

## Macrokinetic theory of electrons in gases

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A closed, macroscopic description of the dynamics of an assembly of electrons under the influence of a space-time-varying field is presented. This is accomplished by approximating the phase-space distribution function in an equivalent space whose coordinates are the infinite set of moments,  $\{m_j; j=1, \dots, \infty\}$ . An attempt has been made to formulate a rigorous procedure for obtaining approximate distributions with varying degrees of space-time resolution and for establishing their range of validity. Expressions are presented for the approximate distribution function and the transport parameters with resolution corresponding to the scale for energy relaxation.

### I. INTRODUCTION

In previous papers,<sup>1,2</sup> the macroscopic behavior of an assembly of electrons has been described using the concept of macrokinetic distribution (MKD) functions. These are velocity-dependent (kinetic) distributions with macroscopic space-time variation. It has been argued that, in general, the variables that characterize the macroscopic dynamics of the electron assembly depend on average properties of the single-particle kinetic distribution (KD),  $f(\mathbf{v}, \mathbf{r}, t)$  (where  $\mathbf{v}$  is velocity,  $\mathbf{r}$  is position, and  $t$  is time) over extended velocity intervals; moreover, that dynamical changes in these average properties occur over space-time scales that are coarser than those of the KD.<sup>1,2</sup> The KD has a space-time resolution corresponding to those of a two-body collision, and thus contains more information than necessary to provide a characterization of the assembly in terms of macroscopic variables. A distribution function with less space-time resolution (coarser) than that of the KD, and equivalent (as far as macroscopic properties) velocity dependence, can equally serve to determine macroscopic properties of the assembly. This distribution is the MKD. The scale of resolution of the MKD is dictated by the characteristic scales of variation of the dynamical macroscopic variables, which scales are self-consistently obtained as appropriate averages over the distribution function.

In formulating a theory for obtaining the MKD, the question arises as to which set of macroscopic variables can be used to specify with some measure the macroscopic scales of variation of the assembly. Moreover, given this set of variables, how can the corresponding (coarse) distribution function be determined and its range of validity assessed? These questions have been briefly treated in Refs. 1 and 2. This treatment has been partially based on physical arguments and on use of the Bogoliubov ansatz,<sup>3</sup> and provides neither rigorous answers to these questions nor a foundation for the establishment of the theory. In this paper, a macrokinetic theory is developed starting from basic principles. It makes use of moments of the KD to specify the macroscopic scales of variation. The theory is formally developed in the next section, and

applied in Sec. III to the description of an electron assembly with a resolution in the scale of energy relaxation.

### II. THEORETICAL FOUNDATIONS

At the kinetic level, the ensemble-averaged dynamic behavior of the assembly is described by the KD,  $f$ , which obeys an equation of the form<sup>3,4</sup>

$$\partial_t f + \mathbf{v} \cdot \nabla f + \frac{q}{m} \mathbf{E} \cdot \nabla_{\mathbf{v}} f = I(f), \quad (1)$$

where  $I(f)$  is the linear scattering operator. Equation (1) is the starting point for classical<sup>1</sup> and semiclassical<sup>5</sup> electron kinetics. Once the distribution function is found, desired space-time-dependent macroscopic properties (which can be measured) can be calculated by velocity averaging over the KD the corresponding microscopic properties.

To formulate a macroscopic description of an assembly of electrons using moments of the distribution to define its scale of resolution, a unique correspondence between the KD and the infinite set of moments,  $\{m_i(\mathbf{r}, t)\}$ ,<sup>6</sup> where  $m_i(\mathbf{r}, t)$  corresponds to a velocity moment of the distribution, which may be a scalar, vector, or tensor, is established. For algebraic simplicity in presenting the formulation of this description, consider a distribution in one-dimensional (1D) velocity and configuration variables,  $(v, x)$ . Expressing the distribution in terms of its characteristic function,  $\phi(s, x, t)$ , where<sup>6</sup>

$$f(v, x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-isv} \phi(s, x, t) ds \quad (2a)$$

and using the series representation for  $\phi$ ,<sup>6</sup>

$$\phi(s, x, t) = \sum_{j=0}^{\infty} \frac{m_j(x, t)}{j!} (is)^j. \quad (2b)$$

A formal expression can be obtained for the distribution in terms of its moments; namely,

$$f(v, x, t) = \sum_j m_j(x, t) g_j(v) \quad (2c)$$

with

$$g_j(v) = \frac{1}{j!} (-1)^j \partial_v^j \delta(v),$$

where  $\delta(v)$  is the Dirac delta function. Equation (2c) indicates that the space-time dependence of the distribution may be regarded as implicit through its moments. To exhibit this dependence, the arguments of the distribution may be rewritten as follows:

$$f(v, x, t) = f(v, \{m_j(x, t)\}) = f(v, \{m_j\}). \quad (2d)$$

An alternate (formal) approach to Eq. (1) for obtaining  $f$  is to use Eq. (2a) and the equations for the  $\{m_j\}$ 's. These are obtained from Eq. (1) by taking velocity moments.<sup>1,2</sup> In 1D, these are

$$\partial_t m_j + \partial_x m_{j+1} - a j m_{j-1} = \int v^j I(f) dv, \quad (3a)$$

with

$$a = \frac{q}{m} E$$

and

$$m_s = \int v^s f dv.$$

An integral without limits implies integration over all velocity space.

To obtain a formal closed set of equations for the  $\{m_j\}$ 's, substitute the expansion for  $f$ , Eq. (2c), into (3) to obtain

$$\partial_t m_j + \partial_x m_{j+1} - a j m_{j-1} = - \sum_v C_{jv} m_v \quad (3b)$$

with

$$C_{jv} = - \int v^j I(g_v) dv. \quad (3c)$$

Regard the sequence  $\{m_j\}$  as being arranged according to increasing values of  $|C_{jj}|$  (this corresponds to an ordering of the sequence of moments), and consider time scales such that

$$|\partial_t m_j| < |C_{jj} m_j| \quad \text{for } j > k, \quad (4)$$

where  $k$  is the highest moment not satisfying this inequality. Equation (3b) for  $j > k$  can be rewritten in the form

$$\partial_x M_h + A M_h = B M_k, \quad (5a)$$

where  $M_h$  and  $M_k$  are column vectors whose components are the moments  $m_j$ ,  $j > k$  and  $m_i$ ,  $1 < i \leq k$ , respectively; and,  $A$  and  $B$  are matrices whose elements are obtained from the coefficients in Eq. (3b). Treating the term proportional to  $M_k$  as a source term, Eq. (5a) can formally be solved for  $M_h$ ,

$$M_h(x, t) = \exp \left[ \int_0^x A(x', t) dx' \right]_+ M_h(0, t) + \sum_i T_i \partial_x^i M_k(x, t) \quad (5b)$$

where

$$T_i = \sum_j \int_0^x dx_1 \int_0^{x_1} dx_2 \cdots \int_0^{-x_{j-1}} dx_j A(x_1, t) \cdots A(x_j, t) \int_0^{x_j} B(\xi, t) \frac{(\xi - x)^i}{i!} \quad (5c)$$

and the subscript  $+$  indicates a space-ordered product of matrices [similar to Eq. (5c)]. Thus, in the region where the contribution from the first term can be neglected (this requirement determines how far from the boundary, at  $x=0$ , the results are valid), Eq. (5b) establishes that

$$m_{j>k} = \mathcal{F}(\{m_{s=k_j, \dots, 1}\}, \{\partial_x^i m_{s=k_j, \dots, 1}; i=1, \dots, \infty\}), \quad (6)$$

where  $\mathcal{F}(\ )$  represents a function of. Using this observation, a distribution function,  $f_M^{(k)}$  can be defined with resolution in the time scale of Eq. (4). Using Eq. (6) in Eq. (2d), this distribution has a functional dependence of the form

$$f_M^{(k)} = f(v, \{m_{s=k, \dots, 1}\}, \{\partial_x^i m_{s=k, \dots, 1}; i=1, \dots, \infty\}). \quad (7)$$

The transition from Eq. (2d) to Eq. (7) can be given a geometrical interpretation. Consider  $f$  to be a vector in the infinite  $\{m_{j=1, \dots, \infty}\}$  space. Equation (7) represents an approximation to  $f$  where the contribution from the coordinates  $m_j$ ,  $j > k$  are approximated (for times  $> C_{jj}^{-1}$ ) by the  $i$ th space derivative of the lower moments,  $\partial_x^i m_j$ ,  $j \leq k$ . This procedure corresponds to an approximation

in the infinite  $\{m_j\}$  space as opposed to a projection in  $v$  space, in which a finite subset of a complete set of  $v$ -space functions are used to represent the phase-space distribution.<sup>4,7,8</sup> Moreover, Eq. (7) represents a variation from the Bogoliubov<sup>3</sup>-Chapman-Enskog<sup>9</sup> ansatz in that the derivatives of the moments are explicitly treated as independent coordinates that are used to properly account for the contribution from the higher-order moments.

The discussion leading to Eq. (7) suggests a procedure for obtaining a macroscopic description of the electron assembly. For a given scale of resolution specified by  $k$  in Eq. (4) (or equivalently, for a given finite set of moments), a distribution function,  $f_M^{(k)}$ , is defined whose functional dependence is given by Eq. (7). A formal expression for  $f_M^{(k)}$  can be obtained by substituting Eq. (5b) into Eq. (2a). Each value of  $k$  defines a scale of resolution [assuming no degeneracy in the  $C_{vj}$ , Eq. (3c), otherwise the number is accordingly reduced]. The set of  $f_M^{(k)}$  have been collectively named macrokinetic distributions (MKD).<sup>2</sup> This name refers to the fact that these are velocity-dependent (kinetic) distributions with macroscopic space-time resolution.

An alternate approach than using Eq. (2c) for obtaining a working expression for the MKD is to solve its

defining differential equation. This equation can be obtained from Eq. (1) by noting that in the scale of resolution of Eq. (4) (and returning to 6D space),<sup>1,2</sup>

$$f(\mathbf{v}, \mathbf{r}, t) \equiv f_M^{(k)}.$$

It is convenient to define the normalized  $i$ th spatial derivative of  $m_j$ ,  $G_{ij}$ , which is symbolically written as  $\nabla^i m_j / m_j$  (where  $\nabla$  is the spatial gradient, and the nature of the  $\nabla^i$  operation depends on whether  $m_j$  is a scalar, vector, or tensor) and rewrite Eq. (7) as

$$f_M^{(k)} = f(\mathbf{v}, \{m_j = k, \dots, 1\}, \{G_{ij} = k, \dots, 1; i = 1, \dots, \infty\}). \quad (8)$$

With this dependence,

$$\partial_t f = \sum_{j=1}^k \left[ \partial_{m_j} f_M^{(k)} \partial_t m_j + \sum_i \partial_{G_{ij}} f_M^{(k)} \partial_t G_{ij} \right], \quad (9a)$$

$$\nabla f = \sum_{j=1}^k \left[ \partial_{m_j} f_M^{(k)} \nabla m_j + \sum_i \partial_{G_{ij}} f_M^{(k)} \nabla G_{ij} \right], \quad (9b)$$

$$\nabla_{\mathbf{v}} f = \nabla_{\mathbf{v}} f_M^{(k)}. \quad (9c)$$

Using the 3D version of Eq. (3a) for the  $m_j$ 's and Eqs. (9a)–(9c) in Eq. (1), the defining equation for  $f_m^{(k)}$  is obtained.<sup>1</sup>

For electrons in gases, the sequence  $\{m_j\}$  [arranged as indicated in the statement following Eq. 3(c)] is given by  $(n, n\bar{\epsilon}, n\mathbf{u}, \dots)$ , where  $n$ ,  $\bar{\epsilon}$ , and  $\mathbf{u}$  are the electron density, mean energy, and average velocity, respectively, and the ellipses corresponds to higher-order moments.<sup>1</sup> This is a consequence of the fact that  $C_{11} < C_{22} < C_{33} < \dots$ , where the  $C_{jj}^{-1}$ 's are the characteristic time scales of  $n$  ( $j=1$ ),  $n\bar{\epsilon}$  ( $j=2$ ),  $n\mathbf{u}$  ( $j=3$ ), and so on.<sup>10</sup> The macrokinetic description of the electron assembly with a resolution corresponding to  $C_{11}^{-1}$  [ $k=1$  in Eq. (4)], yields the theory of drift and diffusion,<sup>1,2</sup> which is based on the continuity equation [Eq. (10b) below]. Macrokinetic descriptions with resolution in the  $C_{22}^{-1}$  time scale has been discussed by Roumeliotis and Cram<sup>11</sup> and in the  $C_{33}^{-1}$  time scale have been discussed by Kunhardt, Wu, and Penetrante.<sup>1</sup> However, the MKD that has been used to close the moment equations in this last case is obtained

from that corresponding to the  $C_{22}^{-1}$  time scale.

In this paper, the theory corresponding to the  $C_{22}^{-1}$  time scale, i.e., that of energy relaxation, is developed from the theory presented in this section. It provides a suitable description of the evolution of the assembly for fields that are changing with time at rates up to  $C_{22}$ . In this time scale, the  $M_k$  vector in Eq. (5a) only contains two elements,  $n$  and  $n\bar{\epsilon}$ . The equations corresponding to Eq. (3a) are, in 3D,<sup>1</sup>

$$\partial_t n + \nabla \cdot (n\mathbf{u}) = \nu n, \quad (10a)$$

$$\partial_t (n\bar{\epsilon}) + \nabla \cdot (\epsilon \mathbf{v}) - q\mathbf{E} \cdot n\mathbf{u} = -\nu_{\epsilon} n\bar{\epsilon}, \quad (10b)$$

where

$$n\mathbf{u} = \int \mathbf{v} f_M^{(2)} d\mathbf{v}, \quad (10c)$$

and the angular bracket implies an average over the distribution  $f_M^{(2)}$ ,  $\epsilon = \frac{1}{2}mv^2$ , and  $\nu (=C_{11})$ ,  $\nu_{\epsilon} (=C_{22})$  are the (space-time-dependent) effective ionization, and energy-exchange frequencies, respectively. These frequencies are defined by

$$\nu n = \int I(f) d\mathbf{v},$$

$$-\nu_{\epsilon} n\bar{\epsilon} = \int \frac{1}{2}mv^2 I(f) d\mathbf{v},$$

with  $f = f_M^{(2)}$ . The equation for  $f_M^{(2)}$  is presented in the next section, and is solved (approximately) for the case of a quasi-Lorentz gas model of the collision operator in Eq. (1).<sup>2,12</sup>

### III. DESCRIPTION OF THE ELECTRON ASSEMBLY IN THE ENERGY EXCHANGE TIME SCALE

In the time scale of energy exchange,  $\tau_{\epsilon} (= \nu_{\epsilon}^{-1})$ , Eqs. (4) and (8) lead to

$$f_M^{(2)} = f(\mathbf{v}, n, n\bar{\epsilon}, \{g_i\}, \{h_i\}; i = 1, \dots, \infty),$$

where  $g_i = (\nabla^i n)/n$  and  $h_i = (\nabla^i n\bar{\epsilon})/n\bar{\epsilon}$ , with the same interpretation for the  $\nabla^i$  operation as in Eq. (8). Placing Eqs. (10a) and (10b) and Eqs. (9a) and (9b) (with  $k=2$ ) into Eq. (1), the equation for  $f_M^{(2)}$  is obtained; namely,

$$\mathbf{a}_1 \cdot \nabla n + \mathbf{a}_2 \cdot \nabla n\bar{\epsilon} + \sum_i \mathbf{a}_3 \cdot \nabla g_i + \sum_i \mathbf{a}_4 \cdot \nabla h_i + \partial_n f_M^{(2)} \nu n + \partial_{n\bar{\epsilon}} f_M^{(2)} \left[ q\mathbf{E} \cdot \int \mathbf{v} f_M^{(2)} d\mathbf{v} - \nu_{\epsilon} n\bar{\epsilon} \right] + \frac{q\mathbf{E}}{m} \cdot \nabla_{\mathbf{v}} f_M^{(2)} = I(f_M^{(2)}) + O(\nabla^2), \quad (11a)$$

where  $O(\nabla^2)$  represents terms proportional to the second spatial derivatives of  $n$  and  $n\bar{\epsilon}$ , and

$$\mathbf{a}_1 = - \left[ \partial_n f_M^{(2)} \int \mathbf{v} \partial_n f_M^{(2)} d\mathbf{v} + \partial_{n\bar{\epsilon}} f_M^{(2)} \int \frac{1}{2}mv^2 \mathbf{v} \partial_n f_M^{(2)} d\mathbf{v} - \mathbf{v} \partial_n f_M^{(2)} \right], \quad (11b)$$

$$\mathbf{a}_2 = - \left[ \partial_n f_M^{(2)} \int \mathbf{v} \partial_{n\bar{\epsilon}} f_M^{(2)} d\mathbf{v} + \partial_{n\bar{\epsilon}} f_M^{(2)} \int \frac{1}{2}mv^2 \mathbf{v} \partial_{n\bar{\epsilon}} f_M^{(2)} d\mathbf{v} - \mathbf{v} \partial_{n\bar{\epsilon}} f_M^{(2)} \right], \quad (11c)$$

$$\mathbf{a}_3 = - \left[ \partial_n f_M^{(2)} \int \mathbf{v} \partial_{g_i} f_M^{(2)} d\mathbf{v} + \partial_{n\bar{\epsilon}} f_M^{(2)} \int \frac{1}{2} m v^2 \mathbf{v} \partial_{g_i} f_M^{(2)} d\mathbf{v} - \mathbf{v} \partial_{g_i} f_M^{(2)} \right], \quad (11d)$$

$$\mathbf{a}_4 = - \left[ \partial_n f_M^{(2)} \int \mathbf{v} \partial_{h_i} f_M^{(2)} d\mathbf{v} + \partial_{n\bar{\epsilon}} f_M^{(2)} \int \frac{1}{2} m v^2 \mathbf{v} \partial_{h_i} f_M^{(2)} d\mathbf{v} - \mathbf{v} \partial_{h_i} f_M^{(2)} \right], \quad (11e)$$

with the conditions

$$\int f_M^{(2)} (\frac{1}{2} m v^2) d\mathbf{v} = n \bar{\epsilon},$$

$$\int f_M^{(2)} d\mathbf{v} = n.$$

Equation (11) is the working equation from which various approximations to  $f_M^{(2)}$  can be obtained using perturbation procedures. The perturbation parameter can be taken to be proportional to any of the  $g_i$ 's or  $h_i$ 's which are considered to be small in a given situation. To simplify the algebra (for the sake of clarity), assume that the applied electric field is in the  $z$  direction [ $\mathbf{E} = E_0(z, t) \mathbf{a}_z$ , where  $\mathbf{a}_z$  is a unit vector in the  $z$  direction] and that the spatial variations in energy and density are also in the same direction ( $\nabla \rightarrow \partial_z \mathbf{a}_z$ ). Depending on the magnitude

of the electric field term in Eq. (11a) [last term on the left-hand side (lhs)] as compared to the other terms on the lhs, solutions for  $f_M^{(2)}$  can be obtained that differ in their range of validity. In this paper, the lowest-order solution to Eq. (11) is obtained in the regime where the spatial derivatives are small.

In order to proceed further with the discussion, consider a quasi-Lorentz gas model ( $m/M \ll 1$ ,  $M$  is the mass of a neutral gas atom per molecule) for conditions such that the ionization rate  $\nu$  is zero and the only spatial derivatives of importance are the gradients of density and mean energy (the objective being the investigation of their first-order effects). Moreover, only the contributions from the linear terms in  $f_M^{(2)}$  [the last terms in Eqs. (11b) and (11c)] are to be retained. Transforming variables from  $(v_x, v_y, v_z, n\bar{\epsilon})$  to  $(v_x, v_y, \xi, n, \zeta)$ , with  $\xi = v_z - n\bar{\epsilon}/(mnu)$ ,  $\zeta = (n\bar{\epsilon}/(mnu))$ , and consequently,

$$\partial_{v_z} = \partial_\xi, \quad (12a)$$

$$\partial_{n\bar{\epsilon}} = \frac{1}{mnu} (\partial_\zeta - \partial_\xi) + O(\partial_{n\bar{\epsilon}} nu), \quad (12b)$$

and letting

$$f_M^{(2)} = n f_M(\mathbf{v}, n\bar{\epsilon}),$$

Eq. (11) becomes

$$v_z f_M \partial_z n + v_z n \frac{\partial_z n \bar{\epsilon}}{mnu} (-\partial_\xi f_M + \partial_\zeta f_M) + \frac{n^2}{mnu} qE_0 \int v_z f_M d\mathbf{v} (-\partial_\xi f_M + \partial_\zeta f_M) + n v_\epsilon \frac{n\bar{\epsilon}}{mnu} (\partial_\xi f_M - \partial_\zeta f_M) + \frac{qE_0}{m} n \partial_\xi f_M = n I(f_M), \quad (13a)$$

where the coefficients are yet to be written in terms of  $\xi$  and  $\zeta$ . Since

$$u = \int v_z f_M d\mathbf{v},$$

the last term in the lhs of Eq. (13a) cancels the first contribution in parentheses from the third term; and, dividing through by  $n$ , Eq. (13a) becomes

$$v_z \frac{\partial_z n}{n} f_M + v_z \frac{\partial_z n \bar{\epsilon}}{mnu} (-\partial_\xi f_M + \partial_\zeta f_M) + \frac{v_\epsilon n \bar{\epsilon}}{mnu} \partial_\xi f_M + \left[ \frac{qE_0}{m} - \frac{v_\epsilon n \bar{\epsilon}}{mnu} \right] \partial_\xi f_M = I(f_M). \quad (13b)$$

Writing the coefficients in terms of  $\xi$  and  $\zeta$  (since  $v_z = \xi + \zeta$  and  $n\bar{\epsilon} = \zeta mnu$ ) and rearranging terms, Eq. (13b) reduces to

$$\left[ 1 - \frac{(\xi + \zeta)}{qE_{eq}/m} \frac{\partial_z n \zeta}{n} \right] \partial_\xi f_M - \frac{m}{qE_{eq}} I(f_M) = - \frac{(\xi + \zeta)}{qE_{eq}/m} \frac{\partial_\zeta n}{n} f_M + \left[ - \frac{(\xi + \zeta)}{qE_{eq}/m} \frac{\partial_z(n\zeta)}{n} + \frac{E_0 - E_{eq}}{E_{eq}} \right] \partial_\zeta f_M, \quad (13c)$$

where

$$E_{eq} = \frac{v_\epsilon n \bar{\epsilon}}{qnu}. \quad (13d)$$

Consider situations where

$$\frac{E - E_{eq}}{E_{cd}} < \frac{\xi + \zeta}{qE_{eq}/m} \frac{\partial_z(n\zeta)}{n}, \frac{\xi + \zeta}{qE_{eq}/m} \frac{\partial_z n}{n} < 1. \quad (13e)$$

This defines the range of validity of the solution to Eq. (13c) obtained below. In particular, it imposes a condition on the rate of change of mean energy, Eq. (10b). The ordering of the first inequality is not necessary; its only purpose is to highlight in first order the contribution from the spatial derivatives. As a consequence of the ordering, the second term inside each large parentheses in Eq. (13c) can be neglected in comparison to the corresponding first term, and regular perturbation theory can

be used to solve the resulting equation by treating the rhs as a source. It is convenient to make a further change of variables from  $(v_x, v_y, \xi, n, \zeta)$  to  $(w_x, w_y, w_z, n, n\bar{e})$ , where  $v_x = w_x$ ,  $v_y = w_y$ ,  $(\xi + \zeta) = w_z$ ,  $mnu\zeta = n\bar{e}$ .<sup>13</sup> To obtain an analytic solution to the resulting equation, a spherical harmonics expansion of  $f_M$  in terms of  $\mathbf{w}$  is used, namely,

$$f_M(\mathbf{w}, n, n\bar{e}) = \sum_i f_{M_i}(w, n, n\bar{e}) P_i(\cos\theta).$$

Substituting this expansion in Eq. (13c), using the orthogonality properties of  $P_i(\cos\theta)$ , and keeping only the first two terms in the expansion, the following equations are obtained for the coefficients  $f_{M_0}$  and  $f_{M_1}$ :

$$\frac{1}{3w^2} \partial_w (w^2 a_{\text{eq}} f_{M_1}) - \frac{1}{w^2} \partial_w (\alpha f_{M_0} + \beta \partial_w f_{M_0}) = -\frac{W}{3} \left[ \frac{\partial_z n \bar{e}}{mnu} \partial_w f_{M_0} + \partial_z n \bar{e} \partial_{n\bar{e}} f_{M_1} + \frac{\partial_z n}{n} f_{M_1} \right] \quad (14a)$$

and

$$\frac{3}{5} \frac{w}{v_m} \frac{\partial_z n \bar{e}}{mnu} \partial_w f_{M_1} + f_{M_1} = -\frac{a_{\text{eq}}}{v_m} \partial_w f_{M_0} - \frac{w}{v_m} \left[ \partial_z n \bar{e} \partial_{n\bar{e}} f_{M_0} + \frac{\partial_z n}{n} f_{M_0} \right], \quad (14b)$$

where  $a_{\text{eq}} = qE_{\text{eq}}/m$  and the quasi-Lorentz collision operator has been used; namely,

$$I(f_M) = \frac{1}{w^2} \partial_w (\alpha f_{M_0} + \beta \partial_w f_{M_0}) - v_m f_{M_1} \cos\theta$$

with

$$\alpha = \frac{m}{M} w^3 v_m,$$

$$\beta = \frac{kT}{M} w^2 v_m,$$

$$v_m = N \sigma_m(w) w,$$

with the condition  $\int f_0 w^2 dw = 1$ .  $\sigma_m(w)$  is the momentum transfer cross section,  $N$  and  $T$  are the density and temperature, respectively, of the background gas. Subsequently, the first term in the rhs of Eq. (14b) is neglected with respect to the second term so that

$$f_{M_1} = -\frac{a_{\text{eq}}}{v_m} \partial_w f_{M_0} - \frac{w}{v_m} \left[ \partial_z n \bar{e} \partial_{n\bar{e}} f_{M_0} + \frac{\partial_z n}{n} f_{M_0} \right]. \quad (14c)$$

As pointed out in Ref. 2, Eqs. (14a) and (14c) have a similar form as the equations for  $f_0$  and  $f_1$  obtained by spherical harmonics expansion of the *steady-state* Boltzmann equation<sup>14</sup> with a quasi-Lorentz collision term, and with the  $\partial_z f_1, \partial_z f_0$  terms expressed in terms of the variables  $n\bar{e}$  and  $n$ . The physics of the two sets of equations, however, are strikingly different. Equations (14a) and (14c) are also *time dependent*, in that the “acceleration”  $a_{\text{eq}}$ , is space-time-dependent and only indirectly related to the applied field (recall  $a_{\text{eq}} = v_e n \bar{e} / mnu$ ); whereas the acceleration in the equations for  $f_0$  and  $f_1$  is simply due to the applied field. Note that the corresponding *time-dependent* equations for  $f_0$  and  $f_1$  are actually valid in the same time scale as Eqs. (14a) and (14c), namely, that of energy relaxation. However, the corresponding complete equation in this time scale obtained by projecting in moment space is Eq. (13c), where no specific assumptions have been made re-

garding the velocity dependence of the distribution. In fact, it can account for highly singular distributions in velocity space, as occurs, for example, at very high fields or when inelastic scattering is of the same order as elastic scattering.

The physical interpretation of Eqs. (14a) and (14c) is as follows. The applied field  $\mathbf{E}$  appears as a source term in the moment equations [Eqs. (10)] and as such causes changes in  $n$  and  $n\bar{e}$ . These equations determine the evolution of  $n$  and  $n\bar{e}$  in the scale of energy relaxation, and consequently, serve as “filters” for the applied field in that the fluid variables  $n$  and  $n\bar{e}$  cannot follow any faster variations that the applied field may contain. Thus, the equivalent field, Eq. (13d), corresponds to the “filtered” field that the distribution “sees” that is consistent with the corresponding changes in  $n$  and  $n\bar{e}$ .

In the two-term spherical harmonics and quasi-Lorentz gas approximations, Eq. (10c) for the current density can be written, with use of Eqs. (12) and (14b), as

$$\begin{aligned} nu \mathbf{a}_z = & \left[ -n \int \frac{4\pi}{3} \frac{w}{v_m} a_{\text{eq}} \partial_w f_{M_0} w^2 dw \right. \\ & - n \partial_z n \bar{e} \int \frac{4\pi}{3} \frac{w^2}{v_m} \partial_{n\bar{e}} f_{M_0} w^2 dw \\ & \left. - \partial_z n \int \frac{4\pi}{3} \frac{w^2}{v_m} f_{M_0} w^2 dw \right] \mathbf{a}_z \quad (15a) \end{aligned}$$

or, in terms of transport parameters,

$$nu = Wn + D \partial_z n, \quad (15b)$$

where  $W$  and  $D$  are the drift velocity and diffusion coefficients, respectively, defined as

$$\begin{aligned} W = & - \int \frac{4\pi}{3} \frac{w}{v_m} a_{\text{eq}} \partial_w f_{M_0} v^2 dw \\ & - \partial_z n \bar{e} \int \frac{4\pi}{3} \frac{w^2}{v_m} \partial_{n\bar{e}} f_{M_0} w^2 dw \quad (16a) \end{aligned}$$

and

$$D = - \int \frac{4\pi}{3} \frac{w^2}{v_m} f_{M_0} w^2 dw. \quad (16b)$$

Similarly, using Eqs. (12) and (14b), and the two-term approximation, the mean energy flow,  $\langle \epsilon \mathbf{w} \rangle$  in Eq. (10b), takes the form,

$$\begin{aligned} \langle \epsilon \mathbf{v} \rangle = \langle \epsilon \mathbf{w} \rangle = & -n \int \frac{4\pi}{3} \frac{m}{2} \frac{a_{\text{eq}}}{v_m} w^3 \partial_w f_{M_0} w^2 dw \\ & -n \partial_z n \bar{\epsilon} \int \frac{4\pi}{3} \frac{m}{2} \frac{w^2}{v_m} \partial_{n\bar{\epsilon}} f_{M_0} w^2 dw \\ & -\partial_z n \int \frac{4\pi}{3} \frac{m}{2} \frac{w^4}{v_m} f_{M_0} w^2 dw. \end{aligned} \quad (17)$$

Separating the component proportional to  $\partial_z \bar{\epsilon}$  in Eq. (16), a coefficient of mean energy conduction can be defined in analogy to that of thermal conductivity. This is further discussed below.

The lowest-order solution for  $f_0$  is obtained from Eq. (14a) by neglecting contributions from the rhs. For  $\sigma_m(w)$  proportional to  $w^{-1}$  (i.e., constant collision frequency) and  $(a_{\text{eq}}/v_m)^2 \gg kT/m$ , this solution has the form of a Maxwellian distribution,<sup>10</sup>

$$f_{M_0} = \frac{1}{\pi^{3/2} \theta^3} \exp(-w/\theta)^2, \quad (18a)$$

where

$$\theta = \left[ \frac{2M}{3m} \right]^{1/2} \frac{v_\epsilon}{v_m} \frac{\bar{\epsilon}}{mu}. \quad (18b)$$

It is valid in the regime defined by Eqs. (13e) and (14b). This result can now be used to explicitly evaluate the averages defined in Eqs. (10a)–(10c),  $n\mathbf{u}$  and  $\langle \epsilon \mathbf{w} \rangle$ ,<sup>15</sup> alternatively, Eqs. (16) and (17). From Eqs. (17) and (16a), the drift velocity component of  $n\mathbf{u}$  is

$$W = (1 + \delta) W_0, \quad (19a)$$

where

$$W_0 = \left[ \frac{v_\epsilon \bar{\epsilon}}{v_m m} \right]^{1/2} \quad (19b)$$

and

$$\delta = -\frac{M}{3m} \left[ \frac{v_\epsilon}{v_m} \right]^{1/2} \frac{\partial_z \bar{\epsilon}}{v_m (m \bar{\epsilon})^{1/2}}. \quad (19c)$$

Note that in this time scale, the drift velocity does not explicitly depend on the applied electric field  $E_0$  so that the mobility ( $W/E_0$ ) may not be a useful concept. (This is further discussed below.) Letting  $v_\epsilon \approx \eta v$ , with the energy loss factor  $\eta$  approximately equal to  $2.66m/M$ ,<sup>10</sup> Eqs. (19b) and (19c) become

$$W_0 \approx 1.63(\bar{\epsilon}/M)^{1/2}, \quad (20a)$$

$$\delta \approx 0.38 \left[ \frac{M}{m} \right]^{1/2} \frac{\partial_z \bar{\epsilon}}{v_m \bar{\epsilon}}. \quad (20b)$$

Thus, for example, in situations where  $(M/m) \approx 10^3$ ,  $v_m \approx 10^{11} \text{ sec}^{-1}$ , and  $\partial_z \bar{\epsilon}/\bar{\epsilon} \approx 10^2$  [which can occur at high  $E/N$  (Ref. 16)], the percentage change in drift velocity is of the order of 20%. For such cases, the descrip-

tion of the evolution of an isolated electron swarm in the scale of energy relaxation needs to take into account the effect of energy gradients on the drift velocity. From Eqs. (18) and (16b), the diffusion coefficient is similarly found,

$$D \approx 0.9\bar{\epsilon}/(m v_m). \quad (21)$$

Energy gradients have no effect on the diffusion coefficient in this order of approximation.

From Eqs. (17) and (18), the average of energy flow is found to be

$$\langle \epsilon \mathbf{w} \rangle = \frac{5}{6} M \left[ \frac{v_\epsilon \bar{\epsilon}}{v_m mu} \right] \left[ u - \frac{2}{3} \frac{M}{m} \left[ \frac{v_\epsilon}{v_m} \right]^2 \frac{\bar{\epsilon}}{mu} \frac{\partial_z \bar{\epsilon}}{mu v_m} \right] n$$

and with the use of Eq. (19)

$$\langle \epsilon \mathbf{v} \rangle \approx \frac{5}{6} M W_0^2 u + J_Q, \quad (22)$$

where  $J_Q$  plays the role of mean energy current, and has the form of Fourier's law

$$J_Q = -\kappa \partial_z \bar{\epsilon} \quad (23)$$

with  $\kappa$ , the mean energy conductivity, defined by

$$\kappa = \frac{5}{9} \left[ \frac{M}{m} \right]^2 \left[ \frac{v_\epsilon}{v_m} \right]^2 n \frac{\bar{\epsilon}}{v}. \quad (24a)$$

For  $v_\epsilon/v_m \approx 2.66m/M$ ,

$$\kappa = 3.99n\bar{\epsilon}/v_m$$

or

$$\kappa/D = 4.5mn. \quad (24b)$$

For conditions in which the rate of change of mean energy with respect to time is small in comparison to the last term in Eq. (10b),  $E_{\text{eq}} = E$ ; then, neglecting gradient contributions, Eqs. (13d) and (19b) become

$$\bar{\epsilon} \approx \frac{q^2 E^2}{m v_\epsilon v_m} \quad (25a)$$

and

$$W \approx qE/m v_m \quad (25b)$$

as expected from Eqs. (10). In this limit, only the changes of density with time [Eq. (9a)] are significant. This is the hydrodynamic regime which has been discussed in a previous paper.<sup>2</sup>

Higher-order contributions to  $n\mathbf{u}$  arising from the terms proportional to  $a_i$ ,  $i=1-4$  in Eq. (10a) can be obtained by extending the calculation of  $f_M^{(2)}$  to the next order. In situations where the spatial gradients are strong, the terms proportional to  $\partial_z n$  and  $\partial_z n\bar{\epsilon}$  in Eq. (11a) need to be taken into account in lowest order, as shown in Ref. 2.

Recently, Ingold<sup>17</sup> has obtained expressions for  $W$ ,  $D$ , and  $\langle \epsilon \mathbf{w} \rangle$  by assuming (for  $v_m = \text{const}$ ) a distribution of the form given by Eq. (17), and further assuming  $\theta$  to be proportional to  $\bar{\epsilon}$ . This form of distribution has also been used by Roumeliotis and Cram<sup>11</sup> as an approximate MKD in the  $C_{22}^{-1}$  time scale. These assumptions yield re-

sults that are similar to those presented here for situations where the ratio  $v_e/v_m$  is independent of the mean energy. A subtle difference appears when considering the approach they used for obtaining  $\theta$ . The equation for  $\theta$  is obtained by requiring self-consistency between the mean energy obtained by taking the energy moment of Eq. (17) and the mean energy obtained from Eq. (10b). If Eq. (17) were the exact distribution, then this requirement must be true. However, since it is an approximate distribution, Eq. (10b) should be used to define  $\bar{\epsilon}$ , while the approximate distribution should be used to approximate [in lowest order in the case of Eq. (17)] the value for the unknown parameters in Eq. (10b). To achieve self-consistency, higher-order corrections to Eq. (17) would have to be used. An issue that remains to be addressed is the sensitivity of the solution to Eq. (10b) to errors in the value of the parameters.

#### IV. CONCLUDING REMARKS

A closed, macroscopic description of the dynamics of an assembly of electrons under the influence of space-time varying fields has been presented. This has been accomplished by approximating the distribution function  $f$  in a space whose coordinates are the infinite set of moments,  $\{m_j; j=1, \dots, \infty\}$ . For a given scale of resolution [defined by Eq. (4)], it has been shown that moments with faster variations can be formally expressed in terms of the slower moments and their spatial derivatives [Eq. (5)]. Thus, an approximate distribution function  $f_M^{(k)}$  can be obtained in the alternate space whose coordinates are the slower moments and their derivatives [Eq. (7)]. To each resolution scale corresponds a different  $f_M^{(k)}$ , distinguished by the index  $k$ . These distributions have been called macrokinetic distributions (MKD) since they are distributions in velocity space with macroscopic space-time resolution. The distribution obtained via the Bogoliubov<sup>3</sup>-Chapman-Enskog<sup>9</sup> ansatz corresponds to one of these distributions for  $k=3$ .

The approach presented in this paper is conceptually different from those that approximate the phase-space distribution by using projections in  $\mathbf{v}$  space.<sup>4,7,8,14</sup> In these projections, the dependence of  $f$  on  $\mathbf{v}$  may be severely altered in velocity ranges that may significantly contribute in the calculations of transport parameters

and rate coefficients.<sup>18</sup> What is desired for this purpose is a distribution with no *a priori* assumptions made regarding its velocity dependence, and possessing a space-time resolution which at least corresponds to that of the macroscopic description to which these parameters and coefficients pertain. This upper limit is provided by the MKD. Note that the use of the MKD does not preclude the possibility for using truncated expressions in velocity space to obtain an approximate solution to Eq. (11) for the MKD. This has in fact been done in Sec. III. However, other approaches (including computational) are available for obtaining such a solution.

In the scale of the electron energy exchange time, the description of the assembly is given (for constant collision frequency) by Eqs. (10), (11), and (17). In this time scale, the electron density and mean energy are independent variables that specify the dynamics of the assembly. The applied electric field influences the velocity distribution only through its effect on the mean energy. For applied fields with space-time variations in the scale of the mean energy, Eq. (10b) must be used to determine the behavior of  $n\bar{\epsilon}$ .  $n\bar{\epsilon}$  in turn determines the equivalent field [Eq. (13b)] that drives the MKD corresponding to this scale of resolution. This MKD is used in the calculation of the energy relaxation time in a self-consistent manner.

To illustrate the approach formally outlined in Sec. II, expressions for the MKD in the regime defined by the energy exchange rate have been derived in Sec. III for the case of collisions with cross section proportional to  $w^{-1}$ . Expressions for the unknown averages defined in Eqs. (9) have been obtained [Eqs. (19) and (22)]. In particular, the drift velocity [Eq. (16b)] diffusion coefficient [Eq. (16c)], and the mean energy conductivity [Eq. (24a)] have been explicitly evaluated. Thus, Eqs. (9a) and (9b) form a closed set that can be used to describe the macroscopic dynamics of the assembly. From the solutions to these equations, other macroscopic variables can be obtained (in this scale of resolution) from the MKD [Eq. (18)].

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<sup>13</sup>This transformation expresses the new equation in terms of the original coordinates, although the velocity variable is now called  $w$  to indicate the new conditions. The reason for the transformation is to be able to write the quasi-Lorentz gas collision operator in the simple form given in Eq. (14a).

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