

# Multiterm spherical tensor representation of Boltzmann's equation for a nonhydrodynamic weakly ionized plasma

R. E. Robson, R. Winkler, and F. Sigeneger

*Institut für Niedertemperatur-Plasmaphysik, D-17489 Greifswald, Germany*

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The Boltzmann equation corresponding to a general “multiterm” representation of the phase space distribution function  $f(\mathbf{r}, \mathbf{c}, t)$  for charged particles in a gas in an electric field was reformulated entirely in terms of spherical tensors  $f_m^l$  some time ago, and numerous applications, including extension to time varying and crossed electric and magnetic fields, have followed. However, these applications have, by and large, been limited to the hydrodynamic conditions that prevail in swarm experiments and the full potential of the tensor formalism has thus never been realized. This paper resumes the discussion in the context of the more general nonhydrodynamic situation. Geometries for which a simple Legendre polynomial expansion suffices to represent  $f$  are discussed briefly, but the emphasis is upon cylindrical geometry, where such simplification does not arise. In particular, we consider an axisymmetric cylindrical column of weakly ionized plasma, and derive an infinite hierarchy of integrodifferential equations for the expansion coefficients of the phase space distribution function, valid for both electrons and ions, and for all types of binary interaction with neutral gas molecules.

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## I. INTRODUCTION

The Boltzmann equation corresponding to the phase space distribution function  $f(\mathbf{r}, \mathbf{c}, t)$  of each charged particle component of a weakly ionized gas can be written as

$$(\partial_t + \mathbf{c} \cdot \nabla + \mathbf{a} \cdot \partial_{\mathbf{c}} + J)f = 0. \quad (1)$$

Here  $\mathbf{a} = q\mathbf{E}/m$  is the force per unit mass acting on a particle of charge  $q$ , mass  $m$  due to an electric field  $\mathbf{E}$ . The operator  $J$  acts in velocity space and accounts for the rate of change of  $f$  due to various types of collisions between charged particles and neutral gas molecules. It is a scalar operator and it is also linear, as long as the degree of ionization is sufficiently low so that collisions between charged particles are negligible. There have been many methods advanced for the solution of Eq. (1) over the years, and a review of the literature to the mid 1980s was given by Robson and Ness [1]. In Ref. [1], Eq. (1) was reformulated in a very general way, entirely in terms of spherical tensors  $f_m^l$ , where  $l=0,1,2,3,\dots$  and  $m = -l, \dots, l$ , with attention being focused upon collisions that do not conserve particle number, and their effect upon measured transport coefficients. Numerous applications, to both ions and electrons, including extension to crossed electric and magnetic fields [2], have followed, and the recent review by White *et al.* [3] summarizes the literature to the present time. Note that explicit expressions for  $J$ , including simplified forms corresponding to limiting cases of very light or very heavy charged particles, are widely known—see, for example, Refs. [4,5], but are not needed for the present study.

The analysis presented in Ref. [1] had swarm experiments [4] specifically in mind, and consequently was slanted towards the *hydrodynamic regime*, where the macroscopic space-time dependence of  $f(\mathbf{r}, \mathbf{c}, t)$  is assumed to be projected onto a lower level through a linear functional dependence upon the number density  $n(\mathbf{r}, t)$  [5]. Swarm experi-

ments determine transport coefficients, which are unfolded using this hydrodynamic kinetic theory formalism to yield ion-molecule interaction potentials or electron-molecule impact cross sections [6]. This procedure is generally independent of the type of geometry, since all space dependence is accounted for by  $n(\mathbf{r}, t)$ , which in turn can be found by solving a diffusion equation. It is at this level that geometry appears, in the form of appropriate initial and boundary conditions for the diffusion equation, corresponding to the experiment at hand. Put another way, hydrodynamic kinetic theory generally (but not always [7]) has nothing to do with geometry or experimental arrangement *per se*.

This contrasts with the modern day demands for a rigorous *nonhydrodynamic* kinetic theory for low-temperature plasmas, where, although kinetic equations of the same mathematical *form* as in the swarm case apply for each charged species (as long as the degree of ionization is not too high, as already noted), the focus is often on the need to understand the behavior in the neighborhood of sources and boundaries, and otherwise on geometry in general. Large gradients may prevail, fields may vary in space and time, and hydrodynamic kinetic theory may consequently not be of much use. Configuration space and velocity coordinates must be treated on an equal footing: geometry and kinetic theory are thus intertwined, a fact that was well known to neutron transport theorists a long time ago [8]. The extensive analysis that has been carried out in recent times for electrons in low-temperature plasmas in planar geometry [9], using a simple Legendre polynomial representation of the distribution function, does not carry over to other geometries in a straightforward way. Higher order tensor spherical harmonics representation of the velocity distribution appears unavoidable, and spherical notation appears to offer advantages over the equivalent Cartesian representation [10–12] (see notes on tensors in the Appendix). Fortunately, most of the hard work has already been done in Ref. [1], and the present paper resumes the discussion at this point and deals in par-

ticular with cylindrical geometry. The aim is to develop a general framework for solving the Boltzmann equation, valid for both ions and electrons and all important types of binary charged particle–neutral molecule collisions, and yielding equations that can ultimately be solved using an appropriate numerical technique, for example, finite differences, Galerkin method, etc. The emphasis in the present paper is on a derivation of the hierarchy of equations, and applications will be reported in later papers.

The discussion proceeds from the general form of the multiterm representation of the phase space distribution in spherical harmonics  $Y_m^l$  in Sec. II, and circumstances are considered where this reduces to a simple Legendre polynomial expansion. In Sec. III, we specialize to cylindrical geometry, and give the hierarchy of equations corresponding to the axially symmetric case. A further reduction of the number and complexity of equations in the hierarchy results when axial fields and gradients can be neglected.

## II. THE BASIC FORMALISM

### A. General representation of the Boltzmann equation in the spherical harmonic basis

The starting point for most modern-day solutions of Boltzmann’s equation is the now familiar decomposition of the charged particle phase space distribution function in terms of spherical harmonics in velocity space (these are defined in the Appendix according to the phase convention of Fano and Racah [13]), the so-called “multiterm” expansion,

$$f(\mathbf{r}, \mathbf{c}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^l f_m^{(l)}(\mathbf{r}, c, t) Y_m^{(l)}(\hat{\mathbf{c}}), \quad (2)$$

which in turn is used to decompose the Boltzmann equation (1). Truncation of the infinite summation at  $l=l_{\max}$  corresponds to the “ $l_{\max}+1$ -term approximation,” or in neutron transport parlance, the “ $P_{l_{\max}}$  approximation” [8]. After substitution of Eq. (2) into Eq. (1), multiplication by  $Y_m^{(l)}(\hat{\mathbf{c}}) \equiv Y_m^{(l)}(\hat{\mathbf{c}})^*$ , and integration over all directions  $\hat{\mathbf{c}}$  of velocity space, the following infinite hierarchy of coupled integrodifferential equations for the expansion coefficients  $f_m^{(l)}$  results [see Ref. [1], Eq. (22), but note that we are *not* now taking  $\mathbf{E}$  to be along the  $z$  direction only]:

$$\begin{aligned} \partial_t f_m^{(l)} + \sum_{l' m' \mu} (l' m' 1 \mu | l m) \langle l \| c^{[1]} \| l' \rangle G_{\mu}^{(11)} f_{m'}^{(l')} \\ + \sum_{l' m' \mu} (l' m' 1 \mu | l m) \langle l \| \partial_c^{[1]} \| l' \rangle a_{\mu}^{(1)} f_{m'}^{(l')} = -J_l(f_m^{(l)}), \end{aligned} \quad (3)$$

where  $l=0,1,2,\dots,\infty$ ;  $m=-l,\dots,l$ . Values of the Clebsch-Gordan coefficients  $(l' m' 1 \mu | l m)$  are given by Condon and Shortley [14] and are of a particularly simple form. We have assumed that the collision operator  $J$  is a linear, scalar operator in velocity space, with spherical components  $J_l$ . The explicit form of the latter is not needed here,

and in any case they are well known, e.g., the approximate differential-finite difference form favored for light ions and electrons [4,5,9]. The reduced matrix elements  $\langle l \| \dots \| l' \rangle$  were calculated in Ref. [1] and are shown below

$$\begin{array}{lll} l' & \langle l \| c^{[1]} \| l' \rangle & \langle l \| \partial_c^{[1]} \| l' \rangle \\ l+1 & c \sqrt{\frac{l+1}{2l+1}} & \sqrt{\frac{l+1}{2l+1}} \left[ \frac{\partial}{\partial c} - \frac{l-1}{c} \right] \\ l-1 & c \sqrt{\frac{l}{2l+1}} & \sqrt{\frac{l}{2l+1}} \left[ \frac{\partial}{\partial c} + \frac{l+2}{c} \right] \\ \text{otherwise} & 0 & 0. \end{array}$$

Limits for the summations are normally not shown, it being implicitly understood that they run over all values of the indices for which the summand is nonzero. In Eq. (3) the “selection rules” are thus

$$l' = l \pm 1,$$

$$m' = m - \mu, \quad \mu = 0, \pm 1.$$

The gradient tensor operator  $G_{\mu}^{(11)}$  and field vector  $a_{\mu}^{(1)}$  components are defined in Ref. [1] for Cartesian coordinates and also in Eq. (31) below for cylindrical polar coordinates.

We could go on to include a magnetic field as Ness has done [2] by adding an appropriate term to the left-hand side of Eq. (3) (essentially the matrix elements of the angular momentum operator of quantum mechanics), but for the present the interest is only in electric fields.

In practice both the infinite summation (2) and the hierarchy (3) are truncated at some finite value  $l_{\max}$ , with the “two term” approximation corresponding to  $l_{\max}=1$ . Further decomposition of the coefficients  $f_m^{(l)}(\mathbf{r}, c, t)$  in speed space by some standard method (e.g., finite difference, polynomial expansion, etc.), and of course appropriate representation in time and spatial coordinates, is necessary to effect a solution. We emphasize that equations (3) [and the “multiterm” expansion (2) from which they derive] are quite independent of any such considerations, and can be used as the launching point for any study of charged particles, be it hydrodynamic or nonhydrodynamic, in whatever geometry desired.

### B. Some quantities of physical interest

The main quantities of physical interest are the number density  $n$ , mean energy  $\epsilon$ , mean velocity  $\mathbf{v}$ , and energy flux  $\mathbf{j}$ . If velocity space averaging is denoted by the angular brackets  $\langle \dots \rangle$ , then in spherical tensor notation these are as follows.

Number density:

$$n = \int f(\mathbf{r}, \mathbf{c}, t) d\mathbf{c} = \sqrt{4\pi} \int_0^{\infty} f_0^{(0)}(\mathbf{r}, c, t) c^2 dc. \quad (4)$$

Mean energy:

$$\begin{aligned}\epsilon &= \left\langle \frac{1}{2} mc^2 \right\rangle = \frac{1}{n} \int \frac{1}{2} mc^2 f(\mathbf{r}, \mathbf{c}, t) d\mathbf{c} \\ &= \frac{1}{n} \sqrt{4\pi} \int_0^\infty f_0^{(0)}(\mathbf{r}, c, t) \frac{1}{2} mc^4 dc.\end{aligned}\quad (5)$$

Mean velocity:

$$\begin{aligned}v_m^{(1)} &= \langle c_m^{(1)} \rangle = \frac{1}{n} \int c_m^{(1)} f(\mathbf{r}, \mathbf{c}, t) d\mathbf{c} \\ &= \frac{1}{n} \sqrt{\frac{4\pi}{3}} \int_0^\infty f_m^{(1)}(\mathbf{r}, c, t) c^3 dc.\end{aligned}\quad (6)$$

Mean energy flux:

$$\begin{aligned}j_m^{(1)} &= \left\langle \frac{1}{2} n m c^2 c_m^{(1)} \right\rangle = \int \frac{1}{2} m c^2 c_m^{(1)} f(\mathbf{r}, \mathbf{c}, t) d\mathbf{c} \\ &= \sqrt{\frac{4\pi}{3}} \int_0^\infty f_m^{(1)}(\mathbf{r}, c, t) \frac{1}{2} m c^5 dc.\end{aligned}\quad (7)$$

In the above the spherical components are defined as in Eq. (A7) of the Appendix for  $m=0, \pm 1$ . The corresponding Cartesian components could, if desired, be found by inverting these equations.

This concludes the general discussion. The specialization to particular geometry now follows.

### C. When can a simple Legendre polynomial expansion be used?

#### 1. Plane parallel geometry

If there is only one preferred direction  $\hat{\mathbf{a}}$  in a physical system, then there is only one way in which we can form a tensor of rank  $l$  from it, and that is through a spherical harmonic. Thus for any arbitrary tensor  $f_m^{(l)}$  associated with such a system, we must have

$$f_m^{(l)} = F_l Y_m^{(l)}(\hat{\mathbf{a}}), \quad (8)$$

where  $F_l$  is scalar coefficient. This is the case for planar systems, for example, where  $\hat{\mathbf{a}}$  defines the direction of field and gradient normal to the electrodes, taken to be the  $z$  axis for simplicity. After substituting in Eq. (2) and using the addition theorem for spherical harmonics (A5), we obtain the familiar Legendre polynomial expansion

$$f = \sum_{l=0}^{\infty} f_l(z, c, t) P_l(\cos \chi), \quad (9)$$

where  $\cos \chi = \hat{\mathbf{a}} \cdot \hat{\mathbf{c}}$  and  $f_l = [(2l+1)/4\pi] F_l$ . Although we could generate the equations for  $f_l(z, c, t)$  by substituting Eq. (8) into the general representation (3), the usual procedure (and the simplest one) is to substitute the expansion (9) directly into the Boltzmann equation (1), and to equate coefficients of Legendre polynomials. Either way we arrive at the familiar chain of equations,

$$\begin{aligned}\partial_c f_{l+} + \sum_{p=\pm 1} \Delta_l^{(p)} \left[ c \partial_z + a_z \left( \partial_c + p \frac{l + \frac{3p+1}{2}}{c} \right) \right] f_{l+p} \\ = -J_l(f_l) \quad (l=0,1,2, \dots, \infty),\end{aligned}\quad (10)$$

where the coefficients are defined by  $\Delta_l^{(+)} = (l+1)/(2l+3)$  and  $\Delta_l^{(-)} = l/(2l-1)$ .

### 2. Spherical geometry

Consider a plasma confined in a spherical container for which any fields and gradients are directed in the radial direction  $\hat{\mathbf{r}} \equiv \hat{\mathbf{a}}$  only. This forms an axis of rotational symmetry and therefore similar considerations apply as in the case of plane geometry. In particular, the distribution function can be represented by a Legendre polynomial expansion in terms of  $f_l(r, c, t)$  similar to Eq. (9). Upon substitution of this into the Boltzmann equation (1) the following hierarchy results:

$$\begin{aligned}\partial_r f_{l+} + \sum_{p=\pm 1} \Delta_l^{(p)} \left[ c \left( \partial_r + p \frac{l + \frac{3p+1}{2}}{r} \right) \right. \\ \left. + a_r \left( \partial_c + p \frac{l + \frac{3p+1}{2}}{c} \right) \right] f_{l+p} = -J_l(f_l) \\ (l=0,1,2, \dots, \infty).\end{aligned}\quad (11)$$

Note the symmetry with respect to interchange of  $c$  and  $r$  on the left-hand side in this case. A similar result was obtained previously by Sigeneer *et al.* [15]. In both cases described above, the number of equations and unknowns corresponding to truncation at  $l=l_{\max}$  is simply  $l_{\max}+1$ .

## III. CYLINDRICAL GEOMETRY

### A. Axial symmetry and tensor structure

Let  $\mathbf{r} = (\rho, \varphi, z)$  and  $\mathbf{c} = (c, \theta_c, \varphi_c)$  denote cylindrical coordinates in configuration space and spherical coordinates in velocity space, respectively. To make matters as simple as possible, we assume rotational symmetry about the axis of the cylinder, with no azimuthal field or gradients. However, this does *not* mean that the distribution of velocities also has this property, as was already pointed out in Ref. [1], since any radial field or gradient provides a preferred direction  $\hat{\boldsymbol{\rho}}$  in velocity space, in a plane perpendicular to the cylinder's axis, along which charged particles flow preferentially. In this case, the phase space distribution function must have the form

$$f(\mathbf{r}, \mathbf{c}, t) = f(\rho, z; c, \theta_c, \varphi_c - \varphi; t), \quad (12)$$

where the dependence upon the *difference* of the azimuthal angles reflects the requirement for invariance of the *shape* of the velocity distribution with respect to rotations about the axis of the cylinder. This has the immediate consequence that the tensor expansion coefficients must have the property

$$f_m^{(l)} = N_{lm} F_{l,m} e^{-im\varphi}, \quad (13)$$

where the factor

$$N_{lm} = (-i)^l (-1)^{(m+|m|)/2} \left( \frac{4\pi(l+|m|)!}{(2l+1)(l-|m|)!} \right)^{1/2}$$

has been extracted merely for convenience. The distribution function follows from Eqs. (2) and (13),

$$f = \sum_{l=0}^{\infty} \sum_{m=-l}^l F_{l,m}(\rho, z; c; t) P_l^{|m|}(\cos \theta_c) e^{im(\varphi_c - \varphi)}, \quad (14)$$

where  $P_l^{|m|}(\cos \theta_c)$  is an associated Legendre function (see Appendix), and  $f$  clearly has the functional dependence prescribed by Eq. (12). When Eq. (13) is substituted into the general hierarchy (3), it is found that the equations are invariant under the transformation  $m \rightarrow -m$  provided that

$$F_{l,-m} = F_{l,m}. \quad (15)$$

This very important result is simply a consequence of the symmetry of the distribution function in the  $c_x - c_y$  plane in directions normal to the radial vector  $\hat{\rho}$ , i.e., Eq. (14) can depend upon only the *magnitude* of  $\varphi_c - \varphi$ . This, together with properties of spherical harmonics [see Eq. (A1) of the Appendix], leads directly to Eq. (15). It means that *it is necessary to calculate  $F_{l,m}$  (and hence  $f_m^{(l)}$ ) with only non-negative values of  $m = 0, 1, 2, \dots, l$  in the axisymmetric case.* Note that from now on  $F_{l,m}$  will be considered the quantities of primary importance, and the hierarchy (3) will be expressed in terms of these quantities accordingly. In general, they are functions of speed, time, radial and axial coordinates, i.e.,

$$F_{l,m} = F_{l,m}(\rho, z; c; t), \quad (16)$$

although we shall not always make this dependence explicit.

## B. The quantities of physical interest

### 1. Moments

The moments of physical interest follow from Eqs. (4)–(7), (13), and (A8).

Number density:

$$n = 4\pi \int_0^{\infty} F_{0,0} c^2 dc. \quad (17)$$

Mean energy:

$$\epsilon = \frac{1}{n} 4\pi \int_0^{\infty} F_{0,0} \frac{1}{2} mc^4 dc. \quad (18)$$

Mean axial velocity:

$$v_z = \frac{1}{n} \frac{4\pi}{3} \int_0^{\infty} F_{1,0} c^3 dc. \quad (19)$$

Mean radial velocity:

$$v_\rho = \frac{1}{n} \frac{8\pi}{3} \int_0^{\infty} F_{1,1} c^3 dc. \quad (20)$$

Axial energy flux:

$$j_z = \frac{4\pi}{3} \int_0^{\infty} F_{1,0} \frac{1}{2} mc^5 dc. \quad (21)$$

Radial energy flux:

$$j_\rho = \frac{8\pi}{3} \int_0^{\infty} F_{1,1} \frac{1}{2} mc^5 dc. \quad (22)$$

To this list we add the following second rank tensor, whose physical meaning is the traceless part of the momentum flux:

$$\Pi = nm \left\langle \mathbf{cc} - \frac{c^2}{3} \mathbf{1} \right\rangle.$$

The connection with the spherical components of the distribution function may be found using Eqs. (49) and (50) of Ref. [16]. The nonzero components are then expressible in cylindrical components as follows:

$$\begin{aligned} \Pi_{\rho\rho} &= \alpha m \int_0^{\infty} [12F_{2,2} - F_{2,0}] c^4 dc, \\ \Pi_{zz} &= 2\alpha m \int_0^{\infty} F_{2,0} c^4 dc, \end{aligned} \quad (23)$$

$$\Pi_{\rho z} = \Pi_{z\rho} = 6\alpha m \int_0^{\infty} F_{2,1} c^4 dc,$$

$$\Pi_{\varphi\varphi} = -\Pi_{zz} - \Pi_{\rho\rho},$$

where  $\alpha = 4\pi/15$ .

All these integral quantities are in general functions of  $z$ ,  $\rho$ , and  $t$ . One evaluates the integrals over speeds  $c$  after solving the hierarchy of equations below for  $F_{l,m} \equiv F_{l,m}(\rho, z; c; t)$ .

### 2. Balance equations

Before proceeding to the hierarchy of equations for the  $F_{l,m}$ , it is interesting to write down the balance equations for the above moments. These have an existence independent of the Boltzmann equation and are very useful in serving to provide an integral consistency check for any tensor representation. Thus quite generally we have the following equations [17].

(i) The equation of continuity:

$$\partial_t n + \frac{1}{\rho} \partial_\rho (\rho n v_\rho) + \partial_z (n v_z) = -R_{coll}. \quad (24)$$

(ii) The energy balance equation:

$$\begin{aligned} \partial_t(n\epsilon) + \frac{1}{\rho} \partial_\rho(\rho n j_\rho) + \partial_z(n j_z) - n q v_\rho E_\rho - n q v_z E_z \\ = -R_{coll}^\epsilon. \end{aligned} \quad (25)$$

(iii) Radial momentum balance equation:

$$\begin{aligned} \partial_t(n m v_\rho) + \frac{2}{3} \partial_\rho(n \epsilon) - n q E_\rho + \left( \partial_\rho + \frac{2}{\rho} \right) \Pi_{\rho\rho} + \frac{\Pi_{zz}}{\rho} + \partial_z \Pi_{\rho z} \\ = -R_{\rho, coll}. \end{aligned} \quad (26)$$

(iv) Axial momentum balance equation:

$$\begin{aligned} \partial_t(n m v_z) + \frac{2}{3} \partial_z(n \epsilon) - n q E_z + \left( \partial_\rho + \frac{1}{\rho} \right) \Pi_{\rho z} + \partial_z \Pi_{zz} \\ = -R_{z, coll}. \end{aligned} \quad (27)$$

In these equations the terms on the right-hand side represent the rate of loss of particle number, energy, radial and axial components of momentum, respectively.

### 3. Collision loss terms

We now express the right-hand side of each of the above balance equations in terms of the spherical components of the distribution function and the corresponding spherical components of the collision operator.

(i) Rate of particle loss:

$$R_{coll} = \int J(f) d\mathbf{c} = 4\pi \int_0^\infty J_0(F_{0,0}) c^2 dc. \quad (28)$$

(ii) Rate of loss of energy:

$$R_{coll}^\epsilon = \int \frac{1}{2} m c^2 J(f) d\mathbf{c} = 4\pi \int_0^\infty \frac{1}{2} m c^4 J_0(F_{0,0}) dc. \quad (29)$$

(iii) Rate of loss of momentum:

$$\mathbf{R}_{coll} = \int m \mathbf{c} J(f) d\mathbf{c} = R_{\rho, coll} \hat{\boldsymbol{\rho}} + R_{z, coll} \hat{\mathbf{z}},$$

where the radial and axial components are given by

$$\begin{aligned} R_{\rho, coll} &= \frac{8\pi}{3} \int_0^\infty m c^3 J_1(F_{1,1}) dc, \\ R_{z, coll} &= \frac{4\pi}{3} \int_0^\infty m c^3 J_1(F_{1,0}) dc, \end{aligned} \quad (30)$$

respectively.

### C. The hierarchy of equations for $F_{l,m}$

As mentioned previously, Eqs. (3) apply to any geometry. The gradient tensor and field terms can be found from Table I of Ref. [1], and for the special case of cylindrical coordinates  $(\rho, \varphi, z)$  are

$\mu$	$G_\mu^{(11)}$	$a_\mu^{(1)}$	
0	$-i\partial_z$	$-ia_z$	
+1	$\frac{e^{-i\varphi}}{\sqrt{2}} \left( i\partial_\rho + \frac{1}{\rho} \partial_\varphi \right)$	$\frac{ia_\rho}{\sqrt{2}} e^{-i\varphi}$	
-1	$\frac{e^{i\varphi}}{\sqrt{2}} \left( -i\partial_\rho + \frac{1}{\rho} \partial_\varphi \right)$	$\frac{-ia_\rho}{\sqrt{2}} e^{i\varphi}$	(31)

where  $a_z = qE_z/m$  and  $a_\rho = qE_\rho/m$  denote axial and radial field terms, respectively. Even though there is axial symmetry in configuration space, it is essential to retain the azimuthal derivatives  $\partial_\varphi$  when dealing with the distribution function, as explained in Sec. III A. The general spherical harmonic representation of Boltzmann's equation is converted into one appropriate for cylindrical geometry by substitution of Eqs. (13) and (31) into Eq. (3):

$$\begin{aligned} \partial_t F_{l,m} + \sum_{l'} i^{-1} \frac{N_{l'm}}{N_{lm}} (l' m 10 | lm) \langle l \| c^{[1]} \| l' \rangle \partial_z F_{l',m} + \frac{1}{\sqrt{2}} \sum_{l'} i \frac{N_{l'm-1}}{N_{lm}} (l' m - 1 11 | lm) \langle l \| c^{[1]} \| l' \rangle \\ \times \left[ \partial_\rho - \frac{m-1}{\rho} \right] F_{l',m-1} + \frac{1}{\sqrt{2}} \sum_{l'} i^{-1} \frac{N_{l'm+1}}{N_{lm}} (l' m + 1 1 - 1 | lm) \langle l \| c^{[1]} \| l' \rangle \left[ \partial_\rho + \frac{m+1}{\rho} \right] F_{l',m+1} \\ + a_z \sum_{l'} i^{-1} \frac{N_{l'm}}{N_{lm}} (l' m 10 | lm) \langle l \| \partial_c^{[1]} \| l' \rangle F_{l',m} + \frac{a_\rho}{\sqrt{2}} \sum_{l'} i \frac{N_{l'm-1}}{N_{lm}} (l' m - 1 11 | lm) \langle l \| \partial_c^{[1]} \| l' \rangle F_{l',m-1} \\ + \frac{a_\rho}{\sqrt{2}} \sum_{l'} i^{-1} \frac{N_{l'm+1}}{N_{lm}} (l' m + 1 11 | lm) \langle l \| \partial_c^{[1]} \| l' \rangle F_{l',m+1} = -J_l(F_{l,m}) \quad (l=0,1,2,\dots,\infty; \quad m=0,1,2,\dots,l). \end{aligned} \quad (32)$$

If the expansion and hierarchy are truncated at  $l=l_{\max}$ , there results  $N=\frac{1}{2}(l_{\max}+2)(l_{\max}+1)$  equations and the same number of unknowns. The above can be written in a far more concise form after substituting for the reduced matrix elements and Clebsch-Gordan coefficients,

$$\begin{aligned} \partial_t F_{l,m} + \sum_{p=\pm 1} \Delta_{lm}^{(p,0)} \left[ c \partial_z + a_z \left( \partial_c + p \frac{l + \frac{3p+1}{2}}{c} \right) \right] F_{l+p,m} \\ + \sum_{p=\pm 1, q=\pm 1} \Delta_{lm}^{(p,q)} \left[ c \left( \partial_\rho + q \frac{(m+q)}{\rho} \right) \right. \\ \left. + a_\rho \left( \partial_c + p \frac{l + \frac{3p+1}{2}}{c} \right) \right] F_{l+p,m+q} = -J_l(F_{l,m}) \end{aligned} \quad (l=0,1,2,\dots,\infty; \quad m=0,1,2,\dots,l), \quad (33)$$

where the coefficients are defined below:

$$\begin{aligned} \Delta_{lm}^{(+,0)} &= \frac{l+m+1}{2l+3}, \quad \Delta_{lm}^{(-,0)} = \frac{l-m}{2l-1}, \\ \Delta_{lm}^{(+,+)} &= \frac{(l+m+2)(l+m+1)}{2(2l+3)}, \quad \Delta_{lm>0}^{(+,-)} = -\frac{1}{2(2l+3)}, \\ \Delta_{l0}^{(+,-)} &= \frac{(l+1)(l+2)}{2(2l+3)}, \\ \Delta_{lm}^{(-,+)} &= -\frac{(l-m-1)(l-m)}{2(2l-1)}, \quad \Delta_{lm>0}^{(-,-)} = \frac{1}{2(2l-1)}, \\ \Delta_{l0}^{(-,-)} &= -\frac{l(l-1)}{2(2l-1)}. \end{aligned}$$

It is clear that field and gradient terms step the  $l$  index by  $\pm 1$ . However, while the axial field and gradient leave the  $m$  index unchanged, the radial field and gradient each step the  $m$  index by  $\pm 1$ . It is implicit in these equations that any term  $F_{l,m}$  for which  $m>l$  should be set to zero, and that any coefficient with  $m<0$  should be related to its counterpart with positive  $m$  through Eq. (15).

By multiplying the  $(l,m)=(0,0)$  member of the hierarchy in succession by  $4\pi$  and  $4\pi\frac{1}{2}mc^2$  and integrating over all speeds  $c$ , we obtain the equations of continuity and energy balance (24) and (25), respectively. If the  $(l,m)=(1,1)$  and  $(1,0)$  members are multiplied by  $(8\pi/3)mc$  and  $(4\pi/3)mc$ , respectively, and integrated over all speeds  $c$ , the radial and axial momentum balance equations (26) and (27) are regained. Such consistency considerations are important for establishing the integrity of the hierarchy.

#### D. Radial field and gradient only

Suppose now there is neither axial field nor axial gradient, with the field and any spatial dependence being entirely in

the radial direction  $\hat{\rho}$ . We cannot take  $F_{l,m}$  as simply proportional to a spherical harmonic with  $\hat{\rho}$  as its argument, since all directions are *not* equivalent with respect to rotations about the radial direction. In other words, a Legendre polynomial representation of  $f$  in velocity space does not suffice. The only simplification we can make is through the observation that the distribution of velocities (14) must be invariant under a reflection through the  $x$ - $y$  plane, i.e.,  $f$  does not change under the transformation  $\theta_c \rightarrow \pi - \theta_c$  or simply  $\cos \theta_c \rightarrow -\cos \theta_c$ . The properties of the Legendre functions [see Eq. (A2) of the Appendix] then lead to the result

$$F_{l,m} = (-1)^{l+m} F_{l,m}, \quad (34)$$

or, in other words,

$$l+m = \text{even}. \quad (35)$$

If one omits the  $z$ -dependent terms in the general hierarchy (33), we find that the resulting chain of equations separates into two subsystems, coupling  $F_{l,m}$  for which  $l+m$  is even or odd, respectively. The condition (35) tells us then that we need only consider the former, as the latter are identically zero. We have then

$$\begin{aligned} \partial_t F_{l,m} + \sum_{p=\pm 1, q=\pm 1} \Delta_{lm}^{(p,q)} \left[ c \left( \partial_\rho + q \frac{(m+q)}{\rho} \right) \right. \\ \left. + a_\rho \left( \partial_c + p \frac{l + \frac{3p+1}{2}}{c} \right) \right] F_{l+p,m+q} \\ = -J_l(F_{l,m}) \end{aligned} \quad (l=0,1,2,\dots,\infty; \quad m=0,1,2,\dots,l; \quad l+m = \text{even}), \quad (36)$$

which is a hierarchy of equations for the quantities  $F_{0,0}, F_{1,1}, F_{2,2}, F_{2,0}, \dots$ , from which all quantities of physical interest can be found directly from Sec. III B. For example, the first two members of the hierarchy are

$$\partial_t F_{0,0} + \frac{2}{3} \left[ \frac{c}{\rho} \partial_\rho (\rho F_{1,1}) + \frac{a_\rho}{c^2} \partial_c (c^2 F_{1,1}) \right] = -J_0(F_{0,0}) \quad (37)$$

and

$$\begin{aligned} \partial_t F_{1,1} + \frac{1}{2} [c \partial_\rho F_{0,0} + a_\rho \partial_c F_{0,0}] + \frac{6}{5} \left[ \frac{c}{\rho^2} \partial_\rho (\rho^2 F_{2,2}) \right. \\ \left. + \frac{a_\rho}{c^3} \partial_c (c^3 F_{2,2}) \right] - \frac{1}{10} \left[ c \partial_\rho F_{2,0} + \frac{a_\rho}{c^3} \partial_c (c^3 F_{2,0}) \right] \\ = -J_1(F_{1,1}). \end{aligned} \quad (38)$$

After appropriate moments of these equations are taken with respect to speed, there follow the equations of continuity, energy, and (radial) momentum balance, as shown in Sec. III B (axial terms vanish).

The next two members of the hierarchy, corresponding to  $l=2, m=0$  and  $l=2, m=2$ , are, respectively,

$$\begin{aligned} \partial_t F_{2,0} + \frac{12}{7} \left[ \frac{c}{\rho} \partial_\rho (\rho F_{3,1}) + \frac{a_\rho}{c^4} (c^4 F_{3,1}) \right] - \frac{2}{3} \left[ \frac{c}{\rho} \partial_\rho (\rho F_{1,1}) \right. \\ \left. + c a_\rho \partial_c \left( \frac{F_{1,1}}{c} \right) \right] = -J_2(F_{2,0}) \end{aligned} \quad (39)$$

and

$$\begin{aligned} \partial_t F_{2,2} + \frac{15}{7} \left[ \frac{c}{\rho^3} \partial_\rho (\rho^3 F_{3,3}) + \frac{a_\rho}{c^4} (c^4 F_{3,3}) \right] - \frac{1}{14} \left[ c \rho \partial_\rho \left( \frac{F_{3,1}}{\rho} \right) \right. \\ \left. + \frac{a_\rho}{c^4} \partial_c (c^4 F_{3,1}) \right] + \frac{1}{6} \left[ c \rho \partial_\rho \left( \frac{F_{1,1}}{\rho} \right) + c a_\rho \partial_c \left( \frac{F_{1,1}}{c} \right) \right] \\ = -J_2(F_{2,2}). \end{aligned} \quad (40)$$

Lower-order equations are obviously coupled to higher equations in both  $l$  and  $m$  indices and truncation to finite size is required to effect a solution. In the “ $l_{\max}+1$  term approximation” we set  $F_{l,m}=0$ ,  $m=0,1,2,\dots,l$ , for all  $l>l_{\max}$ . Thus, for example, for  $l_{\max}=3$ , one has all the above equations and the final two

$$\begin{aligned} \partial_t F_{3,1} - \frac{1}{5} \left[ \frac{c}{\rho^2} \partial_\rho (\rho^2 F_{2,2}) + c^2 a_\rho \partial_c \left( \frac{F_{2,2}}{c^2} \right) \right] \\ + \frac{1}{10} \left[ c \partial_\rho F_{2,0} + c^2 a_\rho \partial_c \left( \frac{F_{2,0}}{c^2} \right) \right] = -J_3(F_{3,1}), \end{aligned} \quad (41)$$

$$\partial_t F_{3,3} + \frac{1}{10} \left[ c \rho^2 \partial_\rho \left( \frac{F_{2,2}}{\rho^2} \right) + c^2 a_\rho \partial_c \left( \frac{F_{2,2}}{c^2} \right) \right] = -J_3(F_{3,3}), \quad (42)$$

making a total of six equations in six unknowns. In general, for truncation at  $l=l_{\max}$  there are either  $N=\frac{1}{4}(l_{\max}+1)(l_{\max}+3)$  or  $N=\frac{1}{4}(l_{\max}+2)^2$  such quantities and equations, depending upon whether  $l_{\max}$  is odd or even, respectively.

In this scheme, the values of  $m$  are automatically limited once an upper bound is placed upon  $l$ , and there is no need for any further truncation condition. However, for practical purposes, and based upon the experience for electrons in crossed electric and magnetic fields [2,3], separate truncation in  $m$  may prove to be worthwhile. This would reduce the number of equations and the corresponding time required to effect a numerical solution. However, we have reached the end of what can be done analytically, and there are no more symmetries to be exploited. That is, no further reduction is possible, and nothing further can be said without specification of the plasma configuration, including initial and boundary conditions, and an appropriate method of numerical solution of the equations.

Special cases of both hierarchy equation systems (33) and (36) related to the cylindrical plasma geometry have already

been reported over the last decade, but these have mostly been limited to the two-term approximation, obtained by truncation of the hierarchy of equations (33) taking  $F_{l,m}=0$  for  $l \geq 2$  and for all corresponding  $m$ . In recent studies of plasma kinetics [18] the further simplification to time-independent states and axial uniformity has made for a stationary, one spatial dimension problem. The calculations were carried out with a view to model the radially dependent electron properties in the plasma column of cylindrical dc glow discharges. The two-term treatment was recently extended [19] to include two spatial dimensions, with axial as well as radial space dependence, and in this way a study of axial relaxation processes in a dc plasma column, with radial space-charge confinement of electrons was made possible. Furthermore, we note that a very recent multiterm treatment using Cartesian tensors and Mathematica [12], dealing with the special case of radial fields and gradients only, has been developed to study the effect of increasing the order of approximation on the electron kinetics in specific cylindrical hollow cathodes. A hierarchy of Cartesian tensor equations to rank 5 was generated with the help of Mathematica, which has been checked up to rank 3 to be fully equivalent to the truncated ( $l_{\max}=3$ ) hierarchy (37)–(42). In contrast, the spherical tensor-based hierarchies (33) and (36) are completely specified in a straightforward way to *all* orders, and are thus in a form suitable for immediate coding for computational purposes.

#### IV. CONCLUDING REMARKS

This paper started with a very general, infinite hierarchy of integrodifferential equations (3), representing Boltzmann’s equation for any charged species in a weakly ionized plasma, obtained by decomposition of the corresponding phase space distribution function in velocity directions, using spherical harmonics and spherical tensor notation [1,16]. As in Ref. [1] the goal has been to lay the foundations for future numerical calculations, by deriving the simplest possible set of equations, involving the maximum number of independent variables consistent with the geometry at hand, and to do this in the most transparent and general way possible. Unlike analysis of the hydrodynamic regime, where spatial and temporal dependence is projected onto a different level (using, for example, a density gradient expansion [5]), the present paper treats configuration and velocity space on an equal footing, and is therefore suitable for *nonhydrodynamic* situations.

First of all we briefly considered two relatively simple cases, corresponding to plane parallel and spherical geometry, respectively, where a Legendre polynomial expansion suffices to represent the distribution function, with a corresponding simplified hierarchy of equations for the expansion coefficients. Then we moved on to the more interesting case of an axisymmetric, cylindrical column of plasma, and derived the corresponding hierarchy of equations (33) for the components of the distribution function, from which all quantities of physical interest may be derived. When there is neither axial field nor axial gradient a significantly simplified hierarchy (36) results.

These spherical tensor-based equations are very general, and can be solved with standard forms of the collision operators  $J_l$ , incorporating all types of binary charged particle–gas molecule interactions [4–6], once further representations in configuration and speed (or energy) space are made, and the temporal dependence dealt with accordingly. Any desired numerical technique can be used in this respect. For example, for electrons, for which the  $J_l$  can be considerably simplified [4,5,9], a finite difference representation in speed space, similar to the one that has met with great success for planar geometry [9,20], could be employed. Sonine polynomial decomposition in speed space (leading to an overall representation in terms of Burnett functions in velocity space) is another option for both electrons and ions [21]. Quantities of physical interest can then be obtained as integrals of the solutions of these equations according to Eqs. (17)–(23).

We have highlighted the practical advantages that these spherical tensor-based equations offer over existing Cartesian counterparts, which have so far only been generated for relatively low orders with the aid of Mathematica and for the specific case of axial homogeneity. In contrast, the hierarchies (33) and (36) are ready for immediate coding to any desired order in numerical applications. A reformulation in terms of Cartesian tensors with only two indices [22] could also be an interesting alternative.

Looking to the future, one sees the need for a multiterm representation of the *nonlinear* Boltzmann equation, which arises in cases where the degree of ionization is such that Coulomb collisions between charged particles can no longer be neglected. There are two important general considerations here.

(i) First, from the point of view of the mathematical reformulation, we emphasize that since the symmetries in velocity and configuration space are unaltered, the complete left-hand side of the kinetic equation, plus the linear charge particle–neutral collision term on the right-hand side, as shown in the present paper, remain intact—it is the spherical harmonic representation of the new nonlinear collision terms on the right-hand side that requires attention. In performing the corresponding tensor analysis we might expect to again usefully draw on the results of Kumar [16], who has given an exact representation of the nonlinear Boltzmann elastic collision operator in the Burnett function basis, using the Talmi transformation. An alternative approach, without the Talmi transformation, and using a representation of the velocity distribution function in terms of generalized tensor Hermite polynomials, has been given by Suchy [23].

(ii) Second, a note of warning must be given when it comes to approximating the charge-charge Boltzmann collision operator by a Fokker-Planck operator. If the velocity distribution is nearly isotropic, making the two-term approximation reasonable, use of the Fokker-Planck operator seems perfectly in order. Such cases have been treated recently [24,25]. However, when the distribution function is anisotropic, necessitating the use of multiterm analysis, there is a question mark over the accuracy of the Fokker-Planck operator, as it neglects contributions from higher- $l$  terms [26]. Discussion of both these points is left to a future paper.

In summary, this paper both complements and generalizes the multiterm, hydrodynamic formulation for swarms given in Ref. [1]. Just as the latter work laid the foundation for many subsequent numerical calculations of transport coefficients for both ions and electron swarms (see the review by White *et al.* [3]), it is hoped that the present paper will be helpful for future applications to low-temperature plasmas.

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## APPENDIX

### 1. Notes on the use of irreducible spherical tensors

It is generally accepted that the equations of physics take their simplest form when expressed as relations between irreducible tensorial sets, and that such representation is very useful for exploitation of any symmetries that might prevail. If one follows this prescription, one expects to obtain equations that involve the minimum possible number of independent quantities required to describe the system, thus enhancing both the transparency of the theory for purposes of physical insight, and the economy of subsequent computational effort. The standard reference on the subject is the treatise by Fano and Racah [13]. While Cartesian irreducible tensors are still sometimes used in kinetic theory [11,12], they appear unwieldy when dealing with quantities of even moderately high rank, and spherical tensors  $f_m^{(l)}$  seem to offer greater advantages. This is because there are only two indices  $l=0,1,2,3,\dots$  and  $m=-l,\dots,l$  to contend with, whatever the rank  $l$ , whereas with Cartesian tensors the number of indices usually increases with the rank. In addition, transformations under rotations of the coordinate frame are most concisely expressed in the spherical format. Note, however, that it is also possible to formulate Cartesian tensors in such a way that only two indices appear [22], and a representation of the Boltzmann's equation in this basis may also be possible. It is to be emphasized that the difference between the two types of tensorial formulations is one of practicality and economy, rather than of principle.

Spherical tensors were originally a product of atomic and nuclear physics, and found their way into the kinetic theory of gases in the mid 1960s, in a series of papers by Kumar [16,27], who discussed the connection between spherical and Cartesian tensors. However, he confined the applications to near equilibrium situations and to the Chapman-Enskog method of solution of the Boltzmann equation in particular. Since that time irreducible spherical tensors have become an integral part of the kinetic theory of charged particles in gaseous media far from equilibrium. The theory of electron transport in the hydrodynamic regime, for so long confined by the limitations of representation of the velocity distribution function by only the first two terms of a spherical harmonic expansion [4], has in particular blossomed with the aid of irreducible tensorial set theory, to the point where nowadays the coupling and recoupling of fields and gradients



in multiterm analysis of the Boltzmann equation is carried out as a matter of course in computation of hydrodynamic transport coefficients [1–3].

## 2. Tensor notation and identities

The tensor formalism and convention followed here is set out in detail by Fano and Racah [13], in the papers by Kumar [16,17], and in the key reference [1], and only essential definitions will be given here. A contrastandard tensor  $f_m^{[l]}$  of rank  $l$  is a set of  $2l+1$  objects ( $m = -l, \dots, l$ ), which transform under rotations of the coordinate frame like a spherical harmonic,

$$Y_m^{[l]}(\theta, \varphi) = i^l (-1)^{(m+|m|)/2} \left( \frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!} \right)^{1/2} \times P_l^{|m|}(\cos \theta) e^{im\varphi},$$

where the associated Legendre functions are defined by

$$P_l^{|m|}(\cos \theta) = \frac{(-1)^l}{2^l l!} (\sin \theta)^{|m|} \frac{d^{l+|m|}}{d \cos \theta^{l+|m|}} (1 - \cos^2 \theta)^l.$$

It can be seen from these definitions that

$$Y_{-m}^{[l]}(\theta, 0) = (-1)^m Y_m^{[l]}(\theta, 0) \quad (\text{A1})$$

and

$$P_l^{|m|}(-\cos \theta) = (-1)^{l+m} P_l^{|m|}(\cos \theta) \quad (\text{A2})$$

are identities that have been used in obtaining Eqs. (14) and (25), respectively. Normally we abbreviate the angular dependence by writing  $\hat{\mathbf{r}} = (\theta, \varphi)$  and denote the spherical harmonic accordingly by  $Y_m^{[l]}(\hat{\mathbf{r}})$ . The corresponding standard tensor is simply the complex conjugate, and is denoted by

$$f_m^{(l)} = f_m^{[l]*}.$$

We can have tensor *operators*, for example, the gradient operator  $G_\mu^{(s,l)}$  defined by equation (31) and Table I of Ref. [1]. Any two tensors,  $f_{m_1}^{[l_1]}$  and  $g_{m_2}^{[l_2]}$  can be coupled according to the prescription

$$(f_{m_1}^{[l_1]}, g_{m_2}^{[l_2]})_m^{[l]} = \sum_{m_1, m_2} (l_1 m_1 l_2 m_2 | l m) f_{m_1}^{[l_1]} g_{m_2}^{[l_2]}, \quad (\text{A3})$$

where the sum is over all allowed values of the  $m$  indices and  $(l_1 m_1 l_2 m_2 | l m)$  is a Clebsch-Gordan or Wigner coefficient, which vanishes unless  $m = m_1 + m_2$  and  $l_1 + l_2 \geq l \geq |l_1 - l_2|$ . These coefficients have orthogonality properties that are outlined in many textbooks on angular momentum theory as well as in Refs. [1] and [16], and are tabulated for lower orders by Condon and Shortley [14].

When two spherical harmonics of the same argument are coupled, the result is another spherical harmonic,

$$[Y^{[l_1]}(\hat{\mathbf{r}}), Y^{[l_2]}(\hat{\mathbf{r}})]_m^{[l]} = \sigma(l_1, l_2, l) Y_m^{[l]}(\hat{\mathbf{r}}), \quad (\text{A4})$$

where

$$\sigma(l_1, l_2, l) = i^{l_1 + l_2 - l} \left( \frac{(2l_1 + 1)(2l_2 + 1)}{4\pi(2l + 1)} \right)^{1/2} (l_1 0 l_2 0 | l 0).$$

In deriving Eq. (9) we used the addition theorem for spherical harmonics,

$$P_l(\hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2) = \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_m^{(l)}(\hat{\mathbf{r}}_1) Y_m^{[l]}(\hat{\mathbf{r}}_2). \quad (\text{A5})$$

The standard spherical components of an arbitrary vector  $\mathbf{a}$  are represented by

$$a_m^{(1)} = \sqrt{\frac{4\pi}{3}} a Y_m^{[1]}(\hat{\mathbf{a}}), \quad m = 0, \pm 1 \quad (\text{A6})$$

and are related to Cartesian components by

$$a_0^{(1)} = -i a_z,$$

$$a_{\pm 1}^{(1)} = \frac{1}{\sqrt{2}} (\pm i a_x + a_y), \quad (\text{A7})$$

while for cylindrical coordinates

$$a_{\pm 1}^{(1)} = \pm \frac{i a e^{\mp i \varphi}}{\sqrt{2}}. \quad (\text{A8})$$

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