v), \]  

substituted into formula H.8, yield the expansion coefficients of an excitation collision integral characterized by energy conservation H.21 and the differential cross-section \( q^{\text{ex}}(v, \psi') \):

\[ S_n^{\text{ex}}(t, z, v) = N_s(z)v\left( \left( \frac{v'}{v} \right)^2 Q_n(v')f_n(t, z, v') - Q_0(v)f_n(t, z, v) \right). \]  

**H.3 Ionization collisions**

Electron-atom collisions may cause ionization of the target atom and result in the production of an additional electron. Energy conservation in an ionization process can be written as

\[ v_1^2 + v_2^2 = v'^2 - \varepsilon_{io}^2, \]  

where \( v' \) is the velocity of the impact electron, \( v_1 \) and \( v_2 \) are the velocities of the scattered and produced electron, and \( \varepsilon_{io} = \frac{m_e v_{in}^2}{2} \) is the energy of ionization.

To find reasonable requirements to the distribution of the velocities of the scattered electrons, let’s for a moment suppose that we can somehow label the scattered and produced electrons as electron 1 and electron 2. Let’s consider the scattered and produced electrons obtained in an ionizing collision by an impact electron of a certain
fixed impact velocity \( v' \). The velocities of the scattered and produced electrons will satisfy the equation

\[ v'^2 - v_{io}^2 = v_1^2 + v_2^2 = \nu^2 = \text{const} \geq 0. \quad (H.28) \]

If electron 1 is scattered into a velocity interval \([v, v + dv]\), electron 2 is found in the velocity interval \([(\nu^2 - v^2)^{1/2} - (\nu^2 - v^2)^{-1/2}v dv, (\nu^2 - v^2)^{1/2}]\), with the corresponding volumes \(4\pi v^2 dv\) and \(4\pi v(\nu^2 - v^2)^{1/2}dv\) in the velocity space. Let’s denote the density functions of electrons 1 and 2 as \(\rho_1(v, \nu)\) and \(\rho_2(v, \nu)\). Suppose a large number of electrons, \(n\), are scattered and we find \(dn = n4\pi v^2 dv \rho_1(v, \nu)\) of the electrons of type 1 in the interval \([v, v + dv]\). The same number of electrons of type 2 has to be found in the interval \([(\nu^2 - v^2)^{1/2} - (\nu^2 - v^2)^{-1/2}v dv, (\nu^2 - v^2)^{1/2}]\) so that \(dn = 4\pi v(\nu^2 - v^2)^{1/2}dv \rho_1(v, \nu)\).

Hence, we obtain

\[ v \rho_1(v^2, \nu^2) = (\nu^2 - v^2)^{1/2} \rho_2(\nu^2 - v^2, \nu^2) \quad (H.29) \]

which by the substitution

\[ u^2 = \nu^2 - v^2 \quad (H.30) \]

can be transformed into

\[ u \rho_2(u^2, \nu^2) = (\nu^2 - u^2)^{1/2} \rho_1(\nu^2 - u^2, \nu^2). \quad (H.31) \]

Using formulas H.29, H.31 and substitution H.30, we can see that normalization
of $\varrho_1$ on the interval $[0, \nu]$

$$4\pi \int_0^\nu dv v^2 \varrho_1(v^2, \nu^2) = 1 \quad \text{(H.32)}$$

leads to the simultaneous normalization of $\varrho_2$

$$4\pi \int_0^\nu dv v^2 \varrho_2(v^2, \nu^2) = 4\pi \int_0^\nu dv v (v^2 - v^2)^{\frac{1}{2}} \varrho_1(v^2 - v^2, \nu^2) \quad \text{(H.33)}$$

$$= -4\pi \int_0^\nu du u^2 \varrho_1(u^2, \nu^2) = 1,$$

and the assumption

$$4\pi \int_0^\nu vdvdv^4 \varrho_1(v^2, \nu^2) = \varepsilon \quad \text{(H.34)}$$

leads to

$$4\pi \int_0^\nu dvv^4 \varrho_2(v^2, \nu^2) = 4\pi \int_0^\nu dv v^2 (v^2 - v^2)^{\frac{1}{2}} \varrho_1(v^2 - v^2, \nu^2) \quad \text{(H.35)}$$

$$= -4\pi \int_0^\nu du u^2 (v^2 - u^2) \varrho_2(u^2, \nu^2) = v^2 - \varepsilon.$$

Taking into account the results of the previous discussion, we can formulate the requirements to the density function $\varrho(v^2, \nu^2)$. Because we clearly cannot label the scattered electrons as 1 and 2, we assume their velocity distributions to be identical

$$\varrho_1(v^2, \nu^2) = \varrho_2(v^2, \nu^2) = \varrho(v^2, \nu^2) \quad \text{(H.36)}$$
with the consequence that (see formula H.31)

\[ v_\varphi(v^2, \nu^2) = (\nu^2 - v^2)^\frac{1}{2} \varphi(\nu^2 - v^2, \nu^2). \quad (H.37) \]

We notice that the above equation is symmetric around \( \frac{\nu^2}{2} \):

\[ \left( \frac{\nu^2}{2} + v^2 \right)^\frac{1}{2} \varphi(\frac{\nu^2}{2} + v^2, \nu^2) = \left( \frac{\nu^2}{2} - v^2 \right)^\frac{1}{2} \varphi(\frac{\nu^2}{2} - v^2, \nu^2). \quad (H.38) \]

When both the scattered and produced electrons have the same density distribution \( \varphi(v^2, \nu^2) \), conservation of electron density

\[
4\pi \int_0^{\nu} dv \ v^2 (\varphi_1(v^2, \nu^2) + \varphi_2(v^2, \nu^2)) = 2 \quad (H.39)
\]

requires the normalization

\[
4\pi \int_0^{\nu} dv \ v^2 \varphi(v^2, \nu^2) = 1, \quad (H.40)
\]

and the energy conservation

\[
4\pi \int_0^{\nu} dv \ v^4 (\varphi_1(v^2, \nu^2) + \varphi_2(v^2, \nu^2)) = \nu^2, \quad (H.41)
\]

requires that

\[
4\pi \int_0^{\nu} dv \ v^4 \varphi(v^2, \nu^2) = \frac{\nu^2}{2}. \quad (H.42)
\]
It is convenient to set

$$\varrho(v^2, \nu^2) = 0 \text{ for } \nu^2 < 0 \text{ or } \nu^2 < v^2,$$  \hfill (H.43)

that is when $v^2$ or $\nu^2$ go outside their domain of definition given by formula H.28.

The above discussion serves to prove that the introduced density function $\varrho(v^2, \nu^2)$ both conserves density as given by formula H.40 and energy in the form

$$\nu^2 = 8\pi \int_0^\nu dv \, v^4 \varrho(v^2, \nu^2) = v^2 - \nu^2_{io},$$  \hfill (H.44)

as follows from formulas H.28 and H.42. The above formula and formula H.40 will also hold if the upper limit of integration $\nu$ is replaced by $\infty$ because of definition H.43.

Our next goal is to calculate rates H.8 for ionization. We can still use formula H.1 and its $P_N$ approximation H.3 for the electrons leaving some region in the velocity space. To determine the analogs of formulas H.2 and H.7 for the incoming electrons for ionization, we consider a simple case when the ionization cross-section does not depend on the direction of $v'$, and $v_1, v_2$ are isotropically distributed. In this case, the ionization scattering is characterized exclusively by the total cross-section $Q_{io}^0(v)$.

The total number $\Delta_{d^3v}^{out}$ of impact electrons scattered out of the region $[v', v' + dv]$ in the velocity space can be found using H.1 integrated over $d\omega'$

$$\Delta_{d^3v}^{out} = dt \, d^3r \, d^3v' \, S_{0}^{\text{out,io}}(t, r, v') = dt \, d^3r \, d^3v' N_{s}(r) v' f_0(t, r, v') Q_{0}^{io}(v),$$  \hfill (H.45)

where $d^3v' = 4\pi dv' \, v'^2$. 

Ionization produces $\Delta_{d^{3}v'}^{\text{out}}$ of additional electrons. The total of $2\Delta_{d^{3}v'}^{\text{out}}$ of the scattered and produced electrons is spread over the velocity region $[0, \nu]$, with $\nu = (v'^2 - v_{io}^2)^{\frac{1}{2}}$. Out of the total of $2\Delta_{d^{3}v'}^{\text{out}}$ of the scattered electrons

$$\Delta_{d^{3}v'}^{\text{in}} \rightarrow d^{3}v = 2d^{3}v \varrho(v'^2, v'^2 - v_{io}^2)\Delta_{d^{3}v'}^{\text{out}}, \text{ where } d^{3}v = 4\pi dv v^2,$$

(H.46)

arrives into the interval $[v, v + dv] \subset [0, \nu]$ in the velocity space. The total number of electrons, landing in the volume $d^{3}v$ as a result of ionization scattering in the volume $v' \geq v_{io}$, during time $dt$, can be found by integration

$$dt \ d^{3}r \ d^{3}v \ S_{n}^{\text{in},io}(t, \mathbf{r}, \mathbf{v}) = \int_{v' \geq v_{io}} \Delta_{d^{3}v'}^{\text{in}} \rightarrow d^{3}v \ (H.47)$$

$$= dt \ d^{3}r \ d^{3}v N_s(\mathbf{r}) 8\pi \int_{v_{io}}^{\infty} dv' v'^3 \varrho(v'^2, v'^2 - v_{io}^2)Q_0(v')f_0(t, \mathbf{r}, v').$$

For the isotropic directional velocity distribution of the scattered electrons

$$S_{n>0}^{\text{in}} = 0,$$

(H.48)

and, the expansion coefficients of the in-scattering collision integral are

$$S_{n}(t, z, v) = N_s(z)\left(\delta_{0,n}8\pi \int_{v_{io}}^{\infty} dv' v'^3 \varrho(v'^2, v'^2 - v_{io}^2)Q_0(v')f_0(t, \mathbf{r}, v') - vQ_0(v)f_{n}(t, z, v)\right).$$

(H.49)

The expansion coefficients of the out-scattering collision integral are given by
equation H.3:

\[ S_{n}^{io, \text{out}}(t, z, v) = N_s(z) v Q_n^{io}(v) f_n(t, z, v). \] (H.50)

The expansion coefficients of an ionization collision integral characterized by the total cross-section \( Q_0(v) \) and the density function of the scattered and produced electrons \( \varrho(v^2, v'^2 - v_{io}^2) \) is given by formula H.8

\[ S_{n}^{io}(t, z, v) = N_s(z) \left( \delta_{0,n} \frac{8\pi}{\nu_0^2} \int_{v_{io}}^{\infty} dv' \, \frac{v'^3}{v'^2 - v_{io}^2} \varrho(v^2, v'^2) Q_0^{io}(v') f_0(t, r, v') - v Q_0^{io}(v) f_n(t, z, v) \right). \] (H.51)

The above formula holds if \( v_{io} \) is replaced by 0. The replacement is possible due to the definition of \( \varrho(v^2, \nu^2) \) given by formula H.43. Formula H.51 also supports particle and energy conservation in the form given by expressions H.40 and H.44.

In what follows, we always assume that the velocities of the electrons scattered in ionization collisions are distributed uniformly in energy (as in reference [17]) so that

\[ 4\pi dv \, \varrho(v^2, \nu^2) = \text{const} \, d(\nu^2) \text{ or } \varrho(v^2, \nu^2) = \frac{\text{const}}{2\pi
u}. \] Normalization H.40 determines the value of \( \text{const} = 1/\nu^2 \), resulting in

\[ \varrho(v^2, \nu^2) = \frac{1}{2\pi \nu^2 v}. \] (H.52)
Bibliography


