# **Anisotropy of the electron component in a cylindrical magnetron discharge. I. Theory of the multiterm analysis**

I. A. Porokhova, $^{1,2}$  Yu. B. Golubovskii,<sup>1</sup> and J. F. Behnke<sup>2</sup>

1 *Saint-Petersburg State University, Ulianovskaia, 1, 198504, St. Petersburg, Russia*

2 *EMA-University, Greifswald, Domstrasse 10a, 17487 Greifswald, Germany*

(Received 23 May 2004; revised manuscript received 29 November 2004; published 22 June 2005)

A general multiterm representation of the phase space electron distribution function in terms of spherical tensors is used to solve the Boltzmann kinetic equation in crossed electric and magnetic fields. The problem is formulated for an axisymmetric cylindrical magnetron discharge with the homogeneous magnetic field being directed axially and the electric field between the coaxial cathode and anode varying in radius only. A spherical harmonic representation of the velocity distribution function in Cartesian coordinates becomes especially cumbersome in the presence of the magnetic field. In contrast, the employment of a spherical tensor representation leads to a compact hierarchy of equations that accurately take into account the spatial inhomogeneities and anisotropy of the plasma in crossed fields. To describe the spatially inhomogeneous plasma the hierarchy of the kinetic equations is formulated in terms of the total energy and the radial coordinate. Appropriate boundary conditions at the electrodes for the tensor expansion coefficients are obtained.

DOI: 10.1103/PhysRevE.71.066406 PACS number(s): 52.25.Dg, 52.25.Fi, 52.25.Xz

# **I. INTRODUCTION**

Owing to their various practical applications in creating and etching thin films, magnetron sputtering discharges remain the focus of many experimental and theoretical studies. To simulate the physical processes in magnetron discharges various hydrodynamic  $[1,2]$ , particle-in-cell (PIC) Monte Carlo  $[3-5]$ , and hybrid methods  $[6]$  have been developed as well as the nonhydrodynamic methods based on the solution of the Boltzmann nonlocal kinetic equation  $[7]$ .

A detailed description of the nonlocal nonhydrodynamic behavior of electrons in a spatially inhomogeneous plasma by a strict kinetic analysis can be reached by two alternative ways: the first way is to use PIC MCC (Monte-Carlo collisions) methods, and the second way is to solve the Boltzmann kinetic equation by decomposition of the phase space distribution function using orthogonal functions or small parameters. Particle simulation techniques have proved their efficiency and flexibility for complicated configurations of fields and plasma geometries. Their disadvantages are connected mainly with large numerical expenditures required to reduce the statistical fluctuations in order to obtain detailed information about the velocity distribution function. Decomposition methods are usually limited to a simple geometry but require essentially smaller calculation expenditures and give detailed and stable solutions.

The electron distribution function in an inert gas discharge plasma is weakly anisotropic, if the ratio of the directed to average velocities is small. In such cases a description based upon the two-term decomposition of the Boltzmann equation is sufficient. This is the situation for the positive column in inert gases. In the cathode region, where the energy losses in inelastic collisions strongly exceed those in elastic impacts, and in the anode region, where electrons fall on the absorbing surface, the distribution becomes anisotropic and multi-term expansion treatments (or MCC methods) are required. For many molecular gases, as for ions, the distribution function is strongly anisotropic in general  $[8]$ . Running a few steps forward, we note that the multiterm analysis presented in Secs. II–V is valid for both electrons and ions.

A comprehensive theoretical analysis of the spatially inhomogeneous Boltzmann kinetic equation in electric and magnetic fields is given in Refs.  $[9,10]$  using Cartesian tensors to decompose the phase space distribution function. However, direct applications of these theories seemed impossible. Robson and Ness  $[11]$  suggested decomposing the distribution function and the Boltzmann kinetic equation in a spherical harmonics series in velocity space, with the expansion coefficients being the spherical tensors. An infinite hierarchy of equations for the tensor coefficients was obtained for electric  $\lceil 11 \rceil$  and magnetic field  $\lceil 12 \rceil$  situations and applied then to hydrodynamic description of charged-particle swarms  $[13,14]$ .

In a recent paper  $\lceil 15 \rceil$  the multiterm theory  $\lceil 11 \rceil$  was reformulated and generalized to nonhydrodynamic plasma conditions. Chains of equations for the distribution function expansion coefficients in the presence of electric field and gradients were obtained for the plane, spherical, and cylindrical geometries. This formed the basis for nonhydrodynamic nonlocal multiterm studies of low-temperature plasmas.

In the present study the multiterm spherical tensor representation developed in  $[15]$  for cylindrical discharges is extended, using the results of Ref.  $[12]$ , to include a magnetic field. This nonhydrodynamic theory is used to describe anisotropic phenomena in a cylindrical magnetron discharge in an axially uniform magnetic field and a radially nonuniform electric field. The obtained hierarchy of the kinetic equations for the tensor expansion coefficients of the electron distribution function in crossed electric and magnetic fields accurately takes into account the spatial inhomogeneities of plasma, contains a reasonable number of equations, and can be solved numerically. Macroscopic quantities including second and third rank tensors for momentum and energy fluxes are discussed. The important problem of appropriate setting of boundary conditions for expansion coefficients with even and odd indices *l* is considered for the cylindrical geometry and the tensor formalism used. In the following paper the general theory developed here is applied to a real magnetron discharge in argon, and the anisotropy visualizations are illustrated on particular examples.

#### **II. THE BASIC EQUATIONS**

The Boltzmann kinetic equation for the phase space distribution function  $f(\mathbf{r}, \mathbf{v}, t)$  of charged particles has the following form:

$$
[\partial_t + \mathbf{v} \cdot \partial_{\mathbf{r}} + (\mathbf{a} + \mathbf{v} \times \mathbf{\Omega}) \cdot \partial_{\mathbf{v}}] f(\mathbf{r}, \mathbf{v}, t) = -J(f), \qquad (1)
$$

where  $\mathbf{a}=e\mathbf{E}/m_{\alpha}$  is the acceleration of a particle with the mass  $m_{\alpha}$  and charge *e* in the electric field **E**, and  $\Omega$  $=$ *e***B**/ $m_\alpha$  is the frequency of the cyclotron rotation in the magnetic field **B**. The collision operator *J* characterizes the rate of change of the function *f* due to collisions of charged particles with neutral atoms. The plasma is assumed to be weakly ionized, so that the collisions between charged particles are negligible.

The multiterm representation  $[11]$  of the Boltzmann equation starts with the following decomposition of the phase space distribution function  $f(\mathbf{r}, \mathbf{v}, t)$  in terms of spherical harmonics in velocity space with the basis of spherical coordinates  $\mathbf{v}=(v,\varphi_v,\theta_v)$ :

$$
f(\mathbf{r}, \mathbf{v}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_m^{(l)}(\mathbf{r}, v, t) Y_m^{[l]}(\mathbf{v}/v),
$$
 (2)

where  $l=0,1,2...$ , $\infty$ ,  $m=-l,...,l$ . According to the tensor formalism of Fano and Racah [11,16] a standard tensor  $f_m^{(l)}$  is the complex conjugate of the contrastandard irreducible tensor  $f_m^{[l]}$  of rank *l* whose  $2l+1$  objects transform under rotations of the coordinate frame like the spherical harmonics

$$
Y_m^{[l]}(\mathbf{v}/v) = i^l(-1)^{(m+|m|)/2} \left[ \frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!} \right]^{1/2}
$$

$$
\times P_l^{|m|}(\cos \theta_v) e^{im\varphi_v},
$$

with the associated Legendre functions defined by

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

The spherical components of an arbitrary vector **b** can be written in terms of the spherical harmonics as

$$
b_m^{(1)} = \sqrt{\frac{4\pi}{3}} b Y_m^{(1)}(\mathbf{b}/b), \quad m = 0, \pm 1. \tag{3}
$$

The spherical components of the velocity vector

$$
v_0^{(1)} = -iv P_1^0(\cos \theta_v),
$$
  

$$
v_1^{(1)} = iv P_1^1(\cos \theta_v)e^{-i\varphi_v}/\sqrt{2},
$$

$$
v_{-1}^{(1)} = -iv P_1^1(\cos \theta_v) e^{i\varphi_v}/\sqrt{2}
$$

are related to the Cartesian basis of configuration space  $(x, y, z)$  by

$$
v_z = v \cos \theta_v = iv_0^{(1)},
$$
  

$$
v_x = v \sin \theta_v \cos \varphi_v = -i[v_1^{(1)} - v_{-1}^{(1)}]/\sqrt{2},
$$
  

$$
v_y = v \sin \theta_v \sin \varphi_v = [v_1^{(1)} + v_{-1}^{(1)}]/\sqrt{2},
$$

and to the basis of cylindrical coordinates  $(r, \varphi, z)$  by

$$
v_r = v_x \cos \varphi + v_y \sin \varphi
$$
  
=  $-i[v_1^{(1)} e^{i\varphi} - v_{-1}^{(1)} e^{-i\varphi}]/\sqrt{2}$   
=  $\frac{v}{2} P_1^1(\cos \theta_v) (e^{-i(\varphi_v - \varphi)} + e^{i(\varphi_v - \varphi)}),$  (4)

$$
v_{\varphi} = -v_x \sin \varphi + v_y \cos \varphi
$$
  
=  $[v_1^{(1)} e^{i\varphi} + v_{-1}^{(1)} e^{-i\varphi}]/\sqrt{2}$   
=  $i\frac{\nu}{2} P_1^1(\cos \theta_v) (e^{-i(\varphi_v - \varphi)} - e^{i(\varphi_v - \varphi)}),$  (5)

$$
v_z = v_z = iv_0^{(1)} = vP_1^0(\cos \theta_v).
$$
 (6)

According to papers by Robson and Ness  $[11,12]$ , decomposition of the Boltzmann equation using the multiterm representation of  $f$  in the form of expansion  $(2)$  is performed in the following way.

The presence of a magnetic field is described by the operator  $\mathbf{L} = \mathbf{v} \times \partial_{\mathbf{v}}$  [12], which satisfies the identity (**v**  $\times \Omega$ )  $\partial_v = -\Omega \cdot L$ . After substitution of expansion (2) into the kinetic equation  $(1)$ , multiplication on the left by the complex conjugate spherical harmonic  $Y_m^{(l)}(\mathbf{v}/v)$ , and integration over all directions of velocity space  $\mathbf{v}/v$ , the following infinite hierarchy of equations for the coefficients  $f_m^{(l)}$  is obtained:

$$
\partial_t f_m^{(l)} + \sum_{l'm'\mu} (l'm'1\mu |lm) \langle l||v^{[1]}||l'\rangle G_{\mu}^{(1)} f_{m'}^{(l')}
$$
  
+ 
$$
\sum_{l'm'\mu} (l'm'1\mu |lm) \langle l||\partial_v^{[1]}||l'\rangle a_{\mu}^{(1)} f_{m'}^{(l')}
$$
  
- 
$$
\sum_{l'm'\mu} \Omega_{\mu}^{(1)} (l'm'1\mu |lm) \langle l||L^{[1]}||l'\rangle f_{m'}^{(l')}
$$
  
= 
$$
-J_l(f_m^{(l)}).
$$
 (7)

Here,  $G^{(11)}_{\mu}$ ,  $a^{(1)}_{\mu}$ , and  $\Omega^{(1)}_{\mu}$  are the gradient operator, the acceleration due to the electric field, and the cyclotron frequency in irreducible tensor notation, the values in parentheses are the Clebsch-Gordan coefficients and the values in angular brackets are the reduced matrix elements. The right hand side of Eq.  $(7)$  contains the spherical components  $J_l$  of the collision operator. Summation indices follow the rules



FIG. 1. Schematic representation of an axially homogeneous cylindrical magnetron discharge in crossed radial electric and axial magnetic fields.

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

The hierarchy of equations  $(7)$  can be applied to hydrodynamic or nonhydrodynamic situations and used for any configuration of electric and magnetic fields. The Clebsch-Gordan coefficients  $\left(l'm'1\mu\right)$  have a simple form and are tabulated, for instance, in Ref.  $\vert$ 17. The reduced matrix elements were calculated in  $[11,12]$ . Further simplification of Eq.  $(7)$  is connected with the choice of the form of expansion coefficients  $f_m^{(l)}$  with respect to discharge geometry and field configuration.

# **III. APPLICATION TO CYLINDRICAL GEOMETRY OF MAGNETRON DISCHARGE**

Cylindrical geometry of the magnetron discharge under consideration  $(Fig. 1)$  assumes rotational symmetry about the axis of the cylinder and the absence of azimuth fields and gradients. Radial electric field and gradients provide a preferred direction **r**/*r* in velocity space.

As was shown in Ref.  $[15]$ , in this case the phase space distribution function must have the property

$$
f(\mathbf{r}; \mathbf{v}; t) = f(r, z; v, \theta_v, \varphi_v - \varphi; t),
$$
\n(8)

i.e., it must depend on the difference of the azimuth angle  $\varphi$ <sub>*v*</sub> in velocity space  $\mathbf{v}=(v,\theta_v,\varphi_v)$  and the azimuth angle  $\varphi$  in configuration space with cylindrical coordinates  $\mathbf{r} = (z, r, \varphi)$ . This reflects the invariance of the distribution shape with respect to rotations about the cylinder axis. The tensor decomposition coefficients  $f_m^{(l)}$  by analogy to [15] will be represented in the form

$$
f_m^{(l)}(v,r,\varphi) = N_{l,m} F_{l,m}(v,r) e^{-im\varphi},\tag{9}
$$

with the factor

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

being extracted for convenience purposes. The phase space distribution function takes the representation

$$
f = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} F_{l,m}(r, z; v; t) P_l^{|m|}(\cos \theta_v) e^{im(\varphi_v - \varphi)} \frac{1}{2^{|m|}} \quad (10)
$$

and possesses the angular dependence prescribed by Eq.  $(8)$ .

Expression  $(10)$  differs from the corresponding equation [Eq.  $(14)$ ] in Ref. [15] by the factor  $(2^{|m|})^{-1}$ , which results below in a more physical form for the integrals denoting the

TABLE I. Gradient operator and field terms in cylindrical coordinates.

μ	$G^{(11)}_{\mu}$	$a_{\mu}^{(1)}$	$\Omega^{(1)}_{\mu}$
			$-i\Omega$
	$e^{-i\varphi}/\sqrt{2}(i\partial_r+\partial_\varphi/r)$	$ia_re^{-i\varphi}/\sqrt{2}$	
-1	$e^{i\varphi}/\sqrt{2}(-i\partial_r+\partial_{\varphi}/r)$	$-ia_re^{i\varphi}/\sqrt{2}$	

macroscopic transport coefficients. Another important distinction is that here the expansion coefficients  $F_{l,m}$  are complex quantities in contrast to  $[15]$ , where these functions were real.

The mathematical proof of the validity of representation (9) for a cylindrical discharge in axial magnetic  $\mathbf{B}_z$  and axisymmetric electric  $\mathbf{E} = \mathbf{E}_z + \mathbf{E}_r$  fields is given in the Appendix. Explicit expression for the tensor coefficients  $f_m^{(l)}$  [see Eq.  $(A4)$  and consequences below] requires the following properties for the coefficients  $F_{l,m}$ .

(1) The expansion coefficients  $F_{l,m}$  and  $F_{l,-m}$  are the complex conjugate functions:

$$
\operatorname{Re}(F_{l,m}) = \operatorname{Re}(F_{l,-m}),
$$

$$
\text{Im}(F_{l,m}) = -\text{Im}(F_{l,-m}).\tag{11}
$$

(2) Im $(F_{l,m})$ =0, if *B*=0, independently of the electric field direction.

(3) In crossed  $E_r$ ,  $B_z$  field configuration (see Fig. 1)

$$
F_{l,m} = 0 \quad \text{unless } l + m = \text{even.} \tag{12}
$$

The property  $(11)$  can be obtained directly from Eq.  $(10)$  by requiring the reality of the phase space distribution function  $f$ . The property  $(12)$  reflects the invariance of the distribution function under the transformation  $v_z \rightarrow -v_z$  and the fact that the magnetic field does not influence charged-particle motion in the direction parallel to the field.

The tensor components of the gradient operator  $G_{\mu}^{(11)}$  and vectors of electric  $a_{\mu}^{(1)}$  and magnetic  $\Omega_{\mu}^{(1)}$  fields in Eq. (7) are given in Table I for cylindrical coordinates in the particular case when the electric field and gradients have radial components only and the uniform magnetic field is directed along the axis of the cylinder. These tensor components were calculated in  $[11,12,15]$  for Cartesian, cylindrical, and spherical coordinates for various field directions.

The reduced matrix elements from Eq.  $(7)$  are shown in Table II. In the case of the axially directed magnetic field the magnetic field term is diagonal with respect to the index *l*.

The steady-state regime of the discharge operation will be considered hereinafter. Substitution of decomposition  $(9)$ into Eq. (7), using explicit values for the Clebsch-Gordan coefficients, applying the summation rules and taking into account the properties of the tensor coefficients and the reduced matrix elements listed in Tables I and II results in the following hierarchy:

TABLE II. Reduced matrix elements.

	$\langle l  v^{[1]}  l'\rangle$	$\langle l \vert \partial_r^{[1]} \vert l' \rangle$	$\langle l\ L^{[1]}\ l'\rangle$
$l+1$	$v\sqrt{(l+1)/(2l+1)}$	$\sqrt{(l+1)/(2l+1)}$ $d/dv + (l+2)/v$	
			$-\sqrt{l(l+1)}$
$l-1$	$v\sqrt{l/(2l+1)}$	$\sqrt{l/(2l+1)}$ $d/dv-(l-1)/v$	

$$
\begin{aligned}\n&\left[v\left(\partial_r - \frac{m-1}{r}\right) + a_r\left(\partial_v + \frac{l+2}{v}\right)\right] \frac{F_{l+1,m-1}}{(2l+3)} g_1 \\
&+ \left[v\left(\partial_r - \frac{m-1}{r}\right) + a_r\left(\partial_v - \frac{l-1}{v}\right)\right] \frac{F_{l-1,m-1}}{(2l-1)} g_2 \\
&+ \left[v\left(\partial_r + \frac{m+1}{r}\right) + a_r\left(\partial_v + \frac{l+2}{v}\right)\right] \frac{F_{l+1,m+1}}{(2l+3)} g_3 \\
&+ \left[v\left(\partial_r + \frac{m+1}{r}\right) + a_r\left(\partial_v - \frac{l-1}{v}\right)\right] \frac{F_{l-1,m+1}}{(2l-1)} g_4 \\
&= -i\Omega m F_{l,m} - J_l(F_{l,m}),\n\end{aligned} \tag{13}
$$

where the indices *l* and *m* take the values  $l=0,1,2,..., m$ =−*l*,...,*l*, and the coefficients *gk* are

$$
g_1 = \begin{cases} -1, & m > 0, \\ (l - m + 1)(l - m + 2)/4, & m \le 0, \\ (l - (l + m)(l + m - 1)/4, & m \le 0, \\ -(l + m)(l + m - 1)/4, & m \ge 0, \end{cases}
$$
  

$$
g_3 = \begin{cases} (l + m + 1)(l + m + 2)/4, & m \ge 0, \\ -1, & m < 0, \end{cases}
$$
  

$$
g_4 = \begin{cases} -(l - m - 1)(l - m)/4, & m \ge 0, \\ 1, & m < 0. \end{cases}
$$

The hierarchy of equations  $(13)$  is valid for both electrons and ions and permits one to compute the coefficients  $F_{lm}$  and the relevant macroscopic quantities.

## **IV. MACROSCOPIC QUANTITIES**

The main macroscopic properties of physical interest are the particle number density, mean energy, and particle flux density in the radial and azimuth directions. These quantities can be found by velocity space averaging of the distribution function. Thus, the number density *n* and mean energy  $U_{\alpha}$ are

$$
n = \int f(\mathbf{r}, \mathbf{v}) d\mathbf{v} = \sqrt{4\pi} \int_0^\infty f_0^{(0)}(\mathbf{r}, v) v^2 dv
$$
  
=  $\sqrt{4\pi} \int_0^\infty N_{0,0} F_{0,0} v^2 dv = 4\pi \int_0^\infty F_{0,0} v^2 dv$ , (14)

$$
U_{\alpha} = \frac{1}{n} \int \frac{m_{\alpha} v^2}{2} f(\mathbf{r}, \mathbf{v}) d\mathbf{v} = \frac{4\pi}{n} \int_0^{\infty} F_{0,0} \frac{m_{\alpha} v^2}{2} v^2 dv. \tag{15}
$$

The radial, azimuth, and axial components of the particle flux density result from the velocity space averaging of the distribution function multiplied by the corresponding velocity component

$$
j_{r,\varphi,z} = \int v_{r,\varphi,z} f(\mathbf{r}, \mathbf{v}) d\mathbf{v}.
$$
 (16)

The substitution of expressions  $(4)$ – $(6)$  for the velocity components in cylindrical coordinates and the distribution function expansion  $(10)$  into Eq.  $(16)$  yields

$$
j_r = \int_0^{\infty} v^2 dv \int_0^{2\pi} d\varphi_v \int_0^{\pi} \sin \theta_v d\theta_v \frac{v}{2} P_1^1(\cos \theta_v)
$$
  
 
$$
\times (e^{-i(\varphi_v - \varphi)} + e^{i(\varphi_v - \varphi)}) \sum_{l=0}^{\infty} \sum_{m=-l}^l F_{l,m} P_l^{|m|}(\cos \theta_v) e^{im(\varphi_v - \varphi)} \frac{1}{2^{|m|}}
$$
  

$$
= \frac{4\pi}{3} \int_0^{\infty} \text{Re}(F_{1,1}) v^3 dv,
$$
 (17)

$$
j_{\varphi} = -\frac{4\pi}{3} \int_0^{\infty} \text{Im}(F_{1,1}) v^3 dv,
$$
 (18)

$$
j_z = \frac{4\pi}{3} \int_0^\infty F_{1,0} v^3 dv.
$$
 (19)

In our special case of the axially uniform cylindrical magnetron discharge  $F_{1,0}$  and  $j_z$  equal zero.

In a similar way one can find the higher-order macroscopic quantities responsible for the momentum and energy flux transports. The nonzero components of the second rank tensor

$$
\mathbf{\Pi} = nm_{\alpha} \left\langle \mathbf{vv} - \frac{v^2}{3} \mathbf{I} \right\rangle, \tag{20}
$$

whose physical meaning is the tensor of anisotropic pressure or the traceless part of the momentum flux  $(I$  is the second rank identity tensor), in cylindrical coordinates have the following form:

$$
\Pi_{rr} = m_{\alpha} \int (v_{rr} - v^2/3) f(\mathbf{r}, \mathbf{v}) d\mathbf{v}
$$

$$
= \frac{4\pi}{5} \int_0^\infty \left[ \text{Re}(F_{2,2}) - \frac{1}{3} F_{2,0} \right] m_{\alpha} v^4 dv,
$$

$$
\Pi_{zz} = m_{\alpha} \int (v_{zz} - v^2/3) f(\mathbf{r}, \mathbf{v}) d\mathbf{v} = \frac{4\pi}{5} \int_0^\infty \frac{2}{3} F_{2,0} m_{\alpha} v^4 dv,
$$

$$
\Pi_{\varphi\varphi} = m_{\alpha} \int (v_{\varphi\varphi} - v^2/3) f(\mathbf{r}, \mathbf{v}) d\mathbf{v} = - \Pi_{zz} - \Pi_{rr},
$$

$$
\Pi_{r\varphi} = \Pi_{\varphi r} = m_{\alpha} \int v_{r\varphi} f(\mathbf{r}, \mathbf{v}) d\mathbf{v} = -\frac{4\pi}{5} \int_0^{\infty} \text{Im}(F_{2,2}) m_{\alpha} v^4 dv.
$$

The tensor of the isotropic pressure of particles is

$$
\mathbf{P} = nm_{\alpha} \left\langle \frac{v^2}{3} \mathbf{I} \right\rangle, \quad P_{ii} = \frac{4\pi}{3} \int_0^{\infty} F_{0,0} m_{\alpha} v^4 dv.
$$

In the case of nonzero axial electric field and gradient (for instance, a magnetron discharge of finite length with the ends closed by shields biased at the potential of the plasma or cathode) the components  $\Pi_{rz}$  and  $\Pi_{z\varphi}$  will differ from zero.

The third rank tensor

$$
\Psi = \frac{n m_{\alpha}}{2} \langle \mathbf{v} \mathbf{v} \mathbf{v} - v^2 \mathbf{I} \mathbf{v} \rangle \tag{21}
$$

corresponds to the difference between the energy flux tensor

$$
\widetilde{\Psi} = \frac{n m_{\alpha}}{2} \langle \mathbf{v} \mathbf{v} \mathbf{v} \rangle \tag{22}
$$

and the tensor  $Ij_u$ , where  $j_u$  is the energy flux vector with the components

$$
j_{ur} = \frac{4\pi}{3} \int_0^\infty \text{Re}(F_{1,1}) \frac{m_\alpha v^2}{2} v^3 dv,
$$
  

$$
j_{u\varphi} = -\frac{4\pi}{3} \int_0^\infty \text{Im}(F_{1,1}) \frac{m_\alpha v^2}{2} v^3 dv,
$$
  

$$
j_{u z} = \frac{4\pi}{3} \int_0^\infty F_{1,0} \frac{m_\alpha v^2}{2} v^3 dv.
$$

The nonzero components of the third rank tensor  $(21)$  are

$$
\Psi_{rrr} = \frac{4\pi}{7} \int_0^{\infty} \left[ \frac{3}{2} \text{Re}(F_{3,3}) - \frac{3}{5} \text{Re}(F_{3,1}) - \frac{14}{15} \text{Re}(F_{1,1}) \right]
$$
  
\n
$$
\times \frac{m_a v^2}{2} v^3 dv,
$$
  
\n
$$
\Psi_{r\varphi\varphi} = -\frac{4\pi}{7} \int_0^{\infty} \left[ \frac{3}{2} \text{Re}(F_{3,3}) + \frac{1}{5} \text{Re}(F_{3,1}) - \frac{7}{15} \text{Re}(F_{1,1}) \right]
$$
  
\n
$$
\times \frac{m_a v^2}{2} v^3 dv,
$$
  
\n
$$
\Psi_{rzz} = \frac{4\pi}{7} \int_0^{\infty} \left[ \frac{4}{5} \text{Re}(F_{3,1}) + \frac{7}{15} \text{Re}(F_{1,1}) \right] \frac{m_a v^2}{2} v^3 dv,
$$
  
\n
$$
\Psi_{\varphi rr} = -\frac{4\pi}{7} \int_0^{\infty} \left[ \frac{3}{2} \text{Im}(F_{3,3}) - \frac{1}{5} \text{Im}(F_{3,1}) + \frac{7}{15} \text{Im}(F_{1,1}) \right]
$$
  
\n
$$
\times \frac{m_a v^2}{2} v^3 dv,
$$

$$
\begin{split} \Psi_{\varphi\varphi\varphi} & = \frac{4\pi}{7} \int_0^\infty \Biggl[ \frac{3}{2} \; \mbox{Im}(F_{3,3}) + \frac{3}{5} \; \mbox{Im}(F_{3,1}) + \frac{14}{15} \; \mbox{Im}(F_{1,1}) \Biggr] \\ & \times \frac{m_\alpha v^2}{2} v^3 dv \,, \\ \Psi_{\varphi zz} & = - \; \frac{4\pi}{7} \int_0^\infty \Biggl[ \frac{4}{5} \; \mbox{Im}(F_{3,1}) + \frac{7}{15} \; \mbox{Im}(F_{1,1}) \Biggr] \frac{m_\alpha v^2}{2} v^3 dv \,. \end{split}
$$

The tensor components  $\Psi_{ijk}$  do not change under permutation of indexes. Contraction of tensor  $(21)$  with respect to any pair of indices gives zero:  $\Psi_{irr} + \Psi_{izz} + \Psi_{i\varphi\varphi} = 0$ .

The components of the tensors  $(20)$  and  $(21)$  appear in the momentum and energy flux balance equations.

## **V. TWO-TERM APPROXIMATION**

The well-known two-term representation of the phase space distribution function *f* in cylindrical geometry

$$
f = f_0 + (\mathbf{v}/v)\mathbf{f}_1 = f_0 + (v_z f_{1z} + v_r f_{1r} + v_\varphi f_{1\varphi})/v,
$$

follows from Eqs. (10) and (4)–(6), and property (11), with the definitions  $f_0$ ≡ $F_{0,0}$ ,  $f_{1r}$ ≡Re $(F_{1,1})$ , and  $f_{1\varphi}$ ≡ $-\text{Im}(F_{1,1})$ . The passage to the limit of the two-term approximation can be easily demonstrated by setting  $l=0$ ,  $m=0$  and  $l=1$ ,  $m$  $= \pm 1$  in Eq. (13). The equation for the isotropic part of the distribution function then becomes

$$
[v(\partial_r + 1/r) + a_r(\partial_v + 2/v)](F_{1,-1} + F_{1,1})/6 = J_0.
$$

At  $l=1$ ,  $m=1,-1$ , and  $J_1=-\nu F_{1,m}$  ( $\nu$  is the collision frequency), Eq.  $(13)$  takes the form

$$
[v \partial_r + a_r \partial_v] F_{0,0} = \pm i \Omega F_{1,\pm 1} - \nu F_{1,\pm 1}.
$$
 (23)

At  $l=1$  and  $m=0$  we obtain  $F_{1,0}=0$ .

By extracting the real and imaginary parts from the complex conjugate equations  $(23)$  and using the above definitions, we obtain the following equations for the axial, azimuth, and radial anisotropic parts of the distribution, as well as the equation for the isotropic distribution function:

$$
f_{1z} = 0, \quad f_{1\varphi} = \frac{\Omega}{\nu} f_{1r},
$$

$$
f_{1r} = -\frac{\nu}{\Omega^2 + \nu^2} \left( \nu \frac{\partial f_0}{\partial r} + a_r \frac{\partial f_0}{\partial v} \right),
$$

$$
\frac{\nu}{3} \frac{1}{r} \frac{\partial}{\partial r} r f_{1r} + \frac{a_r}{3} \frac{1}{\nu^2} \frac{\partial}{\partial v} \nu^2 f_{1r} = J_0.
$$

These equations coincide with the conventional ones used in the  $(f_0, f_1)$  approximation for electrons in crossed  $\mathbf{E}_r, \mathbf{B}_z$ fields.

#### **VI. FOUR-TERM APPROXIMATION FOR ELECTRONS**

Equations for the distribution function expansion coefficients in the multiterm approximation follow from the hierarchy (13), with *l*=0,1,2,3, etc., and *m*=−*l*,...,*l*. Truncation of the infinite summation at  $l = l_{\text{max}}$  corresponds to the  $(l=l_{\text{max}}+1)$ -term approximation with all higher expansion coefficients being set to zero.

Hereinafter, we consider the four-term approximation for the electrons. The procedure for ions is analogous.

Electrons with the charge  $-e$  and mass  $m_e$  move in the radial potential  $\varphi(r) = \int_{R_C}^r (-E) dr$  from the cathode of radius  $R<sub>C</sub>$  to anode. The direction of their motion coincides with the *r*-axis direction and is opposite to the direction of the field  $\mathbf{E}_r$ . Equations (13) can be simplified by the transformation of the variables  $(v, r)$  to variables  $(\varepsilon, r')$ , where  $r' = r$  and the total energy  $\varepsilon = U + \Phi(r)$  is the sum of the kinetic *U*  $=m_e v^2/2$  and potential  $\Phi(r) = (-e)\varphi(r)$  energies. Using the transformation rules

$$
\partial_r = \partial_{r'} + eE\partial_{\varepsilon}, \quad \partial_v = m_e v \partial_{\varepsilon},
$$

we come to the following hierarchy for the coefficients  $F_{l,m}(\varepsilon,r) = 2\pi(2/m_e)^{3/2}F_{l,m}(v,r)$ :

$$
\left[U\left(\partial_r - \frac{m-1}{r}\right) - eE\frac{l+2}{2}\right] \frac{\tilde{F}_{l+1,m-1}}{(2l+3)} g_1
$$
  
+ 
$$
\left[U\left(\partial_r - \frac{m-1}{r}\right) + eE\frac{l-1}{2}\right] \frac{\tilde{F}_{l-1,m-1}}{(2l-1)} g_2
$$
  
+ 
$$
\left[U\left(\partial_r + \frac{m+1}{r}\right) - eE\frac{l+2}{2}\right] \frac{\tilde{F}_{l+1,m+1}}{(2l+3)} g_3
$$
  
+ 
$$
\left[U\left(\partial_r + \frac{m+1}{r}\right) + eE\frac{l-1}{2}\right] \frac{\tilde{F}_{l-1,m+1}}{(2l-1)} g_4
$$
  
= 
$$
-i\Omega m (m_e U/2)^{1/2} \tilde{F}_{l,m} - S_l(\tilde{F}_{l,m}).
$$
 (24)

Here, the kinetic energy  $U = \varepsilon - \Phi(r)$  is the dependent variable, and the collision operators  $S_l = (m_e U/2)^{1/2} J_l$ .

The hierarchy  $(24)$  should be converted then into a system of equations written explicitly for required values of *l* and *m*. Equations for the indices *m* and −*m* form complex conjugate pairs. By extracting the real and imaginary parts of  $\tilde{F}_{l,\pm m}$ from the pairs of coupled equations we obtain the following system of equations for the functions  $f_k(\varepsilon, r)$ :

$$
\frac{U}{3} \frac{1}{r} \frac{\partial}{\partial r} r f_1 - \frac{eE}{3} f_1 = S_0, \tag{25}
$$

$$
A_1 f_1 + U \frac{\partial f_0}{\partial r} + \frac{3}{5} U \frac{1}{r^2} \frac{\partial}{\partial r} r^2 f_2 - \frac{U}{5} \frac{\partial f_3}{\partial r} + \frac{3}{10} eE(f_3 - 3f_2) = Gf_6,
$$
\n(26)

$$
A_{2}f_{2} + \frac{15}{14}U\frac{1}{r^{3}}\frac{\partial}{\partial r}r^{3}f_{4} + \frac{U}{3}r\frac{\partial}{\partial r}\frac{f_{1}}{r} - \frac{U}{7}r\frac{\partial}{\partial r}\frac{f_{5}}{r} + eE\left(\frac{1}{6}f_{1} - \frac{15}{7}f_{4} + \frac{2}{7}f_{5}\right) = 2Gf_{7},
$$
(27)

$$
A_2 f_3 + \frac{6}{7} U \frac{1}{r} \frac{\partial}{\partial r} r f_5 - \frac{U}{3} \frac{1}{r} \frac{\partial}{\partial r} r f_1 - eE \left( \frac{1}{6} f_1 + \frac{12}{7} f_5 \right) = 0,
$$
\n(28)

$$
A_3 f_4 + \frac{U}{5} r^2 \frac{\partial f_2}{\partial r} + \frac{eE}{5} f_2 = 3G f_8, \tag{29}
$$

$$
A_3 f_5 + \frac{U}{5} \frac{\partial f_3}{\partial r} - \frac{U}{10} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 f_2 - \frac{eE}{10} (f_2 - 2f_3) = G f_9, \tag{30}
$$

$$
A_1 f_6 + \frac{3}{5} U \frac{1}{r^2} \frac{\partial}{\partial r} r^2 f_7 - \frac{9}{10} eE f_7 = -G f_1,\tag{31}
$$

$$
A_{2}f_{7} + \frac{15}{14}U\frac{1}{r^{3}}\frac{\partial}{\partial r}r^{3}f_{8} + \frac{U}{3}r\frac{\partial}{\partial r}f_{6} - \frac{U}{7}r\frac{\partial}{\partial r}\frac{f_{9}}{r} + eE\left(\frac{1}{6}f_{6} - \frac{15}{7}f_{8} + \frac{2}{7}f_{9}\right) = -2Gf_{2},
$$
(32)

$$
A_3 f_8 + \frac{U}{5} r^2 \frac{\partial f_7}{\partial r} \frac{dF}{r^2} + \frac{eE}{5} f_7 = -3Gf_4,
$$
 (33)

$$
A_3 f_9 - \frac{U}{10} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 f_7 - \frac{eE}{10} f_7 = -Gf_5.
$$
 (34)

Here we use the following designations for the real parts of the components:

$$
\tilde{F}_{0,0} = f_0
$$
, Re( $\tilde{F}_{1,1}$ ) =  $f_1$ , Re( $\tilde{F}_{2,2}$ ) =  $f_2$ ,  
\n $\tilde{F}_{2,0} = f_3$ , Re( $\tilde{F}_{3,3}$ ) =  $f_4$ , Re( $\tilde{F}_{3,1}$ ) =  $f_5$ ,

and for the imaginary parts:

Im
$$
(\tilde{F}_{1,1}) = f_6
$$
, Im $(\tilde{F}_{2,2}) = f_7$ ,  
Im $(\tilde{F}_{3,3}) = f_8$ , Im $(\tilde{F}_{3,1}) = f_9$ .

The coefficients  $A_l$  ( $l \neq 0$ ) and *G* are defined by

$$
S_l(\widetilde{F}_{l,m}) = -A_l \widetilde{F}_{l,m}, \quad A_l(\varepsilon, r) \equiv UNQ_{\Sigma}(U),
$$
  

$$
G(\varepsilon, r) \equiv (m_e U/2)^{1/2} \Omega, \quad \Omega = -eB/m_e,
$$

where  $N$  is the neutral gas density (a cold gas is being considered, which corresponds to the low-temperature cylindrical magnetron discharge in a gas flow) and the total cross section is

$$
Q_{\Sigma} = Q_l + Q^{ex} + Q^{di}.\tag{35}
$$

The collision operator  $S_0$  involves elastic, inelastic, and ionizing collisions of electrons with atoms of an inert gas and can be written in the form

$$
S_0 = S_0^{el}(f_0) + S_0^{ex}(f_0) + S_0^{di}(f_0),
$$

where

$$
S_0^{el}(f_0) = 2 \frac{m_e}{M} \frac{\partial}{\partial \varepsilon} [U^2 N Q^d(U) f_0(U, r)],
$$

066406-6

$$
S_0^{ex}(f_0) = -UNQ^{ex}(U)f_0(\varepsilon, r)
$$
  
+ 
$$
(U + U_{ex})NQ^{ex}(U + U_{ex})f_0(\varepsilon + U_{ex}, r),
$$

$$
S_0^{di}(f_0) = - UNQ^{di}(U)f_0(\varepsilon, r)
$$
  
+  $(U/\beta + U_{di})NQ^{di}(U/\beta + U_{di})f_0(U/\beta + U_{di}, r)/\beta$   
+  $(U/[1 - \beta] + U_{di})NQ^{di}(U/[1 - \beta] + U_{di})$   
 $\times f_0(U/[1 - \beta] + U_{di}, r)/[1 - \beta].$ 

The cross sections appearing in Eq.  $(35)$  and collision operators are  $Q_l$ , the generalized cross sections resulting from an averaging of the differential cross sections over the solid angle of scattering,  $Q^d$ , the momentum transfer cross section,  $Q^{ex}$ , the total excitation cross section with the threshold  $U_{ex}$ , and  $Q^{di}$ , the direct ionization cross section with the ionization potential  $U_{di}$ . The quantities  $\beta$  and 1− $\beta$  denote the fraction in which the remaining kinetic energy of the colliding electron is shared in ionization event between the two outgoing electrons. Inelastic scattering is supposed here to be isotropic. Superelastic collisions do not play a role because of a small excited atom density.

To take into account the anisotropic scattering in elastic collisions the differential cross sections  $\sigma^{el}(U, \cos \theta)$  are needed. This can be simplified by assuming separation of variables  $\vert 18,19 \vert$ , according to which the differential cross sections

$$
\sigma^{el}(U,x) = Q_0^{el}(U)R(x)/(2\pi), \quad x \equiv \cos \theta, \quad -1 \le x \le 1,
$$

are expressed in terms of the total elastic cross section  $Q_0^{el}(U)$  and the scattering profile  $R(x)$ 

$$
R(x) = \frac{1}{a} \exp\left(-\frac{(x - x_c)^2}{x_w^2}\right),
$$
  

$$
a = \int_{-1}^1 \exp\left(-\frac{(x - x_c)^2}{x_w^2}\right) dx.
$$

The values  $x_c = 1$  and  $x_w = 0.5$  for the center and width of the scattering profile correspond to a considerable forward scattering of electrons. The value  $x_w = \infty$  describes the isotropic scattering.

Under this approximation the generalized cross sections are written in the form

$$
Q_l(U) = Q_d(U)(\alpha_n/\alpha_1), \quad \alpha_n = 1 - \int_{-1}^1 R(x)P_n(x)dx,
$$

where  $P_n$  are the Legendre polynomials.

# **VII. BOUNDARY CONDITIONS**

The system of equations  $(25)$ – $(34)$  for the distribution function expansion coefficients should be supplemented by the relevant boundary conditions that correspond to the problem specifics and reflect the processes at the boundaries of the solution region.

The solution region of system  $(25)$ – $(34)$  for the cylindrical magnetron discharge in the plane total energy  $\varepsilon$  and ra-



FIG. 2. Solution region of the system of equations  $(25)$ – $(34)$  in the variables total energy  $\varepsilon$  and coordinate  $r$ . Distribution of the potential  $\varphi(r)$  is typical for the cylindrical magnetron discharge in argon at  $B = 100$  G.

dial coordinate *r* is schematically shown in Fig. 2. The region is limited on top by the boundary *D* ( $\varepsilon = \varepsilon_{\infty}$ ), where all expansion coefficients of the distribution function become negligibly small; on the right by the line  $C (r=R_A)$  corresponding to the anode position; on the left by the boundary  $A(\varepsilon > 0)$  where the electrons are ejected into the plasma from the cathode surface; and on the left and from below by the curve  $B\left[\varepsilon = \Phi(r)\right]$  at which the electron kinetic energy equals zero  $(U=0)$ .

A half-space analysis  $[20-23]$  has shown that, for multiterm expansions, stable numerical solutions result when the boundary conditions are applied alternatively at the anode and cathode, for functions with even and odd *l* indexes. Thus, the boundary conditions for the functions with even *l* indexes (in our designations these are  $f_0$ ,  $f_2$ ,  $f_3$ ,  $f_7$ ) should be specified at the anode, and for the terms with odd *l* (these are  $f_1$ ,  $f_4$ ,  $f_5$ ,  $f_6$ ,  $f_8$ ,  $f_9$ ) at the cathode and on the curve *B*.

The anode boundary conditions must provide a transition from the positive column to the equipotential anode. Conditions at the absorbing surface for expansion coefficients resulting from the spherical harmonic decomposition of the distribution of neutrons in the medium surrounding "black" sphere were first obtained by Marshak  $[24]$ . The main ideas proposed by Marshak are that the hierarchy should be truncated at odd *l* indices, since the even approximations contain singular parts which have no clear physical significance; and that the boundary conditions at the absorbing surface in the *l*-term approximation should follow from the corresponding odd velocity moment of the distribution function. Multiterm studies  $[25,26]$  of the electron distribution function in the anode region have contributed significantly to the field.

Following [26], where the plane anode region was studied by a multiterm Legendre polynomial expansion, we develop



FIG. 3. Spherical coordinates  $(v, \theta_v, \varphi_v)$  in velocity space and cylindrical coordinates  $(z, r, \varphi)$  in configuration space. Figure on the right shows the plane *z*=const. Shaded area of the smaller circle corresponds to the angles  $\varphi$ <sub>v</sub> at which the particle flux goes away from the anode.

a method to deduce the boundary conditions at the radial absorbing boundary of a cylindrical plasma, for the multiterm spherical harmonic representation of the phase space distribution function. Relations for the expansion coefficients at the anode boundary were derived in Ref.  $[26]$  by decomposing the particle fluxes (and higher odd velocity moments) into elementary microscopic fluxes (moments), directed toward and away from the anode surface. The reflection condition applied to these microscopic fluxes resulted in a coupling of the functions with even and odd *l* indices, thus yielding the required boundary conditions.

At first, the procedure to deduce the boundary conditions at the anode will be demonstrated for the first velocity moment that corresponds to the radial flux density of electrons. The radial flux density determined by Eq.  $(17)$  can be represented as a sum of the microscopic flux densities directed towards and away from the anode. To obtain these fluxes in cylindrical geometry a reference to Fig. 3 is useful.

It is seen from Fig. 3 that the electron flux toward the anode  $j_r^+$  is limited by the angles  $\varphi_v$  in the range of the difference  $\varphi$ <sub>*v*</sub>− $\varphi$  from  $-\pi/2$  to  $\pi/2$ , and the flux going away from the anode  $j_r^-$  is given by the angles  $\varphi_v - \varphi$  in the range from  $\pi/2$  to  $3\pi/2$ . The corresponding microscopic particle fluxes can be calculated as

$$
j_r^- = \int_0^\infty v_r v^2 dv \int_{\varphi + \pi/2}^{\varphi + 3\pi/2} d\varphi_v \int_0^\pi \sin \theta_v d\theta_v
$$
  
 
$$
\times \sum_{l=0}^\infty \sum_{m=-l}^l F_{l,m}(r, v, t) P_l^{|m|}(\cos \theta_v) e^{im(\varphi_v - \varphi)} \frac{1}{2^{|m|}},
$$
  

$$
j_r^+ = \int_0^\infty v_r v^2 dv \int_{\varphi - \pi/2}^{\varphi + \pi/2} d\varphi_v \int_0^\pi \sin \theta_v d\theta_v
$$
  

$$
\times \sum_{l=0}^\infty \sum_{m=-l}^l F_{l,m}(r, v, t) P_l^{|m|}(\cos \theta_v) e^{im(\varphi_v - \varphi)} \frac{1}{2^{|m|}}.
$$

In the case of a partial absorption of electrons by the anode surface these microscopic fluxes are related by the reflection condition

$$
\ddot{j_r} = -\xi \ddot{j_r}
$$

with the values of the reflection coefficient  $\xi$  running between zero and unity.

Hereinafter for simplicity reasons all electrons having reached the anode are assumed to be absorbed, i.e.,  $j_r^-=0$  and reflection coefficient  $\xi=0$ . Applying this absorption requirement to each energy of the integrand we obtain the following boundary condition for the expansion coefficients in the twoterm approximation

$$
\sum_{l=0}^{l} \sum_{k=-l}^{l} \frac{1}{2^{|k|}} \gamma_k^{(1)} \alpha_{1l}^{1k} F_{l,k} = 0, \qquad (36)
$$

where

$$
\gamma_k^{(1)} = \int_{\varphi + \pi/2}^{\varphi + 3\pi/2} (e^{i(k-1)(\varphi_v - \varphi)} + e^{i(k+1)(\varphi_v - \varphi)}) d\varphi_v,
$$
  

$$
\alpha_{1l}^{1k} = \int_{-1}^1 P_1^1(x) P_l^k(x) dx.
$$

The condition  $(36)$  in the conventional two-term approximation reads

$$
F_{0,0} = \frac{2}{3} \operatorname{Re}(F_{1,1}).
$$

Similar relationships have been obtained in many two-term studies (e.g.,  $[27–29]$ ).

To obtain the boundary conditions for the four-term approximation one must consider, in a similar way, the radial components of the third velocity moment given by the components  $\tilde{\Psi}_{rrr}$ ,  $\tilde{\Psi}_{r\varphi\varphi}$  and  $\tilde{\Psi}_{rzz}$  of the energy flux tensor (22)

$$
\widetilde{\Psi}_{rkk} = \frac{m_e}{2} \int v_{rkkf}(\mathbf{r}, \mathbf{v}) d\mathbf{v},
$$

where  $v_{rr} = v_r^3$ ,  $v_{r\varphi\varphi} = v_r v_{\varphi}^2$ ,  $v_{rzz} = v_r v_z^2$ .

From the requirement of complete absorption of the energy flux tensor radial components  $\tilde{\Psi}_{rrr}^{\text{}}=0$ ,  $\tilde{\Psi}_{r\varphi\varphi}^{\text{}}=0$ , and  $\tilde{\Psi}^-_{\text{rzz}} = 0$  it follows that

$$
\sum_{l=0}^{l} \sum_{k=-l}^{l} \frac{1}{2^{|k|}} \alpha_{3l}^{3k} (\gamma_k^{(3)} + 3 \gamma_k^{(1)}) F_{l,k} = 0, \qquad (37)
$$

$$
\sum_{l=0}^{l} \sum_{k=-l}^{l} \frac{1}{2^{|k|}} \alpha_{3l}^{3k} (\gamma_k^{(3)} - \gamma_k^{(1)}) F_{l,k} = 0, \qquad (38)
$$

$$
\sum_{l=0}^{l} \sum_{k=-l}^{l} \frac{1}{2^{|k|}} \gamma_k^{(1)} (\alpha_{1l}^{1k} - \alpha_{3l}^{3k} / 15) F_{l,k} = 0, \tag{39}
$$

where

$$
\gamma_k^{(3)} = \int_{\varphi + \pi/2}^{\varphi + 3\pi/2} (e^{i(k-3)(\varphi_v - \varphi)} + e^{i(k+3)(\varphi_v - \varphi)}) d\varphi_v,
$$

TABLE III. Coefficients  $\gamma_k$  in the boundary conditions  $(37)–(39)$  and  $(41)$ .

		$k \t -3 \t -2$		$-1$ 0 1 2 3	
				$\gamma_k^{(1)}$ 0 -4/3 $\pi$ -4 $\pi$ -4/3 0	
$\gamma_k^{(3)}$	$\pi$	$-12/5$ 0 4/3 0 $-12/5$			$\pi$
$\widetilde{\gamma}_{k}^{(1)}$		0 $-8/3$ $-\pi$		0 $\pi$ 8/3	
$\widetilde{\gamma}_{\scriptscriptstyle{k}}^{\scriptscriptstyle{(3)}}$	$-\pi$	$8/5$ 0 0		0 $8/5$	$\pi$

$$
\alpha_{3l}^{3k} = \int_{-1}^{1} P_3^3(x) P_l^k(x) dx.
$$

After substitution of  $\gamma_k^{(n)}$  (cf. Table III) and  $\alpha_{nl}^{nk}$  (n=1,3) (cf. Table IV) in Eqs.  $(37)$ – $(39)$  and cancellation of terms containing the imaginary parts of  $F_{l, \pm k}$ , the boundary conditions for the functions  $f_0 = F_{0,0}$ ,  $f_2 = \text{Re}(F_{2,2})$ , and  $f_3 = F_{2,0}$  take the representation

$$
f_0 = \frac{8}{15}f_1 + \frac{12}{35}f_5 - \frac{6}{7}f_4,
$$
  
\n
$$
f_2 = \frac{4}{15}f_1 - \frac{4}{35}f_5 + \frac{18}{7}f_4,
$$
  
\n
$$
f_3 = -\frac{4}{15}f_1 + \frac{12}{5}f_5 + \frac{6}{7}f_4.
$$
\n(40)

Notice that the condition  $(36)$  holds too.

The boundary condition for the imaginary part of the term  $f_7 = \text{Im}(F_2)$  follows from the absorption requirement for the third rank tensor component  $\tilde{\Psi}_{err} = \tilde{\Psi}_{rr}$  in the form

$$
\sum_{l=0}^{l} \sum_{k=-l}^{l} \frac{1}{2^{|k|}} \alpha_{3l}^{3k} (\widetilde{\gamma}_{k}^{(3)} + 3 \widetilde{\gamma}_{k}^{(1)}) F_{l,k} = 0, \qquad (41)
$$

where

$$
\widetilde{\gamma}_{k}^{(n)} = \int_{\varphi + \pi/2}^{\varphi + 3\pi/2} (e^{i(k-n)(\varphi_{v} - \varphi)} - e^{i(k+n)(\varphi_{v} - \varphi)}) d\varphi_{v}.
$$

Cancellation of the real parts in Eq.  $(41)$ , followed by the substitution of the corresponding coefficients listed in Tables III and IV, results in the relationship

$$
f_7 = -\frac{8}{15}f_6 + \frac{8}{35}f_9 - \frac{12}{7}f_8.
$$
 (42)

The boundary conditions at the anode surface written in the form of Eqs.  $(40)$  and  $(42)$  for the functions with even *l* index in the four-term approximation ensure the solution stability and smooth transition from the inhomogeneous positive column to the equipotential anode.

The presence of the axially directed electric field generates the particle fluxes along the *z* axis. In this case the absorption or reflection conditions should be also set for the axial tensor components  $\tilde{\Psi}_{zzz}$ ,  $\tilde{\Psi}_{z\varphi\varphi}$ ,  $\tilde{\Psi}_{zrr}$ , and  $\tilde{\Psi}_{zz\varphi}$ . In the next six-term approximation for the distribution function the boundary conditions at the anode should be derived from the reflection requirements for the fifth order velocity moment.

The boundary conditions on the cathode side can be set by various methods (e.g.,  $[23,25,30]$ ). The two boundaries *A* and *B* specified in Fig. 2 are to be considered here. Conditions on the boundary *A* ( $\varepsilon$ >0) correspond to the distribution of electrons ejected from the cathode. These electrons are assumed to form a high-energy beam with anisotropic distribution  $f_1(U) = \text{Re}(F_{1,1}) = \exp[-(U - U_m)^2 / (\delta U)^2]$  with a center at the energy  $U_m$  and width  $\delta U$ . The values of the anisotropic functions  $f_6$ ,  $f_4$ ,  $f_5$ ,  $f_8$ , and  $f_9$  should be chosen consistently with the system of equations. This consistency can be reached in the simplest way, by setting  $f_4=0, f_5=0$ ,  $f_8=0, f_9=0,$  and

$$
f_6 = -\frac{(mU/2)^{1/2}\Omega}{NQ_1(U)U}f_1,
$$

valid along with the additional condition  $f_7=0$ . Conditions on the potential curve where  $U=0$  ( $\varepsilon < 0$ ) can be derived by analyzing the system of equations in the limit  $U\rightarrow 0$ . This analysis shows that all anisotropic components must turn into zero on the boundary *B* (Fig. 2):  $f_1 = f_6 = f_4 = f_5 = f_8 = f_9$  $=0$ . However, an employment of the additional requirement  $f_7=0$  can be useful to ensure the solution's stability under nonzero magnetic field conditions. The reason is that the functions  $f_6$ ,  $f_8$ , and  $f_9$  in the vicinity of zero kinetic energy vary approximately as  $\sim U^{-1}$  leading to quick accumulation of small discretization errors present in any numerical scheme.

The balance equations for particle number, energy, and momentum will be considered in the following paper, as well as calculations of the isotropic and anisotropic parts of the distribution function. These and the calculation of additional

	$\alpha_{0l}^{0k}$	$\alpha_{1l}^{1k}$	$\alpha_{2l}^{0k}$	$\alpha_{2l}^{2k}$	$\alpha_{3l}^{3k}$
$l=0, k=0$	2	$\pi/2$	$\theta$	$\overline{4}$	$45\pi/8$
$l=1, k=1$	$\pi/2$	4/3	$-\pi/16$	$9\pi/8$	16
$l=2, k=0$	$\theta$	$-\pi/16$	2/5	$-4/5$	$-45\pi/32$
$l=2, k=2$	$\overline{4}$	$9\pi/8$	$-4/5$	48/5	$225 \pi / 16$
$l=3, k=1$	$\Omega$	$\theta$	$21\pi/64$	$-9\pi/32$	$-48/7$
$l=3, k=3$	$45\pi/8$	16	$-45\pi/32$	$225\pi/16$	1440/7

TABLE IV. Coefficients  $\alpha_{nl}^{mk}$  in the boundary conditions (37)–(39) and (41).

macroscopic quantities will be illustrated on concrete examples of real operating conditions for cylindrical magnetron discharge.

# **VIII. CONCLUSION**

In this paper we have developed a nonhydrodynamic method to treat the anisotropic electron distribution functions in crossed electric and magnetic fields in the presence of spatial inhomogeneities. The method is based on the spherical tensor decomposition  $[11,12,15]$  of the phase space distribution function with further employment of the specific properties of tensor expansion coefficients  $\lceil 15 \rceil$  resulting from the cylindrical symmetry of the discharge. The system of equations describing the spatioenergetic evolution of the distribution function expansion coefficients from cathode to anode in the cylindrical magnetron discharge is obtained. The problem of appropriate boundary conditions at electrodes is considered for cylindrical geometry with respect to even and odd distribution function components written in the spherical tensor notation. The boundary conditions ensuring the solution stability and satisfaction of particle, energy and momentum balance equations are derived at the anode by considering microscopic fluxes of velocity moments directed toward the anode.

An important requirement of decomposition methods is a formulation of the simplest possible system of equations which would give an adequate description of the object on the one hand and could be relatively easily solved analytically or numerically on the other hand. The multiterm treatments of the electron distribution anisotropy using Cartesian tensors become especially awkward in the presence of the magnetic field. The generalization of the spherical tensor decomposition  $[15]$  developed in the present paper for the crossed electric and magnetic fields possesses an elegance and physical transparency. The resulting system of equations for calculations of the distribution function expansion coefficients can be easily obtained from the general hierarchy and contains a reasonable number of equations  $(10, 21, 36)$ equations in four-, six-, and eight-term approximations, respectively). Since the presence of a magnetic field reduces the distribution function's anisotropy, convergence is expected to be reached by the six-term approximation, even for the case of strong electric and weak magnetic fields. Thus, the appropriate and detailed description of the near-electrode regions in weak magnetic fields when the anisotropy is not negligible, can be obtained without use of the PIC MCC methods. A similar method can also be applied to describe anisotropy phenomena in a cylindrical dc discharge in an axial magnetic field.

#### **ACKNOWLEDGMENTS**

The work was financially supported by the DFG SFB 198 Project "Kinetics of partially ionized plasma" and Grants No. PD02-1.2-17 and No. PD03-1.2-123 from the Russian Ministry of Education and Administration of St. Petersburg.

## **APPENDIX**

In this section we prove mathematically the possibility of representing the coefficients  $f_m^{(l)}$  of the spherical harmonics expansion  $(2)$  in the form of Eq.  $(9)$  for cylindrical discharge in electric and axial magnetic field. Then, the expansion coefficients  $F_{l,m}$  will be shown to have properties (11) and (12).

We assume rotational symmetry about the axis of the cylinder, that is, the azimuth gradients and fields are identically zero. In addition, we assume that the spatial gradients  $\partial_r$  are produced by the electric field. In other words, the plasma cannot be inhomogeneous in the direction in which there is no acceleration of particles due to electric field (e.g.,  $\partial_z = 0$ , if  $E_z = 0$ .

A general method to find the tensor coefficients  $f_m^{(l)}$  $[11,12]$  is based on the possibility of representing any tensor  $\bar{f}_m^{(l)}$  by a sum over all possible convolutions of tensors formed from the independent directions in a system. There are two independent directions determined by electric and magnetic fields in the system of cylindrical discharge. The electric field  $E(r, z)$  has axial and radial components generally, and its direction varies with the radial and axial positions. It is convenient to think that the electric field produces two orthogonal independent preferential directions  $\mathbf{E}_z$  and  $\mathbf{E}_r$ , which in accordance with the particular magnitude of  $E_r$  and  $E_z$  combine at every point  $(r, z)$  to give one  $\mathbf{E}(r, z)$ . The directions  $\mathbf{E}_z$  and  $\mathbf{E}_r$  remain independent of position. The magnetic field determines then the third direction. According to Ref.  $[12]$ , the tensor coefficients can be represented quite generally in the following form:

$$
f_m^{(l)} = \sum_{\lambda=0}^{\infty} \sum_{\lambda'=0}^{\infty} \sum_{\lambda''=0}^{\infty} \sum_{\lambda'''=0}^{\infty} \overline{f}(l, \lambda, \lambda', \lambda'', \lambda''')
$$
  
 
$$
\times \left[ [Y^{(\lambda''')}(\hat{\mathbf{E}}_z), Y^{(\lambda)}(\hat{\mathbf{E}}_r)]^{(\lambda')}, Y^{(\lambda'')}(\hat{\mathbf{B}})]_m^{(l)}, \quad (A1)
$$

where  $\bar{f}(l,\lambda,\lambda',\lambda'',\lambda''')$  are scalar coefficients. Parity considerations require  $\bar{f}(l, \lambda, \lambda', \lambda'', \lambda''') = 0$  unless

$$
\lambda''' + \lambda + l = \text{even.} \tag{A2}
$$

It follows, for **B** and  $\mathbf{E}_z$  directed along the *z* axis, that

$$
Y_{\mu''}^{(\lambda'')}(\hat{\mathbf{B}}) = (-i)^{\lambda''} [(2\lambda'' + 1)/4\pi]^{1/2} \delta_{\mu'',0},
$$
  

$$
Y_{\mu'''}^{(\lambda''')}(\hat{\mathbf{E}}_{\mathbf{z}}) = (-i)^{\lambda'''} [(2\lambda''' + 1)/4\pi]^{1/2} \delta_{\mu''',0}.
$$

Using the tensor coupling rule (e.g., Eq.  $(9)$  in [11]) we obtain the following representation:

$$
f_m^{(l)} = \sum_{\lambda=0}^{\infty} \sum_{\lambda'=0}^{\infty} \sum_{\lambda''=0}^{\infty} \sum_{\lambda''=0}^{\infty} \widetilde{f}(l, \lambda, \lambda', \lambda'', \lambda''') (-i)^{\lambda''+\lambda''}
$$
  
 
$$
\times (\lambda'''0\lambda m|\lambda'm)(\lambda'm\lambda''0|lm)Y_m^{(\lambda)}(\widehat{\mathbf{E_r}}).
$$
 (A3)

The functions  $\overline{f}$  and  $\overline{f}$  differ by the factor  $[(2\lambda''+1)(2\lambda''')$  $+1$ ]<sup>1/2</sup>/4 $\pi$ .

Let us reduce Eq.  $(A3)$  to the form of Eq.  $(9)$ . By comparing definitions for  $Y_m^{(\lambda)}$  and  $N_{l,m}$  given in Secs. II and III, we note that

$$
Y_m^{(\lambda)}(\theta,\varphi) = (-1)^l (-i)^{l+\lambda} N_{l,m} e^{-im\varphi} P_{\lambda}^{|m|}(\cos \theta) \sigma_{l,\lambda,|m|},
$$

where  $\sigma_{l,\lambda,|m|}$  is a scalar factor, which does not influence the symmetry properties; the angles  $\theta$  and  $\varphi$  specify the direction of vector  $\mathbf{E}_r$  in the spherical basis  $(r, \theta, \varphi)$ , associated with the cylindrical basis  $(z, r, \varphi)$ , apparently  $\theta = \pi/2$ . By substituting this relation into Eq.  $(A3)$  we see

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

with the expansion coefficients

$$
F_{l,m} = \sum_{\lambda \dots \lambda^m} \tilde{f}(l, \lambda, \dots, \lambda^m) \sigma_{l, \lambda, |m|} (-1)^l (-i)^{l + \lambda + \lambda'' + \lambda^m}
$$
  
 
$$
\times (\lambda^m 0\lambda m |\lambda' m) (\lambda' m \lambda'' 0 |lm) P_{\lambda}^{|m|}(\cos \theta).
$$
 (A4)

The equality (A4) results in a series of important properties for the coefficients  $F_{l,m}$  and the phase space distribution function  $(10)$ .

First, symmetry properties of the Clebsch-Gordan coefficients (e.g., Eq.  $(10)$  in [11]) require the complex conjugation of the coefficients  $F_{l,m}$  and  $F_{l,-m}$  [see Eq. (11)].

- f1g J. W. Bradley and G. Lister, Plasma Sources Sci. Technol. **6**, 524 (1997).
- $[2]$  N. F. Cramer, J. Phys. D  $30$ , 2573 (1997).
- [3] T. A. van der Straaten, N. F. Cramer, I. S. Falconer, and B. W. James, J. Phys. D 31, 191 (1998).
- f4g K. Nanbu, K. Mitsui, and S. Kondo, J. Phys. D **33**, 2274  $(2000).$
- [5] C. H. Shon, J. K. Lee, H. J. Lee, Y. Yang, and T. H. Chung, IEEE Trans. Plasma Sci. **26**, 1635 (1998).
- [6] E. Shidoji, E. Ando, and T. Makabe, Plasma Sources Sci. Technol. **8**, 621 (2001).
- [7] I. A. Porokhova, Yu. B. Golubovskii, J. Bretagne, M. Tichy, and J. F. Behnke, Phys. Rev. E 63, 056408 (2001).
- [8] R. D. White, R. E. Robson, B. Schmidt, and M. A. Morrison, J. Phys. D **36**, 3125 (2003).
- f9g I. P. Shkarofsky, T. W. Johnston, and M. P. Bachynski, *The Particle Kinetics of Plasmas* (Addison-Wesley, Reading, MA,  $1966$ ).
- $[10]$  J. Wilhelm and R. Winkler, Beitr. Plasmaphys. 8, 167  $(1968)$ ; R. Winkler, J. Wilhelm, and V. Schueller, *ibid.* **10**, 51 (1970).
- [11] R. E. Robson and K. F. Ness, Phys. Rev. A  $33$ , 2068 (1986).
- $[12]$  K. F. Ness, Phys. Rev. E 47, 327 (1993).
- [13] R. D. White, K. F. Ness, R. E. Robson, and B. Li, Phys. Rev. E **60**, 2231 (1999).
- f14g R. D. White, R. E. Robson, and K. F. Ness, Phys. Rev. E **60**, 7457 (1999).
- [15] R. E. Robson, R. Winkler, and F. Sigeneger, Phys. Rev. E 65, 056410 (2002).

Second, the associated Legendre function property  $[e.g.,]$ Eq.  $(A2)$  in [15]] imposes an additional condition at  $\theta = \pi/2$  for the field **E**<sub>r</sub>,

$$
\lambda + m = \text{even.} \tag{A5}
$$

In the absence of the axial electric field  $\mathbf{E}_z = \mathbf{0}$ ,  $\lambda''' = 0$ , conditions  $(A2)$  and  $(A5)$  combine to form the constraint  $(12)$ .

Thus, with reference to the axially homogeneous cylindrical magnetron discharge in crossed  $\mathbf{E}_r$  and  $\mathbf{B}_z$  fields (Fig. 1), the expansion coefficients  $F_{l,m}$  possess the properties specified by formulas  $(11)$  and  $(12)$ .

The presence of the axial electric field destroys the constraint  $(12)$ . In the case of only axial electric and magnetic fields, i.e., at  $\lambda = 0$  and  $m=0$ , the coefficients  $f_m^{(l)}$  in Eq. (A3) become real functions with one *l* index, i.e., the limiting case for the plane parallel geometry is realized. The distribution function here is independent of the magnetic field strength. At **B**=0,  $\lambda$ <sup>*n*</sup>=0, condition (A2) forces Im( $F$ <sub>*l,m*</sub>)=0 independently of the electric field configuration.

- [16] U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press, New York, 1959).
- [17] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1953).
- [18] R. Winkler, G. L. Braglia, and J. Wilhelm, Nuovo Cimento Soc. Ital. Fis., D **10**, 1209 (1988).
- [19] F. Sigeneger and R. Winkler, Eur. Phys. J.: Appl. Phys. 19,  $211(2002)$ .
- [20] C. Mark, Technical Rep. No. CRT 338 (Atomic Energy of Canada, 1957); Technical Rep. No. CRT 340 (Atomic Energy of Canada, 1957).
- [21] B. Davison and J. B. Sykes, *Neutron Transport Theory* (Oxford University Press, Oxford, 1957).
- [22] G. Petrov and R. Winkler, J. Phys. D **30**, 53 (1997).
- f23g B. Li, R. D. White, and R. E. Robson, J. Phys. D **35**, 2914  $(2002)$ .
- [24] R. E. Marshak, Phys. Rev.  $71$ , 443 (1947).
- f25g J. P. England and H. R. Skullerud, Aust. J. Phys. **50**, 553  $(1997).$
- [26] D. Loffhagen, F. Sigeneger, and R. Winkler, J. Phys. D 35, 1768 (2002).
- [27] L. L. Alves, G. Gousset, and C. M. Ferreira, Phys. Rev. E 55, 890 (1997).
- f28g E. W. McDaniel, *Collision Phenomena in Ionized Gases* (Wiley, New York, 1964).
- [29] J. H. Ingold, Phys. Rev. E  $56$ , 5932 (1997).
- [30] D. Loffhagen and R. Winkler, J. Phys. D **29**, 618 (1996).