Hydrodynamic description of electron flow to an absorbing anode

L. E. Cram
School of Physics, University of Sydney, New South Wales 2006, Australia
(Received 30 October 1990)

A theory is presented of the nonequilibrium space-time development of a stream of electrons moving through a background medium under the influence of a strong electric field. Nonequilibrium processes are treated by supplementing the usual continuity moment equation with equations describing the velocity and energy moments of the electron distribution. It is shown that the theory is able to reproduce many of the important nonequilibrium effects occurring as an electron stream approaches an absorbing anode, although comparison with detailed solutions of the Boltzmann equation does reveal certain limitations apparently inherent in theories based on moment equations.

I. INTRODUCTION

The phenomena of drift and diffusion through gases and solids of electrons in the presence of an electric field have been studied extensively.[1–3] Most investigations assume that the electron distribution function is close to the "equilibrium" form that would obtain for a steady, uniform flow of electrons through an infinite, homogeneous background medium subject to a constant electric field. Techniques such as the density gradient expansion[2,4] have provided a theoretical description of such flows in terms of a continuity equation involving transport coefficients (drift velocity, diffusion tensor, ionization coefficients, etc.) which depend only on properties of the background medium and the value of the reduced electric field, E/N. This description is found to be very accurate in experiments set up to satisfy closely the requirements of homogeneity and unboundedness.

The presence of large spatial gradients or rapid time changes in the electron number density, the density of the background medium, or the electric field will tend to produce departures from equilibrium, and hence tend to invalidate the use of the usual continuity equation. Techniques that have been introduced to describe electron motion in circumstances where "nonequilibrium" effects are present include analytic[5] or numerical[6,7] solutions of Boltzmann's equation, Monte Carlo simulation,[8] the use of a "memory kernel,"[9] generalizations of the continuity equation,[10,11] and the use of momentum and energy equations to supplement the continuity equation.[12,13]

This paper discusses the use of momentum and energy conservation equations to describe the flow of electrons to an absorbing anode. As shown in Ref. 6 the steep density gradients that occur in this situation lead to significant departures from equilibrium which may be characterized by a spatial variation of the drift velocity and mean energy of the electrons. It is shown here that momentum and energy conservation equations provide a convenient and reasonably accurate description of nonequilibrium effects in this problem. It is suggested that similar equations can be used to provide some insight into nonequilibrium effects in other problems.

II. MOMENT EQUATIONS

It is assumed that the velocity distribution function of the electrons, $f(\mathbf{c},\mathbf{r},t)$, satisfies Boltzmann's equation[2,14]

$$\frac{\partial f}{\partial t}+\mathbf{c}\cdot\frac{\partial f}{\partial \mathbf{r}}+\frac{e\mathbf{E}}{m}\cdot\frac{\partial f}{\partial \mathbf{c}}=\int\int(f'F'-fF)g\sigma(g,\chi)d\hat{\mathbf{g}}\,d\mathbf{V}\ . \tag{1}$$

Here, $\mathbf{E}$ is the impressed electric field, $\mathbf{F}(\mathbf{V})$ the velocity distribution function of the background medium, $\mathbf{g}$ the initial relative velocity, χ the scattering angle, and σ the differential scattering cross section. Primes denote inverse encounters.[14] By multiplying Eq. (1) by any function ψ of the velocity $\mathbf{c}$ and integrating over all velocities $\mathbf{c}$, we may obtain an equation describing the space-time evolution of the quantity

$$\langle\psi\rangle=\frac{1}{n}\int\psi(\mathbf{c})f(\mathbf{c})d\mathbf{c}\ , \tag{2}$$

where $n(\mathbf{r},t)$ is the electron density. The evolution equation is

$$\frac{\partial}{\partial t}(n\langle\psi\rangle)+\frac{\partial}{\partial \mathbf{r}}\cdot(n\langle\mathbf{c}\psi\rangle)-\frac{en\mathbf{E}}{m}\cdot\left\langle\frac{\partial\psi}{\partial\mathbf{c}}\right\rangle=-n\langle J(\psi)\rangle\ , \tag{3}$$

with[14]

$$J(\psi)=\int\int F(\psi'-\psi)g\sigma\,d\hat{\mathbf{g}}'d\mathbf{V}\ . \tag{4}$$

In particular, using $\psi=1$, $m\mathbf{c}$, and $\frac{1}{2}mc^2$ in turn, we obtain the evolution equations

$$\frac{\partial}{\partial t}(n)+\frac{\partial}{\partial \mathbf{r}}\cdot(n\mathbf{v})=-n\langle J(1)\rangle\ , \tag{5}$$

$$\frac{\partial}{\partial t}(mn\mathbf{v})+\frac{\partial}{\partial \mathbf{r}}\cdot(mn\mathbf{v}\mathbf{v}+\mathsf{P})-ne\mathbf{E}=-nm\langle J(\mathbf{c})\rangle\ , \tag{6}$$

$$\frac{\partial}{\partial t}(nU)+\frac{\partial}{\partial \mathbf{r}}\cdot(n\mathbf{v}U+\mathbf{v}+\mathsf{P}+\mathbf{Q})-ne\mathbf{v}\cdot\mathbf{E}=-\tfrac{1}{2}nm\langle J(c^2)\rangle\ . \tag{7}$$

The various moments appearing in these equations are defined by density

$$n=\int f\,d\mathbf{c}\ , \tag{8}$$

mean velocity

$$\mathbf{v}=\langle \mathbf{c}\rangle\ , \tag{9}$$

random velocity

$$\mathbf{C}=\mathbf{c}-\mathbf{v}\ , \tag{10}$$

pressure tensor

$$\mathsf{P}=nm\langle \mathbf{CC}\rangle\ , \tag{11}$$

mean energy

$$U=\tfrac{1}{2}m\langle c^2\rangle=\frac{1}{2n}\mathrm{tr}\mathsf{P}+\tfrac{1}{2}mv^2\ , \tag{12}$$

heat flux

$$\mathbf{Q}=\tfrac{1}{2}nm\langle C^2\mathbf{C}\rangle\ . \tag{13}$$

Equations (5)–(7) may be used to investigate the evolution of the density, momentum, and energy of the electrons provided that the quantities $\mathsf{P},\mathbf{Q}$, and $\langle J\rangle$ can be expressed in terms of n, $\mathbf{v}$, and U. In the present study of steady flow to an absorbing plane anode, the vector equations are reduced to an approximate and closed one-dimensional system as follows:[12,13]

$$\frac{d}{x}(nv)=0\ , \tag{14}$$

$$\frac{d}{dx}(\tfrac{2}{3}nU+\tfrac{2}{3}nmv^2)-enE=-nmv\bar{\nu}\ , \tag{15}$$

$$\frac{d}{dx}[nv(\tfrac{5}{3}U-\tfrac{1}{3}mv^2)]-envE=-2\frac{m}{M}n(U-\tfrac{3}{2}kT_G)\bar{\nu}\ . \tag{16}$$

In passing from Eqs. (5)–(7) to Eqs. (14)–(16) it has been assumed[13] that P is an isotropic, diagonal tensor and that $\mathbf{Q}=0$. On the right-hand side of Eqs. (14)–(16), the quantities M and T_G are the particle mass and temperature, respectively, of the background medium: the algebraic forms follow from Refs. 15 and 16, with the additional assumption that $m\ll M$. We may obtain an approximation to the mean collision frequency $\bar{\nu}$ by adopting momentum-transfer theory,[16] which assumes that

$$\bar{\nu}(U)=N\left[\frac{2U}{m}\right]^{1/2}\sigma_m(U)\ , \tag{17}$$

where N is the background particle density and $\sigma_m(\varepsilon)$ is the momentum transfer cross section at an energy ε.

Equations (15) and (16) imply that in the absence of spatial gradients the "equilibrium" velocity and energy are

$$v_0=\frac{eE}{m\bar{\nu}_0}=\mu_0E\ , \tag{18}$$

$$U_0=\frac{Mev_0E}{2m\bar{\nu}_0}=\tfrac{1}{2}Mv_0^2\ , \tag{19}$$

where μ_0 is the mobility. It is assumed for convenience that $T_g=0$. From Eq. (15) it is possible to deduce that the diffusion coefficient is

$$D_0=\frac{2}{3}\frac{U_0}{m\bar{\nu}_0}=\frac{2}{3}\frac{U_0}{e}\mu_0\ , \tag{20}$$

provided the spatial dependence of v and U is ignored.[16] It is convenient to use these expressions for the equilibrium transport properties to normalize Eqs. (14)–(16). Using the transformations

$$\begin{gathered} n'=n/n_0,\quad v'=v/v_0,\quad U'=U/U_0\ ,\\ \bar{\nu}'=\bar{\nu}(U)/\bar{\nu}(U_0),\quad x'=v_0x/D_0\ , \end{gathered} \tag{21}$$

and a momentum transfer cross section of the form

$$\sigma_m(\varepsilon)=\sigma_0\varepsilon^s\ , \tag{22}$$

we obtain the normalized equations (now omitting the primes)

$$\frac{d}{dx}(nv)=0\ , \tag{23}$$

$$\frac{d}{dx}(nU+\delta nv^2)-n=-U^{s+1/2}\ , \tag{24}$$

$$\frac{d}{dx}(\tfrac{5}{2}U-\delta v^2)-1=-nU^{s+3/2} \tag{25}$$

with $\delta=m/M$. Equation (23) implies that the product nv is a constant and we have chosen the density normalization so that the $nv=1$. The velocity v may now be eliminated from (24) and (25), and first-order coupled differential equations may be obtained for n and U:

$$\frac{dn}{dx}=\frac{(3n-5U^{s+1/2}+2n^2U^{s+3/2})}{5U-9\delta/n^2}\ , \tag{26}$$

$$\frac{dU}{dx}=\frac{2}{5}\left[1-nU^{s+3/2}-2\frac{\delta}{n^3}\frac{(3n-5U^{s+1/2}+2n^2U^{s+3/2})}{5U-9\delta/n^2}\right]\ . \tag{27}$$

III. RESULTS

The coupled ordinary differential equations (26) and (27) have been solved numerically to yield the spatial variation of the density $n(x)$ and mean energy $U(x)$ for several model cross sections. The results have been obtained for a mass ratio $\delta=0$.[17] The method of solution can be illustrated by considering first the level curves of the equation obtained by eliminating the independent variable x from (26) and (27):

$$\frac{dU}{dn}=2U\left[\frac{1-nU^{s+3/2}}{3n-5U^{s+1/2}+2n^2U^{s+3/2}}\right]\ . \tag{28}$$

Figure 1 shows the level curves of Eq. (28) in the (n,U) plane, for the case $s=0$. These curves represent the manifold of solutions of Eqs. (26) and (27) for various boundary conditions. The solution to the absorbing mode prob-

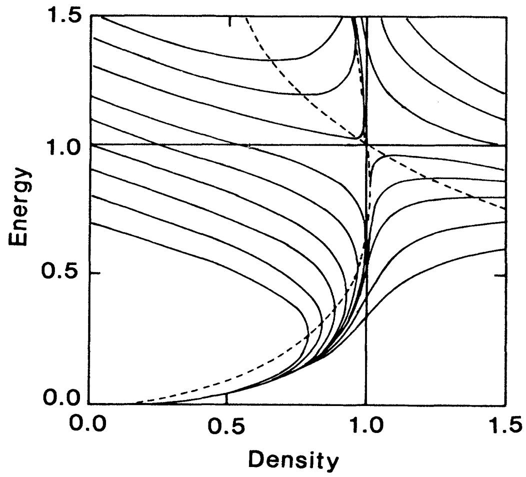

FIG. 1. Level curves of Eq. (28) in the (n, U) plane. Dashed curves show the loci $dU/dn=0$ and $dn/dU=0$. Distance from the anode is a parameter along each level curve, increasing to the right for curves emanating from $n=0$. The solution we seek lies in the top left quadrant, and passes through the equilibrium point $(n, U)=(1,1)$.

lem is the curve which begins at $x=-\infty$ (far from the anode) with the equilibrium solution $(n,U)=(1,1)$ and moves in the positive x direction towards the condition $n=0$ at $x=0$. This curve meets the axis $n=0$ at a point $U=U(0)$, where $U(0)$ is an unknown non-zero number corresponding to the mean energy at the anode.

The value of $U(0)$ is found by Newton-Raphson iteration. Beginning with an estimate $U(0)=U^*$, Eqs. (26) and (27) are integrated towards $x=-\infty$ from the point $(n,U)=(0,U^*)$ at the anode $x=0$, using a fourth-order

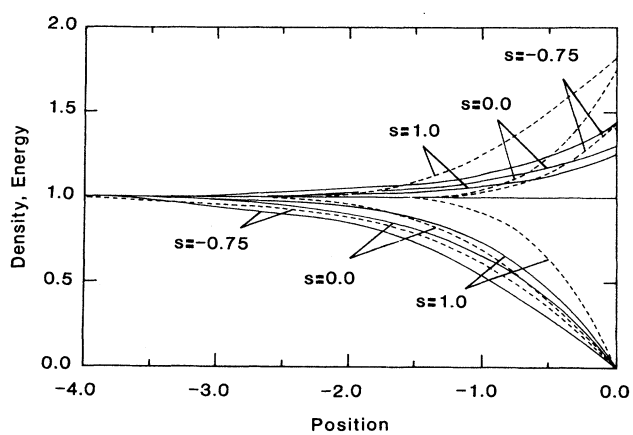

FIG. 2. The variation of normalized energy (upper six curves) and normalized density (lower six curves) with normalized distance from the anode. Dashed curves are drafted from Ref. 6, while the solid curves are solutions to Eqs. (26) and (27). The curves are labeled by the index s used in the collision model.

TABLE I. Comparison between the normalized energy at the anode predicted by (a) the current theory and (b) Ref. 6. The value in equilibrium is 1.0.

s	$U(0)/U(\infty)$ (this paper)	$U/U(\infty)$ (Ref. 6)
1	1.284	1.78
0	1.300	1.75
$-\frac{3}{4}$	1.389	1.47

Runge-Kutta algorithm. The deviation of the solution from the desired values $(n,U)=(1,1)$ for large (negative) values of x ($|x|>10$) can be reduced by systematically adjusting the estimate U^*. It is found that the algorithm converges rapidly, and numerical experiments with a variety of quadrature intervals and initial estimates have shown that solution with an accuracy of 10^{-6} are readily obtained.

Figure 2 shows the calculated run of number density $n(x)$ and mean energy $U(x)$ for the three cases[6] $s=1,0,-\frac{3}{4}$. The equilibrium solution $n(x)=1-e^x$, $U(x)=1$ is also shown, together with solutions drafted from Ref. 6, which were obtained from the Boltzmann equation. Table I compares the values of the mean energy at the anode computed using the present theory with values computed in Ref. 6.

The present theory predicts that the mean electron energy increases towards the absorbing anode. This result disagrees with predictions based on (invalid) equilibrium theory, but agrees qualitatively with the result found in Ref. 6 by solving the Boltzmann equation. The fact that dU/dn is positive for small n and finite U is evident from Eq. (28): the physical intepretation of the effect[6] involves the heating of the electrons by the diffusion current. Moreover, the present theory predicts that the density distributions vary with the index s in a manner qualitatively similar to the solutions of Ref. 6. In view of the economy of the present model compared with many of the alernative methods available for describing non equilibrium behavior,[5-13] the general agreement between the departures from equilibrium predicted by it and by detailed solutions of the Boltzmann equation is very encouraging.

However, as shown in Table I and Fig. 2, the moment equations presented here do not provide an extremely accurate description of nonequilibrium phenomena. The explanation of this shortcoming lies in the fact that the moment equations used here have been truncated ("closed") by the assumptions $\mathbf{Q}=0$ and that P is isotropic. These lead to a simple theory, but cannot treat accurately such effects as the extreme anisotropy of the electron distribution function at the anode (i.e., no inwardly flowing electrons).[6,5] I conjecture that a more complete and accurate theory could be derived by using more complex forms of P and $\mathbf{Q}$, perhaps analogous to the inclusion of viscosity and thermal conductivity in conventional hydrodynamics. However, the Chapman-Enskog or similar methods used to develop higher hydrodynamic theories are unlikely to be useful in the present problem where the equilibrium distribution is non-Maxwellian, and the theory developed in Ref. 10 may provide a clearer path to these more complex and accurate equations.

IV. CONCLUDING REMARKS

Moment equations describing the space-time development of the number density, mean velocity, and mean energy of an electron stream moving under the influence of a strong electric field have been presented. Closing the system of moment equations by the assumptions P is isotropic and $\mathbf{Q}=0$, we find that solutions to the challenging problem of the absorbing anode are readily found, containing much of the important physics. The simple moment equations could thus be used to explore, qualitatively, important nonequilibrium processes in many situations, such as breakdown phenomena, hot electron transport in semiconductors, and high-frequency electric fields.

The simple moment theory does have shortcomings which might be overcome by relaxing the abovementioned assumptions, using approximations to higher moments or the interpolation process exhibited in Ref. 10.

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

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

[3]C. M. Snowden, Rep. Prog. Phys. **48**, 223 (1985).

[4]K. Kumar, Phys. Rep. **112**, 319 (1984).

[5]R. E. Robson, Aust. J. Phys. **34**, 223 (1981).

[6]J. J. Lowke, J. H. Parker, and C. A. Hall, Phys. Rev. A **15**, 1237 (1977).

[7]L. C. Pitchford, Wright-Patterson Air Force Base Technical Report No. AFWAL-TR-85-2016, 1985 (unpublished).

[8]G. L. Braglia and J. J. Lowke, J. Phys. D **12**, 1831 (1979); Tran Ngoc An, E. Marode, and P. C. Johnson, *ibid.* **10**, 2317 (1977).

[9]P. Segur, M. Yousfl, J. B. 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. A. Luessen (Plenum, New York, 1983), p. 331.

[10]E. E. Kunhardt, J. Wu, and B. Penetrante, Phys. Rev. A **37**, 1654 (1988).

[11]N. L. Aleksandrov, A. P. Napartovich, and A. N. Starostin, Fiz. Plazmy **6**, 1128 (1980) [Sov. J. Plasma Phys. **6**, 618 (1980)]; K. K. Thornber, IEEE Electron Device Lett. **EDL-3**, 69 (1982).

[12]J. H. Ingold, J. Appl. Phys. **40**, 55 (1969); **40**, 62 (1969); Phys. Rev. A **40**, 7158 (1989); **42**, 950 (1990).

[13]G. Roumeliotis and L. E. Cram, J. Phys. D **22**, 113 (1989).

[14]S. Chapman and T. G. Cowling, *Mathematical Theory of Non Uniform Gases* (Cambridge University Press, London, 1970).

[15]G. H. Wannier, Bell Syst. Tech. J. **32**, 170 (1953); L. A. Viehland and E. A. Mason, Ann. Phys. (N.Y.) **91**, 499 (1975).

[16]R. E. Robson, J. Chem. Phys. **85**, 4486 (1986).

[17]If the mass ratio $\delta\neq0$, Eq. (27) is singular at the boundary if the condition $n=0$ is imposed there. However, this condition is clearly only an approximation, and more accurate solutions may be obtained by using the concept of an "extrapolation distance" to reflect the physically necessary fact that n is nonzero at the surface of the anode [see J. D. Dudestadt and W. R. Martin, *Transport Theory* (Wiley-Interscience, New York, 1979), Sec. 4.2.1]. Numerical experiments with a range of relevant mass ratios and plausible extrapolation distances show that Eqs. (26) and (27) are well behaved, and that the present results exhibit with minimum complexity the important physical processes embodied in the moment equations.