PHYSICAL REVIEW A VOLUME 37, NUMBER 5 MARCH 1, 1988

Nonequilibrium macroscopic descriptions of electrons in weakly ionized gases

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(Received 16 March 1987)

In this paper a nonequilibrium description of the dynamics of electrons in a background gas under the influence of space-time varying fields is presented. It is obtained by interpolating between a kinetic and a moment formulation. To achieve this, the moment equations have been ordered by using characteristic scales. The ordering is then used to derive, from the kinetic equation, a new equation valid only in the scale of the moment equations. This equation and a finite set of moment equations form a closed system which can be used to describe the dynamics of electrons under various nonequilibrium conditions. Comparisons are presented between results obtained with this formulation and those obtained from a kinetic model.

I. INTRODUCTION

The ensemble-averaged dynamic behavior of an assembly of electrons in a background gas under the influence of a space-time varying field may be described at a microscopic level by the time-dependent distribution function, $f(\mathbf{v},\mathbf{r},t)$ (where $\mathbf{v}$ is velocity, $\mathbf{r}$ is position, and t is time).[1,2] Given the initial state of the assembly, the distribution function at any other time may be obtained from either a kinetic-type equation such as the Boltzmann equation (BE),[3,4] or from Monte Carlo simulations.[5,6] When the fields are changing in space-time, it is, in general, very difficult to obtain the solution to the BE. Moreover, the Monte Carlo approach, although simple to implement, is very time consuming and in some cases (depending on the number of test particles used) prohibitive.[7] Once the distribution function is found, desired macroscopic properties (which can be measured) can be calculated by averaging over the distribution the corresponding microscopic properties.[1,2]

An alternate approach for obtaining the macroscopic properties of the assembly is in terms of moments of the distribution.[1,2] In general, an exact description of the assembly requires an infinite set of moments (this is equivalent to the fact that we need an infinite set of moments to specify the distribution f). These moments obey a hierarchy (infinite set) of equations obtained by taking moments of the BE.[1,2]

In contemplating a description in terms of moment equations, two questions need to be addressed: (1) Can a finite set of moments be used to describe (to some degree of accuracy) the state of the system (this is equivalent to asking under what conditions can a finite set of moments determine to some approximation, the distribution function)?, and (2) given that the previous question is answered in the affirmative, how can a finite set of moment equations be made determinate (since a finite set of moment equations contains more unknowns than equations)? The first question is a well-known problem in statistics and will not be given any attention here.[8] It will be assumed (from physical considerations) that a finite set of moment equations can be used to describe the behavior of the electrons. To assess the accuracy of this finite set, the results for some representative cases must be compared with those obtained from the exact distribution function. This paper focuses on the second question, namely, how to obtain a closed set of moment equations which are valid in the presence of space-time varying fields. A number of approaches have been proposed to accomplish this task. These approaches can be divided into four general categories. They are respectively based on the assumptions that (a) the distribution function can be represented by an expansion in terms of a finite number of Legendre polynomials,[9,10] (b) the distribution function is a displaced Maxwellian,[11] (c) the unknown variables and coefficients appearing in the moment equations are given by phenomenological equations,[12] and (d) the system evolves through a series of equilibrium states so that steady-state results for the unknown parameters can also be used in transient situations.[13] The first approach is closest in spirit to a derivation based on first principles. This is important since it can provide guidance as to where the model is likely to fail.

In Sec. II a mathematical formulation of the problem and the foundation for an approach to its solution are presented. This approach has also been discussed in connection with electron dynamics in semiconductors.[14] In Sec. III closed sets of moment equations are derived for three levels of description. An example is given in Sec. IV to illustrate the capabilities of the model. Some concluding remarks are given in Sec. V.

II. FORMULATION OF THE NONEQUILIBRIUM MACROSCOPIC DESCRIPTION

The state of an assembly of electrons in an ionized medium can be described at a microscopic level by the distribution function $f(\mathbf{v},\mathbf{r},t)$ in $(\mathbf{v},\mathbf{r})$ space. This function obeys the BE; namely,[1-4]

$$\partial_t f+\mathbf{v}\cdot\nabla_r f+\frac{q}{m}\mathbf{E}\cdot\nabla_v f=I'(f)\ , \tag{1}$$

where $\mathbf{E}=E(\mathbf{r},t)$ is the electric field (either externally applied or arising from space-charge), and $I'(f)$ is a nonlinear operator which accounts for collisions of the electrons with neutrals, electrons, and ions. In this paper it is assumed that the neutral and ion distributions are not significantly disturbed by collisions with the electrons and that (two-body) electron-electron interactions are small in some measure. For this case, $I'(f)$ can be linearized.[15] This linear operator is denoted by $I(f)$. No specific form for the operator I need be assumed at this time. This operator describes a number of physical processes (interactions between electrons and background) which occur in different space-time scales. The scales of interest in the formulation of a macroscopic model are the fine-grained (kinetic) scale, where changes occur in a particular collision time and/or distance, and the coarse-grained (hydrodynamic) scale, where changes occur in a macroscopic scale.[16]

At the macroscopic level, the properties of the electrons are given by the "state vector" (of infinite dimension) $\mathbf{S}$, whose components are moments of the distribution.[1,2] That is, $\mathbf{S}=[m_j(\mathbf{r},t);\ j=1,\ldots,N,\ldots\infty]$, where m_j corresponds to a moment of the distribution which may be a scalar, vector, or tensor. The equations for the moments are obtained by taking appropriately weighted integrals (in $\mathbf{v}$ space) of Eq. (1).[1,2] The equations for the first three moments [namely, density $n(\mathbf{r},t)$, mean energy $\bar{\epsilon}(\mathbf{r},t)$, and average velocity, $\mathbf{u}(\mathbf{r},t)$] are

$$\partial_t n+\nabla\cdot(n\mathbf{u})=\nu n \ , \tag{2a}$$

$$d_t(n\bar{\epsilon})+\nabla\cdot\langle\epsilon\mathbf{v}\rangle-q\mathbf{E}\cdot n\mathbf{u}=-\nu_\epsilon n\bar{\epsilon} \ , \tag{2b}$$

$$\partial_t(n\mathbf{u})+\nabla\cdot\langle\mathbf{v}\mathbf{v}\rangle-\frac{q}{m}\mathbf{E}n=-\nu_m n\mathbf{u} \ , \tag{2c}$$

where the bracket implies an average over the distribution, $\epsilon=\frac{1}{2}mv^2$, and ν, ν_ϵ, and ν_m are the (space-time-dependent) effective-ionization, energy-exchange, and momentum-exchange frequencies. These frequencies are defined by

$$\nu n=\int I(f)d\mathbf{v} \ , \tag{3a}$$

$$-\nu_\epsilon n\bar{\epsilon}=\int \tfrac{1}{2}mv^2 I(f)d\mathbf{v} \ , \tag{3b}$$

$$-\nu_m n\mathbf{u}=\int \mathbf{v}I(f)d\mathbf{v} \ . \tag{3c}$$

An integral without limits implies integration over all space. Since it is difficult to ascribe physical significance to higher-order moments, their equations of evolution are seldom written down. The infinite set of moment equations is equivalent to Eq. (1).[1,2]

Because of the difficulty in obtaining solutions to the equations for either $\mathbf{S}$ or f, a description in terms of a finite number of moments is desirable (assuming that this finite system is less difficult to solve), that is, a description in terms of a state vector $\mathbf{S}_N=\{m_j; j=1,\ldots,N\}$. Unfortunately, any finite set of moment equations is not determinate.[1,2] For example, the set of Eqs. (2) contains unknown averages over the distributions (quantities in brackets) and unknown rates [Eqs. (3)]. To calculate these unknowns and thus arrive at a determinate set of equations for $\mathbf{S}_N$, f needs to be found. This implies having to solve Eq. (1), which is exactly what is being avoided.

A similar problem arises in classical gas kinetics, which has been the subject of much investigation.[17–19] For some cases in gas kinetics [namely, those for which the external forces are zero and the spectrum of the corresponding (linearized) collision operator $I(f)$ is either known or significant properties are known], it is possible to obtain formal (exact) expressions for f, i.e., expansions in terms of the eigenvectors of $I(f)$.[17–19] By proper ordering of the terms, these expansions may be truncated resulting in an approximate but manageble expression for f. With this f, a determinate set of macroscopic equations can be obtained.[18] This procedure is mathematically rigorous, and it is possible to assess, *a priori*, the magnitude of truncation errors and the range of validity of the solution. As an example, the one-dimensional initial value problem of a gas of Maxwell molecules has been investigated in some detail using this procedure.[19] In this example (representative of ideal fluids), the spectrum of the operator yields a set of modes that are decaying in time. The three least damped modes have equal decay rates, and are known as hydrodynamic modes [in homogeneous situations, these modes suffer no damping, and collapse into a single mode, i.e., the smallest eigenvalue of $I(f)$ is threefold degenerate]. The modal amplitudes of the hydrodynamic modes correspond to the particle density, average velocity, and mean energy.[19] The hydrodynamic time regime corresponds to time scales for which only these modes need to be considered in the representation of the distribution function (all other modes are exponentially small).

In contrast to classical gas dynamics, very little is known about the properties of either $I(f)$ or the operator $(q/m)\mathbf{E}\cdot\nabla_{\mathbf{v}}-I(f)$ in Eq. (1) for the case of electrons in a weakly ionized gas. In this case, the nature of the interactions between electrons and background makes it very difficult to gain information as to the properties of these operators. Because of this, a more physical approach is proposed. The key to this approach is the use of information from the macroscopic equations to effect the truncation. This is outlined below.

First, the moment equations are ordered according to their characteristic scales. This step requires *a priori* assumptions about the relative magnitude of these scales. They can be made from physical considerations. In any event, the ordering that is used needs to be confirmed after the solution has been found. Equations (2a)–(2c) have been ordered according to their characteristic times. These times are (in decreasing magnitude): τ (effective electron production and/or loss time $=\nu^{-1}$), τ_ϵ (energy-exchange time$=\nu_\epsilon^{-1}$), and τ_m (momentum-exchange time $=\nu_m^{-1}$). The higher moment equations would also have to be ordered accordingly. It is assumed that their characteristic times are smaller than those defined above. Note that, in general, $\tau_\epsilon>\tau_m$ for weakly ionized gases.

Next, the number of moments in the state vector S_N is determined from physical consideration, and from the scale of the desired description. Alternatively, the number of moments that are used determines the coarseness of the macroscopic description. This is because the model is only valid for time scales of the order of the smallest characteristic time contained in the finite set of equations.

Finally, note that the distribution function f, which satisfies Eq. (1), contains information to all orders of time greater than a microscopic collision time.[1,2] This time is, in general, much smaller than the characteristic times in any finite set of moment equations. As far as the moment equations, f contains "too much information." Thus, to obtain a determinate set of moment equations, it is sufficient to use an f which only contains information in the scale of the moment equations. This distribution, the macroscopic distribution function f_M, obeys a "macroscopic-kinetic equation." The equation of evolution for f_M, together with the finite set of moment equations, form a closed set. This set can be used to describe the nonequilibrium dynamics of the electrons in a time scale corresponding to the characteristic times of the moment equations. This description is termed nonequilibrium because f_M may be space-time dependent. In fact, in the time scale of the moments, it is equivalent to f.

A number of procedures can be used to arrive at an equation for f_M. The objective in any of these procedures is to change the scale of Eq. (1) from the microscopic to that of the finite set of moment equations.[20,21] In this paper the technique proposed by Bogoliubov is used.[20] A problem arises when trying to solve the equation for f_M. This has to do with the issue of assignment of initial values to f_M.[17] In this paper it will be assumed that the moments of f_M correspond to the (approximate) macroscopic state. The procedure outlined above is used in Sec. III to obtain closed sets of moment equations valid in three different regimes (time scales).

III. THE NONEQUILIBRIUM MACROSCOPIC EQUATIONS

The approach outlined in Sec. II will now be used to obtain the nonequilibrium macroscopic equations. The characteristic times of the macroscopic equations [Eqs. (2a)–(2c)] can be used to define various levels of descriptions. The most coarse-grained description is valid for times in the order of τ (see Sec. II). From Eqs. (2a)–(2c), since $\nu < \nu_\epsilon < \nu_m$, there is a time for which the mean energy and average momentum of the electrons have relaxed to a state of quasiequilibrium where their subsequent variation is in the scale of τ, i.e., the scale of the density variations. For such times, the macroscopic evolution of the system can be described in a single time scale. Thus, $\mathbf{S}_1 = [n(\mathbf{r},t)]$; that is, the macroscopic state vector contains a single moment, the density.

By analogy with classical gas kinetics (see Sec. II), the time regime for which this description is valid (namely, the longest time scale) is named the hydrodynamic regime. However, in contrast to gas kinetics, the properties of this state can be derived from a single macroscopic variable (instead of three), the density. Note that the evolution of the system to the hydrodynamic regime cannot be determined from the properties of the $\mathbf{S}_1$ state (see below).

Progressively less coarse-grained levels of description can be defined by systematically using an additional moment in the state vector. This assumes that the characteristic times in the moment equations are not degenerate (i.e., equal). In this case, there are times for which the higher-order moments have relaxed to a state in which their scale of variation is the same as the moments being used in the characterization of the macroscopic state. If there was a degeneracy (for example, $\nu_\epsilon^{-1} = \nu_m^{-1}$), then the corresponding moments must be collectively taken as components of the state vector. For cases of interest (electrons in a weakly ionized gas), the characteristic times are not, in general, degenerate.[1,2] Thus, the next less coarse-grained level of description is in terms of $\mathbf{S}_2 = [n(\mathbf{r},t), \bar{\epsilon}(\mathbf{r},t)]$. This is valid for times in the order of ν_ϵ^{-1}. From a practical point of view, the least coarse-grained description of interest is in terms of $\mathbf{S}_3 = [n(\mathbf{r},t), \bar{\epsilon}(\mathbf{r},t), \mathbf{u}(\mathbf{r},t)]$, which is valid for times of the order of ν_m^{-1}.

In contrast to (linear) gas kinetics, these states are not orthogonal, so that there is no one-to-one correspondence with the modes of gas kinetics. The gas kinetics modes evolve independently, and their decay times are given by the eigenvalues of $I(f)$.[18,19] The macroscopic states, on the other hand, evolve sequentially, that is, $\mathbf{S}_3$ evolves into $\mathbf{S}_2$ and subsequently into $\mathbf{S}_1$. However, insight can be gained into the nature of the "kinetic modes" for the electron assembly by comparing the two systems (while keeping in mind the differences between them). Recall that in the gas kinetic hydrodynamic regime (i.e., the longest time scale), three moments are required to describe the system.[18,19] This is due to the degeneracy of the smallest eigenvalue of the corresponding $I(f)$. This degeneracy is reflected in the gas kinetic macroscopic equations by the fact that $\nu = \nu_\epsilon = \nu_m = 0$. Thus, the gas kinetic hydrodynamic regime corresponds to a state $\mathbf{S}_3$. As previously discussed, the macroscopic rates for an electron assembly are not degenerate. Thus, conversely, this may be a reflection on the characteristic time scales of the corresponding (unknown) kinetic modes. In the longest time scale (i.e., hydrodynamic regime), only a single mode survives which corresponds to the $\mathbf{S}_1$ state. The nature of this and the other two modes, and how they combine to yield the $\mathbf{S}_3$ or $\mathbf{S}_2$ states, is yet to be determined.

To make the equations that define the macroscopic states, $\mathbf{S}_i$, $i = 1,2,3$, determinate, the macroscopic-kinetic distribution f_M must be found. To achieve this a macroscopic equation of evolution for f_M in the time scale of the $\mathbf{S}_i$'s needs to be derived and solved. This is carried out below for each level of description of interest; namely, $\mathbf{S}_i$, $i = 1,2,3$.

A. The $\mathbf{S}_1$ state (defined for times $\sim \nu^{-1}$)

In this case, only Eq. (2a) and the equation for $f_M = f_M^1$ in the τ time scale are necessary to describe the evolution of the electrons.[22] These two equations form a closed set. The equation for f_M^1 is obtained by changing the time scale of the BE [Eq. (1)] from the fine-grained to a τ scale. This can be achieved using a technique introduced by Bogoliubov.[20] Mathematically, the change can be accomplished by the following relation:

$$f(\mathbf{v},\mathbf{r},t) = f_M^1[\mathbf{v}, n(\mathbf{r},t)] \ . \tag{4}$$

That is, in the τ scale, the space-time dependence of the distribution is not explicit, but implicit through a dependence on the density. The equation governing the changes in f_M^1 can be found using Eqs. (1) and (2a). From Eq. (4), the changes in f can be written as

$$\partial_t f = \partial_n f_M^1 \partial_t n \ , \tag{5a}$$

$$\nabla_r f = \partial_n f_M^1 \nabla_r n \ , \tag{5b}$$

$$\nabla_v f = \nabla_v f_M^1 \ . \tag{5c}$$

The time derivative of the density may be eliminated from Eq. (5a) by using Eq. (2a). After placing Eqs. (2a) and (5) into Eq. (1), the following equation is obtained for the distribution:

$$\partial_n f_M^1 \left[-\int \partial_n f_M^1 \mathbf{v}\, d\mathbf{v}\cdot\nabla n + \int I(f_M^1) d\mathbf{v} \right] + \mathbf{v}\cdot\nabla n\, \partial_n f_M^1 + \frac{q}{m}\mathbf{E}\cdot\nabla_v f_M^1 = I(f_M^1) \ . \tag{6}$$

The subscript r has been omitted from the spatial gradient. This practice is continued in the rest of the paper. If the deviation from spatial uniformity is small, a parameter δ can be introduced into Eq. (6) which is indicative of this assumption.[16] Using δ as a basis for a perturbation expansion, the distribution may be expressed as

$$f_M^1(\mathbf{v},n) = \sum_i \delta^i f_M^1(\mathbf{v},n) \ .$$

Substituting this expression into Eq. (6) leads, in zeroth order, to the equation

$$\frac{q}{m}\mathbf{E}\cdot\nabla_v f_{M_0}^1(\mathbf{v},n) = I(f_{M_0}^1) - \partial_n f_{M_0}^1 \int I(f_{M_0}^1) d\mathbf{v} \ ,$$

which has the general solution

$$f_{M_0}^1(\mathbf{v},n) = f_{M_0}^1(\mathbf{v}) n(\mathbf{r}',t) \ , \tag{7}$$

where $\mathbf{r}' = \delta\mathbf{r}$, and $f_{M_0}^1(\mathbf{v})$ obeys the equation

$$\frac{q}{m}\mathbf{E}\cdot\nabla_v f_{M_0}^1 = I(f_{M_0}^1) - f_{M_0}^1 \int I(f_{M_0}^1) d\mathbf{v} \ , \tag{8}$$

with the condition

$$\int f_{M_0}^1(\mathbf{v}) d\mathbf{v} = 1 \ . \tag{9}$$

Note that the same symbol has been used for $f_{M_0}^1(\mathbf{v},n)$ and $f_{M_0}(\mathbf{v})$. The context in which they are used determines the argument. Equation (8) has the form of a steady-state, homogeneous Boltzmann equation, and $f_{M_0}^1$ can be identified as the (zeroth-order) steady-state distribution of a homogeneous assembly of electrons in a homogeneous field defined by the value of the field at $\mathbf{r}',t$.[22,23] This is the distribution that exists at $(\mathbf{r}',t)$ if local equilibrium with the field is assumed. A number of techniques are available for solving this equation.[24] $f_{M_0}^1$ can also be obtained using Monte Carlo methods.[7,25]

Noting from Eq. (7) that $\partial_n f_{M_0}^1(\mathbf{v},n) = f_{M_0}^1(\mathbf{v})$, the equation of $O(\delta)$ is found from Eq. (6) to be

$$\frac{q}{m}\mathbf{E}\cdot\nabla_v f_{M_1}^1 - I(f_{M_1}^1) + f_{M_0}^1 \int I(f_{M_1}^1) d\mathbf{v} = f_{M_0}^1 \int f_{M_0}^1 \mathbf{v}\, d\mathbf{v}\cdot\nabla' n - f_{M_0}^1 \mathbf{v}\cdot\nabla' n - n f_{M_0}^1 \int I(f_{M_0}^1) d\mathbf{v} \ , \tag{10}$$

where $\nabla' \rightarrow \delta^{-1}\nabla$, and the last term is an approximation to the corresponding term in Eq. (6).

The right-hand side of Eq. (10) constitutes a source to an equation similar to Eq. (8). After linearization, the solution to Eq. (10) may be formally written as

$$f_{M_1}^1(\mathbf{v},n) = \int G(\mathbf{v},\mathbf{v}') S(\mathbf{v}',n) d\mathbf{v}' \ , \tag{11}$$

where S is the right-hand side of Eq. (10) and G is the Green's function of a linearized Eq. (8). Substituting for S in Eq. (11),

$$f_{M_1}^1(\mathbf{v},n) = f_{M_{10}}^1 n + \mathbf{f}_{M_{11}}^1 \cdot \nabla' n \ , \tag{12a}$$

where

$$\mathbf{f}_{M_{11}}^1 = \int G(\mathbf{v},\mathbf{v}') \left[f_{M_0}^1(\mathbf{v}') \int f_{M_0}^1(\mathbf{v}'')\mathbf{v}'' d\mathbf{v}'' - f_{M_0}^1(\mathbf{v}')\mathbf{v}' \right] d\mathbf{v}' \tag{12b}$$

and

$$f_{M_{10}}^1 = -\int G(\mathbf{v},\mathbf{v}') f_{M_0}^1(\mathbf{v}') \left[\int I[f_{M_0}^1(\mathbf{v}'')] d\mathbf{v}'' \right] d\mathbf{v}' \ . \tag{12c}$$

Since $\int f_{M_1}^1 d\mathbf{v} = 0$ (note that $\int f\, d\mathbf{v} = n$ and $\int f_{M_0}^1 d\mathbf{v}$ has been taken to be one), the $f_{M_1}^1$'s above must satisfy the conditions $\int f_{M_{1i}} d\mathbf{v} = 0$, $i = 0,1$. This implies that $\int G\, d\mathbf{v} = 0$.

The results obtained above can be summarized as follows. The distribution function in the τ scale satisfies Eq. (6). To first order in δ, its solution is given by

$$f_M^1 = f_{M_{00}}^1(\mathbf{v}) n(\mathbf{r}',t) + \delta f_{M_{11}}^1 \cdot \nabla n \ , \tag{13}$$

where

$$f_{M_{00}}^1(\mathbf{v}) = f_{M_0}^1(\mathbf{v}) + \delta f_{M_{10}}^1(\mathbf{v}) \ .$$

This result is the density gradient expansion which has previously been *a priori* assumed for the distribution function.[26] The use of Eq. (13) into Eq. (6) yields a diffusion-type equation for the density,

$$\partial_t n = -(\mathbf{v}_d - \mathbf{v}_{dg})\cdot\nabla' n + \underline{D}\cdot\nabla'\nabla' n + \nu_i n \ , \tag{14}$$

where $\mathbf{v}_d - \mathbf{v}_{dg}$ is the effective drift velocity, $\underline{D}$ is the diffusion tensor, and ν_i is the ionization rate under uniform field conditions at the values of the local field.[23] $\mathbf{v}_{dg}$ is the contribution to the drift velocity resulting from the fact that $\int I(f) d\mathbf{v} \neq 0$. These quantities are defined as

$$\mathbf{v}_d = \int \mathbf{v} f_{M_{00}}^1 d\mathbf{v}, \quad \mathbf{v}_{dg} = \delta \int I(\mathbf{f}_{M_{11}}^1) d\mathbf{v} \ ,$$

$$\underline{D} = -\delta \int \mathbf{v} f_{M_{11}}^1 d\mathbf{v}, \quad \nu_i = \int I(f_{M_{00}}^1) d\mathbf{v} \ .$$

These coefficients depend on the applied field through the

f_{M}'s. They can be tabulated as a function of field by numerically solving for the f_{M}'s and using the above equations. Once these coefficients have been evaluated, Eq. (14) may be used to describe the evolution of the electrons. Thus, in this time scale, the above results correspond to nonequilibrium diffusion theory.

More accurate expressions for the transport parameters can be obtained by explicitly introducing the time scale of the field in the distribution function.[22] That is, by letting $f=f_M^1(\mathbf{v},n(\mathbf{r},t),E(\mathbf{r},t))$. Note that the macroscopic description still corresponds to time scales of the order of ν^{-1}. Using the techniques discussed in this section, transport parameters and rate coefficients can be obtained which explicitly account for field variations.[22] With this method, no *a priori* assumptions need to be made about the form of the distribution as done in Ref. 27. A similar approach can be used to obtain expressions for the transport parameters in the other descriptions (see $\mathbf{S}_2$, and $\mathbf{S}_3$ below) which explicitly account for field variations. This extension of the results presented in this paper will not be discussed further.

B. The $\mathbf{S}_2$ state (defined for times $\sim\nu_\epsilon^{-1}$)

In this case, Eqs. (2a), (2b), and the equation for $f_M=f_M^2$ in the τ_ϵ time scale are used to describe the system.[28] The procedure for obtaining the equation for f_M^2 follows along the same lines as the procedure for f_M^1 (Sec. III A). In this case the change in scale is accomplished by the relation

$$f(\mathbf{v},\mathbf{r},t)=f_M^2(\mathbf{v},n(\mathbf{r},t),\bar{\epsilon}(\mathbf{r},t)) \ . \tag{15}$$

Note that f_M^2 changes in two characteristic time scales, τ and τ_ϵ. From Eq. (15), the changes in f can be written as

$$\partial_t f=\partial_n f_M^2 \partial_t n+\partial_{\bar{\epsilon}} f_M^2 \partial_t \bar{\epsilon} \ , \tag{16a}$$

$$\nabla_{\mathbf{r}} f=\partial_n f_M^2 \nabla n+\partial_{\bar{\epsilon}} f_M^2 \nabla \bar{\epsilon} \ , \tag{16b}$$

$$\nabla_{\mathbf{v}} f=\nabla_{\mathbf{v}} f_M^2 \ . \tag{16c}$$

The time derivative of the density and mean energy may be eliminated from Eq. (16a) by using Eqs. (2a) and (2b). Note that in this scale the average velocity $\mathbf{u}$ is obtained from

$$n\mathbf{u}=\int \mathbf{v} f_M^2 d\mathbf{v} \ . \tag{17}$$

After placing Eqs. (2a), (2b) and (16) in Eq. (1), the following equation is obtained for the distribution function,

$$\begin{aligned}\partial_n f_M^2 &\left[-\int \partial_n f_M^2 \mathbf{v}\, d\mathbf{v}\cdot\nabla n+\int I(f_M^2) d\mathbf{v}\right]+\partial_{\bar{\epsilon}} f_M^2 n^{-1}\\ &\times\left[-\int \partial_n f_M^2 \epsilon \mathbf{v}\, d\mathbf{v}\cdot\nabla n-\int \partial_{\bar{\epsilon}} f_M^2 \epsilon \mathbf{v}\, d\mathbf{v}\cdot\nabla\bar{\epsilon}+\frac{q}{m}\mathbf{E}\cdot\int \mathbf{v} f_M^2\, d\mathbf{v}+\int \epsilon I(f_M^2) d\mathbf{v}\right]\\ &+\mathbf{v}\cdot\nabla n\, \partial_n f_M^2+\mathbf{v}\nabla\bar{\epsilon}\partial_{\bar{\epsilon}} f_M^2+\frac{q}{m}\mathbf{E}\cdot\nabla_{\mathbf{v}} f_M^2=I(f_M^2) \ . \end{aligned}\tag{18}$$

[The term proportional to $\partial_t \ln n$ is assumed to be small and hence has been neglected in Eq. (18). If this is not the case, Eq. (18) should be modified accordingly.] To expedite the algebra in obtaining a solution to Eq. (18), results obtained for f_M^1 [see Eq. (13)] will be used as a guide. That is, let f_M^2 be expressed to first order in spatial gradients by

$$\begin{aligned}f_M^2(\mathbf{v},n,\bar{\epsilon})=&f_{M_0}^2(\mathbf{v},\epsilon)n+\delta f_{M_{10}}^2(\mathbf{v},\bar{\epsilon})n\\ &+\delta f_{M_{11}}^2(\mathbf{v},\epsilon)\cdot\nabla n+\delta f_{M_{12}}^2(\mathbf{v},\epsilon)\cdot\nabla\bar{\epsilon} \ . \end{aligned}\tag{19}$$

The objective for the rest of this section is to arrive at the lowest-order solution for f_M^2. Higher-order approximations and the effect of the gradient terms are to be considered in the future. Thus, only the first term in this expansion will be retained. The equation for $f_{M_0}^2$ is found to be

$$\begin{aligned}f_{M_0}^2 &\left[-\int I(f_{M_0}^2) d\mathbf{v}\right]\\ &+\partial_{\bar{\epsilon}} f_{M_0}^2 \left[\frac{q}{m}\mathbf{E}\cdot\int \mathbf{v} f_{M_0}^2 d\mathbf{v}+\int \epsilon I(f_{M_0}^2) d\mathbf{v}\right]\\ &+\frac{q}{m}\mathbf{E}\cdot\nabla_{\mathbf{v}} f_{M_0}^2=I(f_{M_0}^2) \ . \end{aligned}\tag{20}$$

This is a nonlinear equation for $f_{M_0}^2$. Neglecting the first term (assuming that the effective electron gain integral is small), and using the following definitions:

$$\mathbf{u}=\mathbf{u}_s=\mathbf{u}_s(\bar{\epsilon})=\int \mathbf{v} f_{M_0}^2 d\mathbf{v} \ , \tag{21a}$$

$$-\nu_{\bar{\epsilon}}\bar{\epsilon}=\int \epsilon I(f_{M_0}^2) d\mathbf{v} \ , \tag{21b}$$

Eq. (20) becomes

$$\left[\frac{q}{m}\mathbf{E}\cdot\mathbf{u}_s-\nu_{\bar{\epsilon}}\bar{\epsilon}\right]\partial_{\bar{\epsilon}} f_{M_0}^2+\frac{q}{m}\mathbf{E}\cdot\nabla_{\mathbf{v}} f_{M_0}^2=I(f_{M_0}^2) \ . \tag{22}$$

At this level of approximation to $f_M^2(\mathbf{v},n,\bar{\epsilon})$, Eqs. (22), (2a), and (2b), form the closed set of equations that describes the evolution of the system. $f_{M_0}^2$ is made to satisfy the following normalization conditions (see comment at end of Sec. I):

$$\int f_{M_0}^2 (\tfrac{1}{2} m v^2) d\mathbf{v}=\bar{\epsilon} \ , \tag{23a}$$

$$\int f_{M_0}^2 d\mathbf{v}=1 \ . \tag{23b}$$

The solution to Eq. (22) can be obtained as follows. Performing a change of variables from $(\bar{\epsilon},\mathbf{v})$ to $(\omega,\xi,\mathbf{v}_\perp)$, where

$$\mathbf{v}=v_F \mathbf{a}_F+\mathbf{v}_\perp \ ,$$

(where $\mathbf{a}_F$ is a unit vector parallel to the field direction),

$$\xi = v_F - \bar{\epsilon}/mu_s \ ,$$

$$\omega = \bar{\epsilon}/mu_s \ ,$$

$$v_\perp = v_\perp \ ,$$

and using the chain rule, Eq. (22) becomes [to zeroth order in $\partial_{\bar{\epsilon}} mu_s(\bar{\epsilon})$]

$$\frac{q}{m} E_{\text{eq}} \partial_\xi f^2_{M_0} + \frac{q}{m}(E_{\text{eq}} - E)\partial_\omega f^2_{M_0} = I(f^2_{M_0}) \ , \qquad (24)$$

where

$$\frac{q}{m} E_{\text{eq}} = \frac{\nu_\epsilon \bar{\epsilon}}{mu_s} = \nu_\epsilon \omega \ . \qquad (25)$$

For $(E_{\text{eq}} - E)/E_{\text{eq}}$ small (or $f^2_{M_0}$ a slowly varying function of ω), the lowest-order solution to Eq. (24) satisfies the following equation:

$$\frac{q}{m} E_{\text{eq}} \partial_\xi f^2_{M_0} = I(f^2_{M_0}) \ . \qquad (26)$$

This equation has the form of a steady-state BE with $(q/m)E_{\text{eq}}$ as the source. It is equivalent to Eq. (8) which arises in connection with the description of the $\mathbf{S}_1$ state. Thus, to lowest order, the macroscopic-kinetic distribution function of the $\mathbf{S}_2$ state obeys a steady-state BE in an equivalent field. This observation has a physical interpretation. The actual field E appears as a source term in the moment equations and as such causes changes in the state $\mathbf{S}_2$. These equations describe the evolution of $\mathbf{S}_2$ in their characteristic time scales. Variations in E faster than these time scales are "filtered" by them, that is, as far as changes in $\mathbf{S}_2$ are concerned. Thus, it is the "filtered" field which the state really "sees." This "filtered" field is the equivalent field in Eq. (26).

Equation (26) can be solved numerically with E_{eq} as a parameter. By requiring that

$$\bar{\epsilon} = \int (\tfrac{1}{2} m v^2) f^2_{M_0} d\mathbf{v} \ ,$$

a table for $\bar{\epsilon}$ vs E_{eq} can be generated. Moreover, using Eqs. (3a) and (21), all unknown variables and/or parameters in Eqs. (2a) and (2b) can be tabulated as functions of E_{eq} or equivalently of $\bar{\epsilon}$. In this fashion, $\nu = \nu(\bar{\epsilon})$, $\nu_\epsilon = \nu_\epsilon(\bar{\epsilon})$, and $u = u_s(\bar{\epsilon})$. Once these tables are generated, the system of equations describing the $\mathbf{S}_2$ state becomes determinate (since the unknowns have been determined as functions of the state variables).

C. The $\mathbf{S}_3$ state (valid for times $\sim \nu_m^{-1}$)

In this case, Eqs. (2a)–(2c) and the equation for $f_M = f^3_M$ in the τ_m time scale are used in the description of the system.[28] In the spirit of Eqs. (4) and (15), the distribution function is assumed to depend on space and time as follows:

$$f(\mathbf{v},\mathbf{r},t) = f^3_M(\mathbf{v}, n(\mathbf{r},t), \bar{\epsilon}(\mathbf{r},t), \mathbf{u}(\mathbf{r},t)) \ .$$

Although obtaining an equation for f^3_M is straightforward, its solution is more difficult to find than for the $\mathbf{S}_1$ and $\mathbf{S}_2$ descriptions. This stems from the fact that, even in lowest order, it is an equation in three variables $(\bar{\epsilon}, \mathbf{u}, \mathbf{v})$.

In this paper instead of proceeding to find an equation for f^3_M and obtaining its solution, an approximate expression for f^3_M is presented. This approximation is motivated by Grad's concept of an eigensolution of the BE.[17] A more complete theory [in essence, a more rigorous derivation of an expression similar to Eq. (27) below] is under investigation.

In all cases of interest, the nonequilibrium macroscopic equations are solved using numerical methods. With these methods, the field E in each time step is taken to be constant. Thus, the problem of finding a solution for f_M in a time step corresponds to the approach to equilibrium of an initial distribution in the presence of a constant field (i.e., an initial value problem in each time step). From the discussions in the previous sections, it is known that after a sufficient time, the "initial distribution" will evolve into f^2_M (if the time step is long enough). Thus, an approximate expression for f^3_M can be obtained by assuming that this evolution can be modeled by a relaxation process. Let the macroscopic state $\mathbf{S}_3$ and f^3_M be known at time t_j when the field is $E(\mathbf{r},t_j)$. Note that the field does not change in the interval (t_j, t_{j+1}) and that the distribution $f^3_{Mj}(t_j)$ (i.e., the distribution at time t_j) need not be the equilibrium distribution for the field $E(\mathbf{r},t_j)$. Thus, in the spirit of the above discussion, the distribution at time $t_j + \rho$ (where ρ is a continuous variable) can be written as

$$f^3_M(t_j+\rho) = [f^3_M(t_j) - f^2_M(t_j+\rho)]e^{-\nu_{mj}}\rho + f^2_M(t_j+\rho)$$
$$\text{for } \rho > 0 \ , \qquad (27)$$

where ν_{mj} is the average momentum-exchange frequency in the interval t_j, t_{j+1} [that is, $\nu_{mj}\rho = \int_0^\rho \nu_m(\rho) d\rho$]. That is, f^3_M approaches f^2_M exponentially, due to the relaxation of the fast component $(f^3_M - f^2_M)$ resulting from momentum transfer at an average rate ν_{m_j}. The distribution at the end of the interval is found by letting $\rho = \Delta t$ in Eq. (27). Once $f^3_M(t_{j+1})$ is found, ν, ν_ϵ, and ν_m can be obtained from Eq. (3) at t_{j+1}. With this information, Eqs. (2) are determinate at t_{j+1} and can be used to obtain the state $\mathbf{S}_3$ at t_{j+2}. This procedure is to be repeated at each time interval. Note that to implement this approach f^2_M must also be known at each step. This problem has been discussed in Sec. III C.

A simple alternative to Eq. (27) is to approximate f^3_M by f^2_M in the calculation of the unknown variables in the macroscopic equations [Eqs. (2a)–(2c)]. This substitution in lowest order leads to the phenomenological equations proposed by Shur[29] for space-independent conditions.

IV. EXAMPLE: THE RESPONSE OF A HOMOGENEOUS ASSEMBLY OF ELECTRONS IN NITROGEN TO A STEP CHANGE IN FIELD

In this section the response of a homogeneous assembly of electrons in a background of nitrogen to a step change in electric field is investigated using the theory developed in Sec. III. For the sake of simplicity, ionization by electron impact has been treated as an inelastic process with no particle gain; that is, $n(r,t)=\text{const}$. The evolution of the electrons is discussed in the context of the $\mathbf{S}_3$ time scales. This is dictated by the time scale of the applied field. For this example, Eqs. (2a)–(2c) reduce to

$$\partial_t \bar{\epsilon} = -\nu_\epsilon \bar{\epsilon} + quE , \tag{28a}$$

$$\partial_t u = -\nu_m u + \frac{q}{m} E , \tag{28b}$$

where ν_i, $i=\epsilon,m$, are obtained from Eqs. (3b) and (3c) with $f=f_M^3$.

These equations have been solved numerically using finite difference techniques.[30] At the jth time step, the mean energy $\bar{\epsilon}(j)$ and average velocity $u(j)$ are obtained from the discrete equations, given their values and the rates at the previous time step, $j-1$. After substituting in Eqs. (3b) and (3c) for f_M^3 (Eq. 27), the rates at the jth time step are obtained from

$$\nu_i(j) = [\nu_i(j-1) - \nu_i^{(0)}(j)] e^{-\nu_{mj}\Delta t} + \nu_i^{(0)}(j) , \tag{29}$$

where $i=\epsilon,m$, and the superscripts correspond to rates in the $\mathbf{S}_2$ time scales (see Sec. III C). The $\nu_i^{(0)}$'s are obtained from Eqs. (3b) and (3c), with $f=f_M^2$. f_M^2 is obtained from Eq. (26). This equation is solved using a set of cross-section for electron-N_2 interactions.[31] For simplicity, it has been assumed that the collisions are isotropic. The values for the $\nu_i^{(0)}$'s have been tabulated as a function of mean energy (see discussion in Sec. III B) and are shown in Table I.

In these calculations, ν_{mj} has been approximated by $\nu_m(j-1)$, which is the momentum-exchange frequency at the beginning of the interval. Thus, with $\bar{\epsilon}(j-1)$, $u(j-1)$, and $\nu_i(j-1)$ given, the values of $\bar{\epsilon}(j)$, $u(j)$, and $\nu_i(j)$ are obtained by solving Eqs. (28a), (28b), and (29). This procedure is repeated at each time step.

The evolution of the mean energy and average velocity of the assembly of electrons in N_2 subjected to a step change (of finite rise time) in field is shown in Figs. 1 and 2. The time dependence of the electric field is shown in Fig. 3. The initial field is kept constant for a time such that the electron assembly has attained equilibrium with the field by the time the field begins to change. Also shown in Figs. 1 and 2 are the results obtained using: (a) the Boltzmann equation [Eq. (1)],[32] (b) the $\mathbf{S}_3$ description, i.e., Eqs. (28a) and (28b), with rates determined from the $\mathbf{S}_3$ and $\mathbf{S}_2$ states (i.e., by letting $f_M=f_M^3$ and f_M^2, respectively), and (c) the $\mathbf{S}_1$ state approximation. The evolution of the system from the initial equilibrium state (I) to the final equilibrium state (F) is displayed in $(\bar{\epsilon},u)$ space in Fig. 4. The fast transient (nonequilibrium) behavior obtained with the $\mathbf{S}_3$ approximation is clearly contrasted with those obtained from the $\mathbf{S}_1$ approximation (which in essence yields an evolution through a series of equilibrium states). For fields changing in time scales $<\nu_\epsilon^{-1}$, a description in terms of $\mathbf{S}_1$ is not satisfactory. From these figures, the results obtained from the nonequilibrium macroscopic equations in the $\mathbf{S}_3$ time scale are seen to be remarkably close to those obtained from a kinetic model.

V. CONCLUDING REMARKS

Nonequilibrium descriptions of the dynamics of electrons in a background gas under the influence of space-

TABLE I. Rate coefficients for electrons in N_2 in the $\mathbf{S}_2$ description as function of E_{eq}, or equivalently, as functions of $\bar{\epsilon}$.

E_{eq}/N (TD)	$\bar{\epsilon}$ (ev)	$\nu_\epsilon^{(0)}$ (sec^{-1})	$\nu_m^{(0)}$ (sec^{-1})
100	2.73	4.14×10^{8}	1.56×10^{10}
200	4.892	7.85×10^{8}	1.83×10^{10}
300	6.37	1.28×10^{9}	1.95×10^{10}
400	7.88	1.70×10^{9}	2.11×10^{10}
500	9.178	2.15×10^{9}	2.23×10^{10}
600	10.47	2.58×10^{9}	2.34×10^{10}
800	12.95	3.41×10^{9}	2.55×10^{10}
900	14.115	3.82×10^{9}	2.64×10^{10}
1100	16.645	4.55×10^{9}	2.81×10^{10}
1200	17.573	4.98×10^{9}	2.90×10^{10}
1400	19.9	5.69×10^{9}	3.04×10^{10}
1500	21.925	5.84×10^{9}	3.09×10^{10}
1800	25.465	6.81×10^{9}	3.29×10^{10}
1900	26.578	7.13×10^{9}	3.35×10
2000	27.657	7.45×10^{9}	3.42×10^{10}
2100	28.712	7.75×10^{9}	3.48×10^{10}
2200	29.729	8.14×10^{9}	3.52×10^{10}
2400	31.655	8.79×10^{9}	3.64×10^{10}
2700	34.306	9.84×10^{9}	3.80×10^{10}

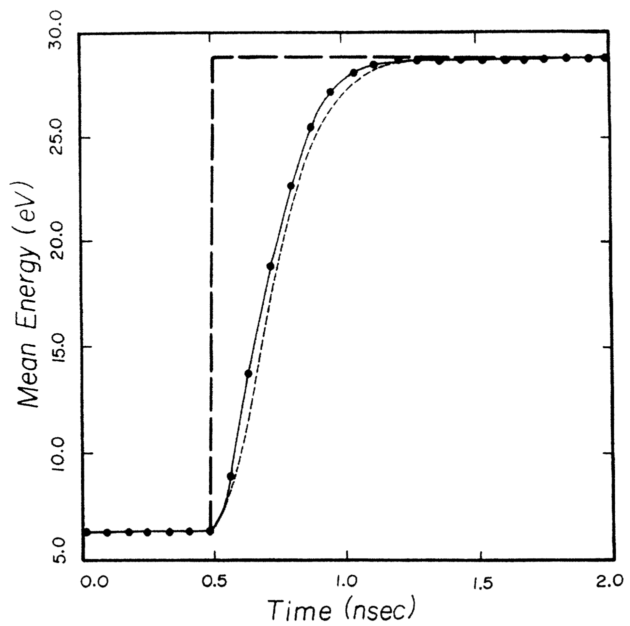

FIG. 1. Evolution of the mean energy of the electron assembly as a consequence of a step change in the applied field (see Fig. 3). In the figures the dotted, solid, short-dashed, and long-dashed lines correspond to the response obtained for the S_3 description, the Boltzmann equation, the S_3 description with rates from the S_2 description, and from the S_1 description, respectively.

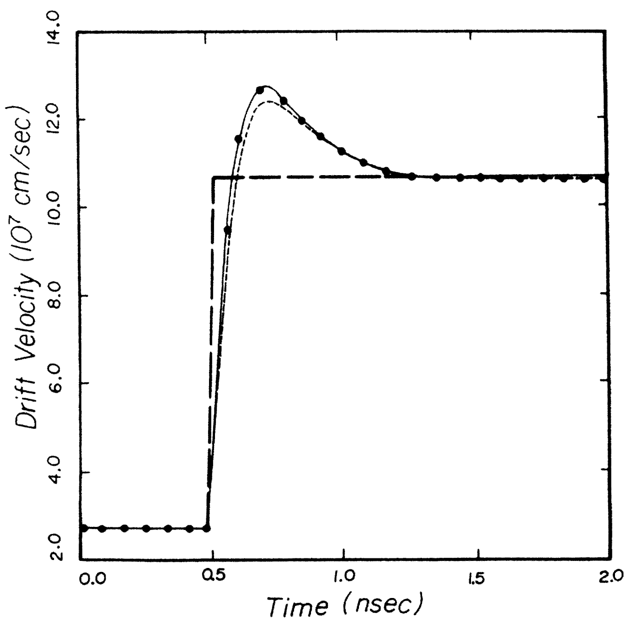

FIG. 2. Evolution of the average velocity of the electron assembly as a consequence of a step change in the applied field (see Fig. 3). The line symbols correspond to those used in Fig. 2.

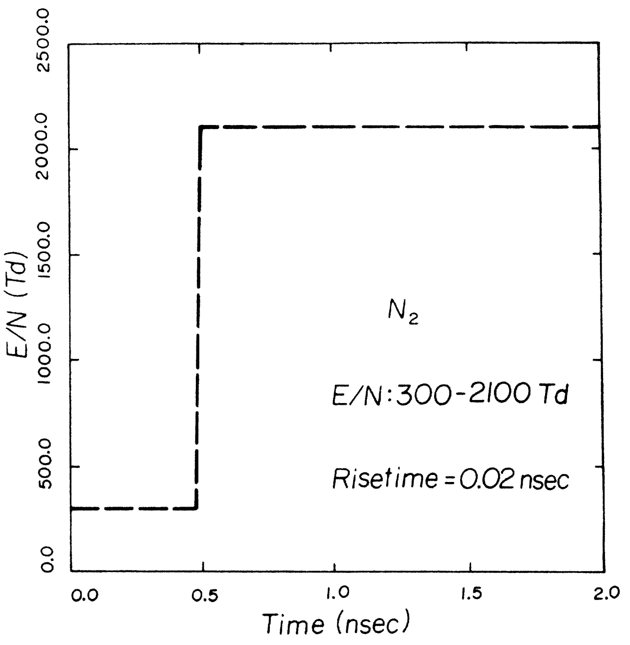

FIG. 3. Time dependence of the applied field.

time varying fields have been presented. These descriptions are valid in different macroscopic space-time scales which are determined from the characteristic scales of the moment equations. The results that have been presented in this paper correspond to the lowest-order solutions of these descriptions. In the fastest scale (S_3), these low-order results have been shown to agree remarkably well with those obtained from a kinetic description. A number of issues remain to be addressed. Among these

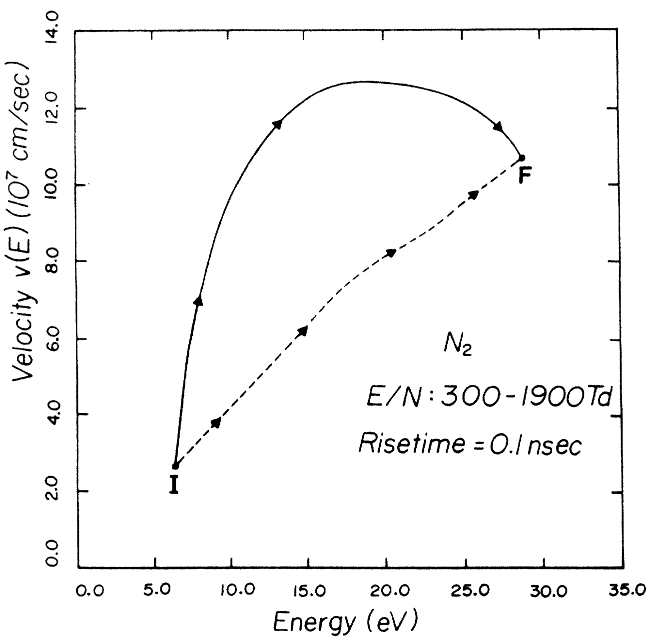

FIG. 4. Phase-space plot of the evolution of the electron assembly. The arrows indicate the direction of evolution. In the figure the solid and dashed lines correspond to the response obtained from the S_3 and S_1 description, respectively.

issues are: (a) the (more) quantitative description of the $\mathbf{S}_3$ state, (b) the relative importance of higher-order terms in the expansions of f_M and of faster time scales ($\mathbf{S}_1$ or higher), and (c) the relationship between a description in terms of $\mathbf{S}_i$ and a modal decomposition of the distribution function. These issues are presently under investigation.

ACKNOWLEDGMENTS

One of the authors (E.E.K.) would like to thank Dr. L. Cram from CSRIO, Australia for a number of very valuable discussions in the early formulation of this work. This work is supported by U. S. Office of Naval Research (ONR).

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[1] M. Mitchner and C. H. Kruger, Jr., *Partially Ionized Gases* (Wiley, New York, 1973).

[2] I. P. Shkarofsky, T. W. Johnston, and M. P. Bachynski, *The Particle Kinetics of Plasmas* (Addison-Wesley, Reading, MA, 1966).

[3] W. P. Allis, in *Handbuch der Physik,* edited by S. Flügge (Springer, Berlin, 1956), Vol. 21, p. 383.

[4] T. Holstein, Phys. Rev. **72**, 1212 (1947).

[5] R. W. L. Thomas and W. R. L. Thomas, J. Phys. B. **2**, 562 (1969).

[6] T. Itoh and T. Musha, J. Phys. Soc. Jpn. **15**, 1675 (1960).

[7] E. E. Kunhardt and Y. Tzeng, J. Comp. Phys. **67**, 279 (1985).

[8] H. Cramer, *Mathematical Methods of Statistics* (Princeton University Press, Princeton, 1946).

[9] S. L. Lin, R. E. Robson, and E. A. Mason, J. Chem. Phys. **71**, 3438 (1979).

[10] B. Shizgal and D. R. McMahon, Phys. Rev. A **32**, 3669 (1985).

[11] K. Blotekjar, IEEE Trans. Electron Devices **ED-17**, 38 (1970).

[12] A. Tran Ngoc, E. Marode, and P. Segur, IEE Conf. Publ. **189**, 59 (1980).

[13] A. J. Davis, C. J. Evans, P. Townsend, and P. M. Woodison, Proc. IEE **124**, 171 (1977).

[14] E. E. Kunhardt (unpublished).

[15] S. I. Sandler and E. A. Mason, Phys. Fluids **12**, 71 (1969).

[16] T. Wu, *Kinetic Equations of Gases and Plasmas* (Addison-Wesley, Reading, MA, 1966).

[17] H. Grad. Phys. Fluids **6**, 147 (1963).

[18] L. Sirovich, Phys. Fluids **6**, 218 (1963).

[19] L. Sirovich, Phys. Fluids **6**, 10 (1963).

[20] N. N. Bogoliubov, in *Studies in Statistical Mechanics,* edited by J. de Boer and G. G. Uhlenbeck (Interscience, New York, 1962).

[21] E. A. Frieman, J. Math Phys. **4**, 410 (1963).

[22] E. E. Kunhardt, Bull. Am. Phys. Soc. **30**, 170 (1985).

[23] L. G. H. Huxley and R. W. Crompton, *The Diffusion and Drift of Electrons in Gases* (Wiley, New York, 1974).

[24] P. Segur, M. Yousfl, J. P. Boeuf, E. Marode, A. J. Davies, and J. G. Evans, in *Electrical Breakdown and Discharges in Gases,* Vol. 89a of *NATO Advanced Study Institute, Series B: Physics,* edited by E. E. Kunhardt and L. H. Luessen (Plenum, New York, 1983), p. 331.

[25] S. L. Lin and J. N. Bardsley, Comp. Phys. Commun. **15**, 161 (1978).

[26] K. Kumar, H. R. Skullerud, and R. E. Robson, Aust. J. Phys. **33**, 343 (1980).

[27] N. L. Aleksandrov, A. P. Napartovich, and A. N. Starostin, Sov. J. Plasma Phys. **6**, 618 (1980).

[28] E. E. Kunhardt, J. Wu, and B. Penetrante, Bull. Am. Phys. Soc. **32**, 1144 (1987).

[29] M. Shur, Electron. Lett. **12**, 615 (1976).

[30] C. W. Gear, *Numerical Initial Value Problems in Ordinary Differential Equations* (Prentice-Hall, New York, 1971).

[31] Y. Tzeng and E. E. Kunhardt, Phys. Rev. A **34**, 2148 (1986).

[32] The Transient Boltzmann calculations have been done using a code provided to us by P. Segur, Université de Toulouse, France.