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The Solution of Nonlinear Boundary-Value Transport Problems in Electron and Plasma Devices*

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A method of solution of the nonlinear Landau-Vlasov equation which occurs in charged particle transport phenomena is described. The method is similar in concept to the Spherical Harmonics Method of neutron transport theory, since the particle distribution function is expanded in orthogonal functions of velocity to obtain an infinite set of partial differential equations. The nonlinearity arises when the particle interactions are taken into account in the force term of the Landau-Vlasov equation. The latter is introduced into the equation iteratively and a numerical integration routine is described to integrate the set of equations resulting from a finite (nth order) truncation of the expansion. The truncated equations, which are for the first n velocity moments of the distribution function, are such that these moments satisfy the untruncated equations also, whereas higher moment equations are modified by a fictitious source term. The convergence of the finite-difference equations and the convergence of the finite-difference solution to the solution of the differential equations is proved for the linear case in which the force is assumed to be known. Computational evidence of the convergence in the nonlinear case is provided, although no mathematical proof has so far been developed.

1. INTRODUCTION

In an invited address [1] in 1962 the first author, while reviewing the existing nonlinear mathematical theory of plasma oscillations, suggested that valuable

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insight and new methods might emerge from a re-examination of the nonlinear theories for existing electron and plasma devices from the viewpoint of transport theory, at least in those instances where it was reasonable to use the Landau-Vlasov equation in spite of its known limitations. (These as described by G. E. Uhlenbeck were also summarized in [1].) This report will present the results obtained to date from this re-examination.

Prior to this work, the nonlinear theories developed for devices of the above type have been almost exclusively based on a ballistic approach involving a Lagrangian formulation in which the overtaking or multistreaming phenomenon is dealt with by introducing the concept of "sheet" or "disc" electrons. In this approach, applied for example to a traveling-wave tube, the electron beam is typically divided into 32 charge sheets, each of which represents the effect of a large number of electrons, and the necessary information is obtained by numerical integration of their motion. Historically, the development of this theory can be found in the book *Thermionic Valves* by Beck [2]. The current state-of-the-art is described in complete detail in a forthcoming book by Rowe [3] who has played a pioneering role in the development of the ballistic approach. Some of his basic contributions and their relations to those of other workers constitute Refs. [4] and [5].

In actual fact little is known about the solution of boundary-value problems even for the usual Boltzmann equation as can be seen by reference to the article by Gross, Jackson, and Ziering [6] who were among the first to introduce the half-range expansions which will play a vital role in the development to be presented here.

Even in the linear approximation, the transport point of view has not received much development to date. Watkins and Rynn [7] formulated it for the traveling-wave tube using Pierce's circuit equation (cf. [8]) and demonstrated that the effects of velocity distribution on the gain were indeed small. Even the achievement of solution of boundary-value problems based on a linearization of the Landau-Vlasov equation in the presence of the Maxwell field equations is a very recent development carried out by Shure [9] for a quite general class of problems, and by Montgomery and Gorman [10] for a more special class.

In contrast to this situation, the solution of nonlinear transport problems as they occur in nuclear reactors has received much attention, as the book by Weinberg and Wigner [11] clearly demonstrates. In particular, considerable success has been achieved by the *Spherical Harmonic Method* as it is described in the full-range approximation by, for example, Kofink [12] and in the half-range approximation by Yvon [13]. An important contribution to this area was made by Krook [14] who was the first to demonstrate that the moment equations were automatically closed at any approximation provided the functions chosen for expansion in velocity, in either the full- or half-range approximation, satisfied a three-term recurrence relation. The mathematical proof of convergence of these methods, even for the neutron case, is in a much less satisfactory state. To the best of our knowledge it has been carried through only for the Milne problem by Kofink [12] who, through the use of delicate and nonuniform convergence arguments, was able to indicate at least a path that could be followed so as to obtain the known Wiener-Hopf solution by passing to the limit in the truncated system resulting from the expansion in Legendre polynomials. In practice, the truncated system has, in turn, to be solved by finite-difference methods. Here, at least for the neutron transport case, Keller and Wendroff [15] and Wendroff [16] were able to establish sufficient conditions for the convergence of a finite-difference scheme to the truncated system. For the numerical integration of the quasi-linear type of equations which arise from the half-range truncated system after appropriate transformation of the equations (Appendix B) a finite-difference approximation has been given by Thomée [30] who establishes sufficient conditions for stability and convergence to the differential equation.

With this much background, it seemed reasonable that it would be possible to carry out a similar development for the Landau-Vlasov equation coupled in a self-consistent nonlinear fashion to one or more of the Maxwell equations. This turned out to be the case, although many unanticipated difficulties arose due to the differences in the physical nature of the problems under consideration, and as a result the theory to be presented here has been slowly evolving since the summer of 1962. While much work still remains to be done before any claim would be justified that a complete rigorous mathematical theory exists, it is believed that sufficient success has been achieved so that a detailed report should now be made available to other scientists in the hope that they can help in filling the existing gaps as well as in extending our results to related problems. In particular, as yet a path has not been discovered which would suggest a way of establishing the convergence of our truncated infinite system to the solution of the full problem. Apart from the delicate considerations which would be as necessary here as in the work of Kofink mentioned above, in the simplest case of full-range expansion in velocity, involving Hermite functions as they are used in the theory of distributions developed by Korevaar [17] and which were shown to be equivalent to the theory of generalized functions as developed by Lighthill [18] and by Widlund [19], one encounters a one-parameter family of infinite noncommuting Jacobi matrices which can be shown to be c-unitary equivalent in the sense of Von Neumann [20] as this theory is presented, for example, in Smirnov [21]. The approximating matrices do converge in the sense of Stone [22] to the infinite matrices, and thus one is confronted with a one-parameter representation of one and the same operator in a Hilbert space which, unfortunately, involves different resolutions of the identity. For the choice of the value zero for this parameter, all is known, for this leads to the Hermite representation as given in either Stone or Smirnov. The details of these considerations are given in Appendix A. Nevertheless, as a result of the methods recently developed by Atkinson and reported in [23] as well as in his recent book [24], there is considerable hope that it may eventually be possible to give a complete and rigorous mathematical theory.

In view of this far from satisfactory situation, one might well ask as to the justification for presenting the report at the present time. The best answer to this at the moment is because of the success obtained in the application of our methods to known steady-state solutions for a number of classical problems. To mention one here which will be discussed in detail in Section 6, Langmuir [25] obtained the steady-state solution for the plane diode in the presence of space charge in 1923 (cf., also Kleynen [26]). Using half-range polynomial expansions in velocity with a fourth-order truncation in both the positive and negative velocity regions (i.e., an 8th order approximation) and beginning with a half-Maxwellian distribution, our method computes the transition to the steady-state anode current, cathode current, and potential distribution which takes place in less than three electron transit times and required less than one minute of computing time on an IBM 7090. The transient behavior as the steady state is approached is illustrated in Figs. 4 and 5.

Before entering into details, it should be mentioned that this work has been reported in a very preliminary form as an invited address at Pennsylvania State University, the proceedings of which constitute [27].

2. General Formulation of the Method

In this section the outline will be indicated, without detailed proofs, of the attack on the Landau-Vlasov equation (often called the collisionless Boltzmann equation)

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + a \frac{\partial f}{\partial v} = 0 \tag{1}$$

which describes a density function $f(x, v, t)$ of an electron beam undergoing an acceleration $a(x, t)$ determined, for example, by space-charge forces and the interaction with a circuit or another particle beam. In the latter case it is necessary of course to consider simultaneously an additional equation of the form Eq. (1) for the other stream of particles. For the moment questions concerning the source of the acceleration term $a(x, t)$ will be left aside and the procedure carried out as if it were known. To reduce Eq. (1) to an infinite set of hyperbolic equations in two independent variables x and t, the density distribution is expanded in terms of orthogonal polynomials in the velocity variable. Since most of the problems to which application of the proposed method is envisaged have a predominant direction of particle streaming, it is advantageous to treat the positive and negative velocity regions of validity of Eq. (1) in a manner first suggested by Yvon [13] for the neutron transport problem. To do this it is necessary to define the kth moments of the distribution function over the half-range,

$$M_k^+ = \int_0^\infty v^k f dv, \tag{2}$$

$$M_k^- = \int_{-\infty}^0 v^k f dv. \tag{3}$$

On multiplying Eq. (1) by v^k and integrating over the ranges $0 \leqslant v \leqslant \infty$ and $-\infty \leqslant v \leqslant 0$ respectively, the upper and lower signs in the following equation are obtained:

$$\frac{\partial M_k^\pm}{\partial t} + \frac{\partial M_{k+1}^\pm}{\partial x} - kaM_{k-1}^\pm = \pm a\delta_{0k} f(x, 0, t). \tag{4}$$

In this equation a partial integration has been carried out on the third term of the left-hand side and it has been assumed that f approaches zero sufficiently rapidly as v approaches both plus and minus infinity. The quantity δ_{0k} is the Kronecker delta

$$\delta_{0k} = 0, \qquad k \neq 0; \qquad \delta_{0k} = 1, \qquad k = 0. \tag{5}$$

An orthogonal power series expansion is now made for $f(x, v, t)$. In order to treat the general case, assume that the polynomials of degree k, $p_k^\pm(v)$, are orthogonal with respect to the weighting function $w^\pm(v)$; that is,

$$\pm \int_0^{\pm\infty} w^\pm(v)\, p_i^\pm(v)\, p_j^\pm(v)\, dv = \delta_{ij}. \tag{6}$$

Certain restrictions are implied on $w^\pm(v)$ in order that this process be possible and in addition it is required that $w^\pm(0) \neq 0$. Without loss of generality, it may be assumed that $w^\pm(0) = 1$. The nth order expansion of f is then

$$f_n^\pm(x, v, t) = w^\pm(v) \sum_{k=0}^{n-1} b_k^\pm(x, t)\, p_k^\pm(v), \tag{7}$$

where the upper and lower signs are valid in the positive and negative regions in this and in all subsequent equations. The coefficients $b_k^{\pm}$ are obtained from Eq. (7) by the formula

$$b_k^{\pm} = \pm \int_0^{\pm\infty} p_k^{\pm}(v) f_n^{\pm}(x, v, t)\, dv, \tag{8}$$

so that in the nth order approximation it is possible to write

$$f_n^{\pm}(x, 0, t) = \int_0^{\pm\infty} \sum_{k=0}^{n-1} p_k^{\pm}(0)\, p_k^{\pm}(v) f_n^{\pm}(x, v, t)\, dv. \tag{9}$$

The Christoffel-Darboux relation (cf., Szegö [28]) can be used to reduce Eq. (9) to

$$f_n(x, 0, t) = \pm \frac{C_{n-1,n-1}^{\pm}}{C_{n,n}^{\pm}} \int_0^{\pm\infty} \left(\frac{p_n^{\pm}(v)\, p_{n-1}^{\pm}(0) - p_{n-1}^{\pm}(v)\, p_n^{\pm}(0)}{v} \right) f dv, \tag{10}$$

where the quantities $C_{k,l}$ occurring in this expression are defined by

$$p_k^{\pm}(v) = \sum_{l=0}^{k} C_{k,l}^{\pm} v^l. \tag{11}$$

Substitution of Eq. (11) into Eq. (10) and the use of Eqs. (2) and (3) yields

$$f_n(x, 0, t) = \left[\frac{C_{n-1,n-1}}{C_{n,n}} \sum_{k=0}^{n-1} (C_{n,k+1} C_{n-1,0} - C_{n-1,k+1} C_{n,0})\, M_k \right]^{\pm}. \tag{12}$$

In general, the two values of $f(x, 0, t)$ given by Eq. (12) for the two signs will not be equal for any finite value of n, thus the question arises of which to use to substitute for the right-hand side of Eq. (4). Examination of Eq. (4) shows that coupling between the positive and negative velocity regions can only occur through $f(x, 0, t)$ in the equation for $k = 0$, and therefore the coupling will be determined by the choice of this expression.

The choice of the sign in Eq. (12) is made by considering the behavior of particles with velocities near zero. If the acceleration $a(x, t)$ is positive, particles having small negative velocities will acquire positive velocities after a short period of time, while particles already having positive velocities will simply be accelerated. Conversely, if the acceleration is negative, particles with small positive velocities will later acquire negative velocities. It is apparent that the coupling is one way and depends on the sign of the acceleration

$a(x, t)$. Therefore a reasonable procedure is to evaluate $f(x, 0, t)$ in Eq. (4) from the negative moments (Eq. (12)) when $a(x, t) > 0$, and from the positive moments when $a(x, t) < 0$, with the result that Eq. (4) becomes

$$\frac{\partial M_k^{\pm}}{\partial t} + \frac{\partial M_{k+1}^{\pm}}{\partial x} - kaM_{k-1}^{\pm}$$

$$= \pm\, a\delta_{0k} \left[\frac{C_{n-1,n-1}}{C_{n,n}} \sum_{k=0}^{n-1} (C_{n,k+1}C_{n-1,0} - C_{n-1,k+1}C_{n,0})\, M_k\right]^{\operatorname{sgn}(-a)},$$

$$k = 0, 1, 2, \cdots n - 1. \tag{13}$$

This can be stated alternatively as follows. Consider the domains of definition of f^+ and f^-, namely, $0 \leqslant x \leqslant d$ (as in a tube problem for example), $0 \leqslant v < +\infty$; $0 \leqslant x \leqslant d$, $0 \geqslant v > -\infty$. These are illustrated in Fig. 1.

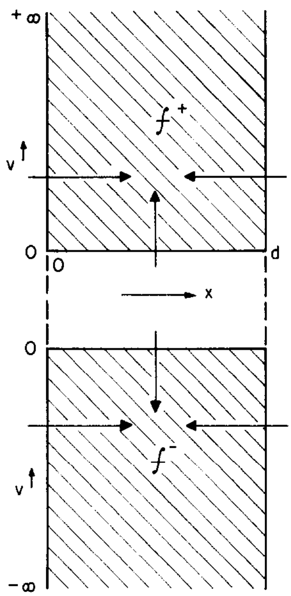

FIG. 1. Domains of f^+ and f^- in phase space.
Arrows represent the inward flow of particles across the boundaries.

It is physically meaningful, and in fact necessary, to specify information about the number of particles entering these two-dimensional phase spaces. The behavior of particles leaving the phase spaces through the boundaries is determined by the interaction of the particles and may not be specified *a priori*. For instance, f^+ must be specified along $x = 0$ for particles having

$dx/dt > 0$, and f^- along $x = d$ for particles having $dx/dt < 0$. Using this same idea of causality, the nonphysical boundary introduced by the use of half-range expansions requires that f^+ must be specified along $v = 0$ for particles having $dv/dt > 0$, i.e., positive acceleration $a(x, t)$. Similar conditions are needed for f^- except that f^- must be specified along $v = 0$ for particles having $dv/dt < 0$. The value of f^+ for $dv/dt > 0$ can only be obtained from the value of f^- computed for $dv/dt > 0$. This is another way of stating that the particles which leave the f^- domain through the upper boundary must enter the f^+ domain through the lower boundary. Correspondingly, particles which leave the f^+ domain through the lower boundary enter the f^- domain through the upper boundary.

Since an nth order approximation is made, it is only possible to derive n independent moment equations for $k = 0, 1, 2, \cdots n - 1$ in Eq. (4). Nevertheless Eq. (4) for $k = n - 1$ involves the moments $M_n^{\pm}$ for which no further equations have been obtained. However, as first shown by Krook [14] for the radiative transfer problem, this moment is in reality linearly dependent upon the previous moments. This can be demonstrated by multiplying Eq. (7) by $p_k^{\pm}(v)$ and integrating over the appropriate half range to give:

$$\pm \int_0^{\pm\infty} w^{\pm}(v) \sum_{k=0}^{n-1} b_k^{\pm} p_k^{\pm}(v)\, p_n^{\pm}(v)\, dv = \pm \int_0^{\pm\infty} f_n(x, v, t) \sum_{k=0}^{n} C_{n,k}^{\pm} v^k dv$$

$$= \sum_{k=0}^{n} C_{n,k}^{\pm} M_k^{\pm}. \tag{14}$$

Because of the orthogonality of the polynomials, the left-hand side of Eq. (14) is clearly zero. Thus

$$M_n^{\pm} = -\frac{1}{C_{n,n}^{\pm}} \sum_{k=0}^{n-1} C_{n,k}^{\pm} M_k^{\pm}. \tag{15}$$

In order to ensure stability in the numerical integration process and to give the correct domain of dependence and influence, it is desirable to transform the moment equations into the characteristic form as originally done by Courant and Lax. For this purpose define

$$m_i^{\pm} = \sum_{j=0}^{n-1} \alpha_{ij}^{\pm} M_j^{\pm}; \qquad M_i^{\pm} = \sum_{j=0}^{n-1} \beta_{ij}^{\pm} m_j^{\pm}, \tag{16}$$

where the matrices $(\alpha_{ij}^{\pm})$ and $(\beta_{ij}^{\pm})$ are mutually inverse. It can be shown by the detailed calculation given in Appendix B that the following expressions are the required ones:

$$\alpha_{ij}^{\pm} = -\frac{\Gamma_i^{\pm}}{\lambda_{i,\pm}^{j+1}} \sum_{l=0}^{j} C_{n,l}^{\pm} \lambda_{i,\pm}^{l}, \tag{17}$$

$$\beta_{ij}^{\pm} = \frac{\lambda_{j,\pm}^{i}}{\Gamma_j^{\pm} p_n^{\pm\prime}(\lambda_{j,\pm})}. \tag{18}$$

In these expressions, $\lambda_{j,\pm}$, $j = 0, 1, 2, \cdots n-1$ are the zeros of $p_n^{\pm}(\lambda)$ arranged in ascending order of magnitude and

$$p_n^{\pm\prime}(\lambda_{j,\pm}) = \frac{dp_n^{\pm}(\lambda)}{d\lambda}\bigg|_{\lambda=\lambda_{j,\pm}}. \tag{19}$$

A similar notation is also used subsequently for the second derivative. The $\Gamma_j^{\pm}$ are arbitrary parameters which may depend on j. If the transformation Eq. (16) is applied to Eq. (13), it can be shown that the resulting expression is

$$\frac{\partial m_k^{\pm}}{\partial t} + \lambda_{k,\pm} \frac{\partial m_k^{\pm}}{\partial x} = a \left[\frac{p_n''(\lambda_k)}{2p_n'(\lambda_k)} m_k - \sum_{\substack{j=0 \\ j\neq k}}^{n-1} \frac{\Gamma_k}{\Gamma_j} \frac{m_j}{\lambda_k - \lambda_j} \right]^{\pm}$$

$$\pm a \left[\frac{\Gamma_k C_{n,0}}{\lambda_k} \right]^{\pm} \left[\frac{C_{n,0} C_{n-1,n-1}}{C_{n,n}} \sum_{j=0}^{n-1} \frac{p_{n-1}(\lambda_j)}{\Gamma_j \lambda_j p_n'(\lambda_j)} m_j \right]^{\mathrm{sgn}(-a)},$$

$$k = 0, 1, 2, \cdots n-1. \tag{20}$$

On the right-hand side of Eq. (20) the $\pm$ and signum signs apply to all terms in the square brackets.

Some simplifications of Eq. (20) result if use is made of the following additional but not very restrictive hypotheses; namely

$$w^-(v) = w^+(-v), \tag{21a}$$

$$\Gamma_i^{\pm} = (-1)^n \left[C_{n,n}^n \prod_{j=0}^{n-1} p_n'(\lambda_j) \right]^{-1/2n}. \tag{21b}$$

The former assumption implies that

$$p_n^-(v) = p_n^+(-v) \tag{22}$$

and that

$$\lambda_{k,-} = -\lambda_{k,+}\,. \tag{23}$$

In Eq. (21b) and the following, the quantities without the superscript $\pm$ are taken with an implied plus sign. Any choice of $\Gamma_i^{\pm}$ which is independent of i will lead to Eq. (24). This specific choice makes det $(\alpha_{ij}) = 1$ although (α_{ij}) is not an orthogonal matrix. Equation (20) then reduces to

$$\frac{\partial m_k^{\pm}}{\partial t} \pm \lambda_k \frac{\partial m_k^{\pm}}{\partial x} = \pm\, a \left[\frac{p_n''(\lambda_k)}{2p_n'(\lambda_k)}\, m_k^{\pm} - \sum_{\substack{j=0\\ j\neq k}}^{n-1} \frac{m_j^{\pm}}{\lambda_k - \lambda_j}\right]$$

$$- \mid a \mid \cdot \frac{C_{n,0}^2 C_{n-1,n-1}}{C_{n,n}} \cdot \frac{1}{\lambda_k} \sum_{j=0}^{n-1} \frac{p_{n-1}(\lambda_j)}{\lambda_j p_n'(\lambda_j)}\, m_j^{\operatorname{sgn}(-a)} \tag{24}$$

In the development to date it is possible to show that the polynomials used (cf. Szegö [28]) obey a three-term recurrence relation of the form

$$vp_n(v) = A_n p_{n+1}(v) + B_n p_n(v) + C_n p_{n-1}(v), \tag{25}$$

and since the derivative $p_n'(v)$ is a polynomial of degree $n - 1$, it can be expressed by

$$p_n'(v) = \sum_{k=0}^{n-1} D_k{}^n p_k(v). \tag{26}$$

With the use of these expressions and Eq. (7) it is straightforward to show that the set of moment equations, Eq. (13), together with Eq. (15) is completely equivalent to the set

$$\frac{\partial b_k^{\pm}}{\partial t} \pm \left(A_{k-1} \frac{\partial b_{k-1}^{\pm}}{\partial x} + B_k \frac{\partial b_k^{\pm}}{\partial x} + C_{k+1} \frac{\partial b_{k+1}^{\pm}}{\partial x} - a \sum_{j=0}^{k-1} b_j^{\pm} D_j{}^k\right)$$

$$= \pm\, a \left[p_k(0) \sum_{l=0}^{n-1} p_l(0)\, b_l\right]^{\operatorname{sgn}(-a)}; \qquad k = 0, 1, 2 \cdots n - 1. \tag{27}$$

In order to find the equation actually satisfied by $f_n(x, v, t)$, as opposed to the Boltzmann equation which is only approximately satisfied by $f_n(x, v, t)$, the operator

$$\frac{\partial}{\partial t} + v \frac{\partial}{\partial x} + a \frac{\partial}{\partial v} \tag{28}$$

is applied to Eq. (7) and Eq. (27) is used. The result is

$$\frac{\partial f_n^{\pm}}{\partial t} + v\frac{\partial f_n^{\pm}}{\partial x} + a\frac{\partial f_n^{\pm}}{\partial v} = \pm\left\{\left[w(v)\frac{C_{n-1,n-1}}{C_{n,n}}p_n(v)\frac{\partial b_{n-1}}{\partial x}\right]^{\pm}\right.$$

$$+\left[aw(v)\sum_{k=0}^{n-1}p_k(0)\,p_k(v)\sum_{j=0}^{n-1}p_j(0)\,b_j(x,0)\right]^{\operatorname{sgn}(-a)}$$

$$-\left[aw(v)\cdot\left(\sum_{k=n}^{\infty}p_k(v)\sum_{j=0}^{n-1}b_jD_j^k\right.\right.$$

$$\left.\left.\left.+\sum_{k=0}^{\infty}p_k(0)\,p_k(v)\sum_{j=0}^{n-1}p_j(0)\,b_j(x,0)\right)\right]^{\mp}\right\}. \qquad (29)$$

The terms on the right-hand side of Eq. (29) represent a fictitious source similar in nature and effect to that which occurs in the neutron transport equation and which has been commented on in detail by Weinberg and Wigner [11] and Kofink [12]. For convergence of Eq. (29) to the Boltzmann equation it is necessary but not sufficient that this term vanishes as n approaches infinity. For n sufficiently large that the positive and negative expressions give the same value at $v = 0$, the term with superscript sgn $(-a)$ in Eq. (29) is nullified by the first n terms of the last double sum on the right-hand side. The lowest remaining polynomial is then $p_n(v)$ which is orthogonal to any power of v lower than n. This means that the moments up to this order are not affected by these remaining source terms.

3. Generalization to the Three-Dimensional Case in the Hamiltonian Formulation

Although no numerical work has yet been undertaken on the extension of the distribution method to two and three dimensions, before entering into the details of the work that has been performed in the one-dimensional case, an outline of the formulation for this generalization will be given.

In two or three dimensions it may be desirable to depart from a Cartesian coordinate system, as, for example, in the important axially symmetric case of a traveling-wave tube. Some care is necessary in the derivation of the Boltzmann equation in a general curvilinear coordinate system. This can be done unambigously by the use of the Hamiltonian formulation.

Let q_1, q_2, q_3 be the generalized coordinates and let total time derivatives be denoted by dots as in the Newtonian notation. Then in terms of the

Lagrangian $L(q_1, q_2, q_3; \dot{q}_1, \dot{q}_2, \dot{q}_3; t)$ the conjugate momenta are defined by

$$p_i = \frac{\partial L}{\partial \dot{q}_i}; \qquad i = 1, 2, 3, \tag{30}$$

and in turn the Hamiltonian $H(q_1, q_2, q_3; p_1, p_2, p_3)$ is defined as

$$H = \sum_{i=1}^{3} p_i \dot{q}_i - L. \tag{31}$$

The general form of the Boltzmann equation for the distribution function $f(q_1, q_2, q_3; p_1, p_2, p_3; t)$ is

$$\frac{\partial f}{\partial t} = [H, f], \tag{32}$$

where the Poisson bracket is, as usual, defined by

$$[H, f] = \sum_{n=1}^{3} \left[\left(\frac{\partial H}{\partial q_i} \right) \left(\frac{\partial f}{\partial p_i} \right) - \left(\frac{\partial H}{\partial p_i} \right) \left(\frac{\partial f}{\partial q_i} \right) \right] \tag{33}$$

The final form of the Boltzmann equation is obtained by using Hamilton's equations

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \qquad \dot{q}_i = \frac{\partial H}{\partial p_i}. \tag{34}$$

Thus Eq. (32) becomes

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} \left[\dot{p}_i \left(\frac{\partial f}{\partial p_i} \right) + \dot{q}_i \left(\frac{\partial f}{\partial q_i} \right) \right] = 0. \tag{35}$$

For the cylindrical coordinate system the electron equations in a quasi-static potential $V(r, \phi, z, t)$ take the following form.

$$q_r = r, \qquad q_\phi = \phi, \qquad q_z = z; \tag{36}$$

$$L = \tfrac{1}{2} m(\dot{r}^2 + r^2\dot{\phi}^2 + \dot{z}^2) + eV; \tag{37}$$

$$p_r = m\dot{r}, \qquad p_\phi = mr^2\dot{\phi}, \qquad p_z = m\dot{z}; \tag{38}$$

$$H = \frac{1}{2m} \left(p_r^2 + \frac{p_\phi^2}{r^2} + p_z^2 \right) - eV. \tag{39}$$

Finally

$$\frac{\partial f}{\partial t} + \frac{1}{m} \left(p_r \frac{\partial f}{\partial r} + \frac{p_\phi}{r^2} \frac{\partial f}{\partial \phi} + p_z \frac{\partial f}{\partial z} \right) + \frac{p_\phi^2}{mr} \frac{\partial f}{\partial p_r}$$
$$+ e \left(\frac{\partial V}{\partial r} \frac{\partial f}{\partial p_r} + \frac{\partial V}{\partial \phi} \frac{\partial f}{\partial p_\phi} + \frac{\partial V}{\partial z} \frac{\partial f}{\partial p_z} \right) = 0. \tag{40}$$

In the case of axial symmetry without rotation, the result is

$$\frac{\partial f}{\partial t} + \frac{1}{m}\left(p_r \frac{\partial f}{\partial r} + p_z \frac{\partial f}{\partial z}\right) + e\left(\frac{\partial V}{\partial r}\frac{\partial f}{\partial p_r} + \frac{\partial V}{\partial z}\frac{\partial f}{\partial p_z}\right) = 0. \tag{41}$$

It should be noted that this is formally the same as the two-dimensional Cartesian case if r is interpreted as x. However, if there is axial symmetry, since by definition, negative values of r are not permitted, a particle passing through the axis $r = 0$ must appear to be specularly reflected, i.e., when $r = 0$,

$$f(r, z; p_r, p_z; t) = f(r, z; -p_r, p_z; t). \tag{42}$$

It can be seen therefore that there is a complete analogy between the axially symmetric situation without rotation and the two-dimensional Cartesian case in which specular reflection of particles occurs at a planar boundary.

The development of a three-dimensional orthogonal polynomial expansion proceeds in a fashion analogous to that given for the one-dimensional case. Three simplifications will however be made for clarity. These are:

1. A Cartesian coordinate system is used.
2. Polynomials orthogonal over the entire range $(-\infty, \infty)$ are used.
3. A single particle species is assumed.

All of these restrictions can be removed.

The electron distribution function is expanded in the following way in terms of polynomials $P_{1i}(v_1)$, $P_{2j}(v_2)$, $P_{3k}(v_3)$ orthogonal over $(-\infty, \infty)$ with respect to the weighting functions $w_1(v_1)$, $w_2(v_2)$, $w_3(v_3)$.

$$f(x_1, x_2, x_3; v_1, v_2, v_3; t) = w_1(v_1)\, w_2(v_2)\, w_3(v_3) \cdot \sum_{i,j,k} b_{ijk}(x_1, x_2, x_3, t)\, P_{1j}(v_1)\, P_{2j}(v_2)\, P_{3j}(v_3). \tag{43}$$

The polynomials satisfy recurrence relations (cf., Szegö [28])

$$v_i P_{i,n} = A_{i,n} P_{i,n+1} + B_{i,n} P_{i,n} + C_{i,n} P_{i,n-1}; \qquad i = 1, 2, 3, \tag{44}$$

and the derivatives can be expressed as

$$P'_{i,n} = \sum_{k=0}^{n-1} D^i_{n,k} P_{i,k}; \qquad i = 1, 2, 3. \tag{45}$$

Equation (43) is substituted into Eq. (35) for the case of Cartesian coordinates and the orthogonal properties are used to obtain the system

$$\frac{\partial b_{i,j,k}}{\partial t} + A_{1,i-1}\frac{\partial b_{i-1,j,k}}{\partial x} + B_{1,i}\frac{\partial b_{i,j,k}}{\partial x} + C_{1,i+1}\frac{\partial b_{i+1,j,k}}{\partial x}$$
$$+ A_{2,j-1}\frac{\partial b_{i,j-1,k}}{\partial y} + B_{2,j}\frac{\partial b_{i,j,k}}{\partial y} + C_{2,j+1}\frac{\partial b_{i,j+1,k}}{\partial y}$$
$$+ A_{3,k-1}\frac{\partial b_{i,j,k-1}}{\partial z} + B_{3,k}\frac{\partial b_{i,j,k}}{\partial z} + C_{3,k+1}\frac{\partial b_{i,j,k+1}}{\partial z}$$
$$- e\left(\frac{\partial V}{\partial x}\sum_{l=0}^{i-1} D^1_{i,l} b_{l,j,k} + \frac{\partial V}{\partial y}\sum_{l=0}^{j-1} D^2_{j,l} b_{i,l,k}\right.$$
$$\left. + \frac{\partial V}{\partial z}\sum_{l=0}^{k-1} D^3_{k,l} b_{i,j,l}\right) = 0. \tag{46}$$

As in the one-dimensional case an orthogonal transformation can be found to reduce the system Eq. (46) to canonical form if one arbitrarily sets $b_{i,j,k} = 0$ for $\max(i, j, k) \geqslant n$. Let the matrix Z^i have elements

$$\begin{aligned}
Z^i_{p,p-1} &= A_{i,p-1}, & p &= 1, 2, \cdots n-1, \\
Z^i_{p,p} &= B_{i,p}, & p &= 0, 1, \cdots n-1, \\
Z^i_{p,p+1} &= C_{i,p+1}, & p &= 0, 1, \cdots n-2, \\
Z^i_{p,q} &= 0, & &\text{otherwise,}
\end{aligned} \tag{47}$$

and let T^i be a matrix which will diagonalize Z^i; i.e.,

$$\sum_{p,q,=0}^{n-1} T^i_{lp} Z^i_{pq} (T^i)^{-1}_{qm} = \lambda_{il}\delta_{lm}. \tag{48}$$

Such a reduction is always possible, the coefficients of T^i are simply expressed in terms of the polynomials $P_{i,j}$ with arguments $\lambda_{i,0}, \lambda_{i,1}, \cdots, \lambda_{i,n-1}$ which are the zeros of $P_{i,n}(v)$. For details see Appendix D. In addition it is necessary to define matrices $\hat{D}^i$ whose elements are

$$\hat{D}^i_{lm} = \sum_{p=0}^{n-1}\sum_{q=p}^{n-1} T^i_{lp} D^i_{pq} (T^i)^{-1}_{qm}. \tag{49}$$

Finally let

$$W_{i,j,k} = \sum_{p,q,r=0}^{n-1} T^1_{ip} T^2_{jq} T^3_{kr} b_{pqr}. \tag{50}$$

The substitution of Eqs. (48), (49), and (50) into Eq. (46) yields

$$\frac{\partial W_{ijk}}{\partial t} + \lambda_{1i}\frac{\partial W_{ijk}}{\partial x} + \lambda_{2j}\frac{\partial W_{ijk}}{\partial y} + \lambda_{3k}\frac{\partial W_{ijk}}{\partial z} - e\sum_{l=0}^{n-1}\left(\frac{\partial V}{\partial x}\hat{D}^1_{il}W_{ljk} + \frac{\partial V}{\partial y}\hat{D}^2_{jl}W_{ilk} + \frac{\partial V}{\partial z}\hat{D}^3_{kl}W_{ijl}\right) = 0. \tag{51}$$

This is in the canonical form with integration of each W_{ijk} along a fixed direction. A possible method of numerical integration is the "alternating directions" procedure of Peaceman and Rachford [29]. However, applications of this method have apparently so far been confined to elliptical and parabolic problems, and the necessary adaption to hyperbolic systems would no doubt require new numerical analysis. It is clear that even in the axially symmetric case, considerably more computation time will be required because each additional dimension introduces two more independent variables.

4. Detailed Derivation for the Half-Range Laguerre Expansions

Since most electron devices usually do not involve a distribution function which is very large for either large positive or negative velocities, the difference between a weighting function exp $(-v/2)$ appropriate for half-range Laguerre expansions and exp $(-v^2/2)$ appropriate for half-range Hermite expansion as used by Gross *et al.* [6] seemed to be more than offset by the well-known set of formulas associated with the half-range Laguerre polynomials in contrast to those for the half-range Hermite polynomials which need step-by-step development. In terms of computers, however, this difference would not be too important, and an investigation of any differences that might arise has been contemplated for future work. However, in order to retain simplicity in the analytical work, half-range Laguerre expansions have been used in all the one-dimensional problems which have so far been attacked.

Laguerre polynomials can be expressed as

$$L_n(z) = \sum_{k=0}^{n}(-1)^k\binom{n}{k}\frac{z^k}{k!}. \tag{52}$$

They satisfy the recurrence relations

$$nL_n(z) = (2n-1-z)L_{n-1}(z) - (n-1)L_{n-2}(z), \tag{53}$$

$$zL_n'(z) = n[L_n(z) - L_{n-1}(z)], \tag{54}$$

and the differential equation

$$zL_n''(z) + (1 - z)L_n'(z) + nL_n(z) = 0. \tag{55}$$

By definition of λ_j

$$L_n(\lambda_j) = 0, \tag{56}$$

and so from Eq. (54)

$$\frac{L_{n-1}(\lambda_j)}{\lambda_j L_n'(\lambda_j)} = -\frac{1}{n}. \tag{57}$$

On identifying the coefficients in the Laguerre polynomial from Eq. (52) it follows that

$$\frac{C_{n,0}^2 C_{n-1,n-1}}{C_{n,n}} \frac{L_{n-1}(\lambda_j)}{\lambda_j L_n'(\lambda_j)} = 1. \tag{58}$$

Also from Eqs. (55) and (56)

$$\frac{L_n''(\lambda_j)}{L_n'(\lambda_j)} = \frac{\lambda_j - 1}{\lambda_j}. \tag{59}$$

The results, Eqs. (58) and (59), are now inserted in Eq. (24) and yield the somewhat simplified equation

$$\begin{aligned} \frac{\partial m_k^\pm}{\partial t} \pm \lambda_k \frac{\partial m_k^\pm}{\partial x} = \pm\, a \left[\left(\frac{\lambda_k - 1}{2\lambda_k}\right) m_k^\pm - \sum_{\substack{j=0 \\ j\neq k}}^{n-1} \frac{m_j^\pm}{\lambda_k - \lambda_j}\right] \\ - \frac{|a|}{\lambda_k} \sum_{j=0}^{n-1} m_j^{\operatorname{sgn}(-a)}, \\ k = 0, 1, 2 \cdots n - 1. \end{aligned} \tag{60}$$

This equation is the one which has been used in all calculations.

5. The Space-Charge-Free Plane Diode

As a first test problem, the methods of Section 4 were used on a plane diode in which electrons were emitted with a half-Maxwellian velocity distribution from the cathode in the presence of a uniform retarding field applied at $t = 0$. That is, the acceleration in Eq. (1) was assumed negative and constant. (Space-charge effects were not included.) The length of the tube was normalized to unity and the boundary and initial conditions used were:

1. $v > 0$,

$$f(0, v, t) = \left(\frac{2}{\sqrt{\pi}}\right) e^{-v^2}, \qquad \text{all} \qquad t \geqslant 0,$$

$$f(x, v, 0) = \left(\frac{2}{\sqrt{\pi}}\right) e^{-v^2}, \qquad 0 \leqslant x \leqslant 1.$$

2. $v < 0$,

$$f(1, v, t) = 0, \qquad \text{all} \qquad t \geqslant 0,$$

$$f(x, v, 0) = 0, \qquad 0 \leqslant x \leqslant 1.$$

The initial values of the moments were computed from Eqs. (2) and (3). The system of equations, Eq. (60), was replaced by the finite-difference scheme as described in Appendix C. As in the neutron transport case, the boundary conditions can only be satisfied approximately in the finite-difference equations. The method used to approximate those given above as well as those for the problem to be discussed in the next section are also to be found in Appendix C. Since the above problem has a known exact solution (given in Appendix E) it was possible to compare the results. For the case $n = 4$ and with a value of $a = -0.4461$, Figs. 2 and 3 compare the computed value of the moment M_0 (charge density) and M_1 (the current density) respectively at the planes $x = 0$ and $x = 1$ with the values calculated from the known closed form solution.

As can always be anticipated in a method involving series approximation, a Gibbs phenomenon will arise in the neighborhood of any sharp discontinuity and the existence of this phenomenon is clearly apparent from the above figures since the agreement is poorest in the neighborhood of the slope discontinuities in the closed form solution.

6. The Langmuir Plane Diode with Space Charge

Any real test of the method outlined in this paper requires the use of some auxiliary force equations which are coupled in a nonlinear but self-consistent way to the equations so far derived in which the acceleration term was always assumed to be known. One of the simplest type of these problems is that of the plane diode in which the effect of space charge is included. As mentioned in the introduction, the steady-state solution for this problem was discovered by Langmuir [25] in 1923 and extensively explored by Kleynen [26] in 1946. To treat this problem here, the acceleration is written

$$a(x, t) = \left(\frac{q}{m}\right) E(x, t), \tag{61}$$

where (q/m) is the charge-to-mass ratio of the particle and $E(x, t)$ is the

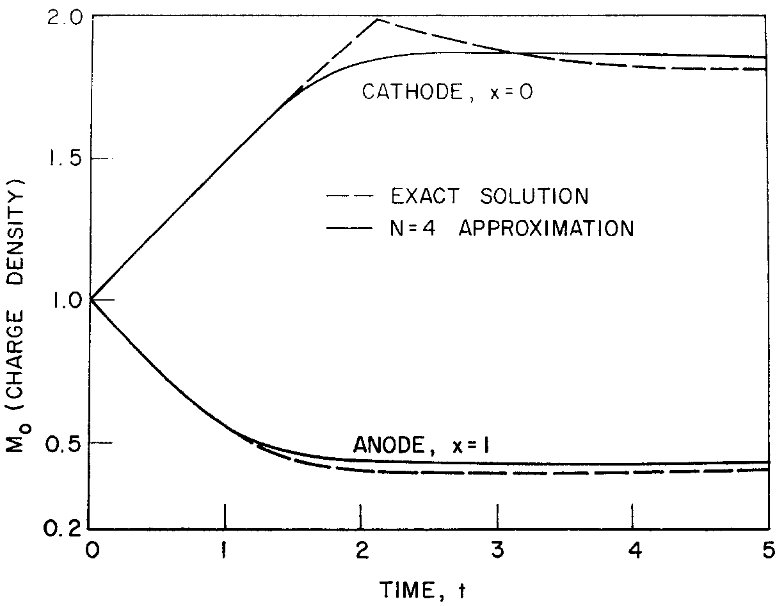

FIG. 2. Charge density at the anode and cathode as a function of time

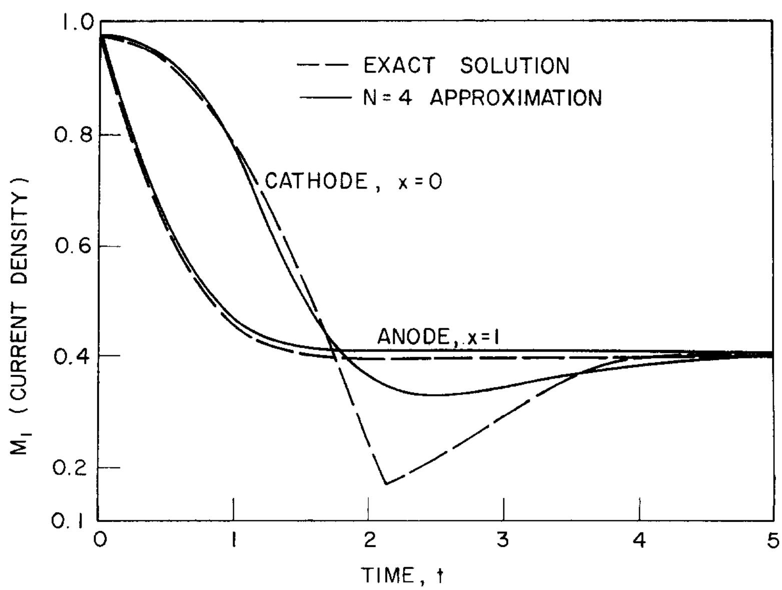

FIG. 3. Current density at the anode and cathode as a function of time

electric field. The quasi-static approximation in which the wave-equation is replaced by Poisson's equation was made and therefore

$$\frac{\partial E}{\partial x} = \frac{\rho}{\epsilon_0}, \tag{62}$$

where

$$\rho = q \int_{-\infty}^{\infty} f(x, v, t)\, dv. \tag{63}$$

Thus

$$E(x, t) = E_{\mathrm{circ}}(x, t) + E_0(t) + \frac{1}{\epsilon_0} \int_0^x \rho(x', t)\, dx' \tag{64}$$

in which E_{circ} is the circuit field and E_0 is the field at $x = 0$ excluding the circuit field. The potential V_d across the region $0 \leqslant x \leqslant d$ is obtained by integrating Eq. (64).

$$-V_d = \int_0^d E_{\mathrm{circ}}\, dx + E_0 d + \frac{1}{\epsilon_0} \int_0^d \int_0^x \rho dx' dx. \tag{65}$$

$V_d(t)$ represents the potential across the device which can be related to the external circuit parameters (e.g., a zero impedance voltage generator). Equation (65) can be used to eliminate $E_0(t)$ from Eq. (64) giving

$$E = E_{\mathrm{circ}} - \int_0^d E_{\mathrm{circ}} \frac{dx'}{d} + \frac{1}{\epsilon_0} \int_0^x \rho dx' - \frac{1}{\epsilon_0} \int_0^d \int_0^{x'} \rho dx'' \frac{dx'}{d} - \frac{V_d}{d}. \tag{66}$$

Equation (66) and the Boltzmann equation

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + a \frac{\partial f}{\partial v} = 0 \tag{67}$$

can be normalized to dimensionless form by taking

$$\begin{aligned}
v &= v_c \tilde{v}, \\
x &= d\tilde{x}, \\
t &= \frac{d}{v_c} \tilde{t}, \\
f &= \frac{m v_c \epsilon_0}{q^2 d^2} \tilde{f}, \\
E &= \frac{m v_c^2}{q d} \tilde{E}, \\
V_d &= \frac{m v_c^2}{q} \tilde{V}_d,
\end{aligned} \tag{68}$$

where v_c is a characteristic velocity. Equation (67) becomes

$$\frac{\partial \tilde{f}}{\partial \tilde{t}} + \tilde{v}\frac{\partial \tilde{f}}{\partial \tilde{x}} + \tilde{E}\frac{\partial \tilde{f}}{\partial \tilde{v}} = 0, \tag{69}$$

and Eq. (66) becomes

$$\tilde{E} = \tilde{E}_{\text{circ}} - \int_0^1 \tilde{E}_{\text{circ}}\, d\tilde{x}' + \int_0^{\tilde{x}}\int_{-\infty}^{\infty} \tilde{f} d\tilde{v} d\tilde{x}' - \int_0^1\int_0^{\tilde{x}'}\int_{-\infty}^{\infty} \tilde{f} d\tilde{v} d\tilde{x}'' d\tilde{x}' - \tilde{V}_d\,. \tag{70}$$

The moment equations derived form Eq. (66) are identical in form to those derived in Sections 2 and 4 provided the unnormalized variables are replaced by the normalized ones and a is replaced by $\tilde{E}$.

The electric field, Eq. (70), is introduced into the computations in an iterative manner. The field for the next time step is initially assumed to remain unchanged while the new value of $f(x, v, t)$ is computed. From this a fresh estimate of the field is obtained and the value of f is recalculated. This is repeated until the change in f is negligible.

This method was applied to the transient analysis of a short circuited diode in which electrons are emitted from the cathode with a half-Maxwellian velocity distribution. If the normalized density function at the cathode is

$$\tilde{f} = \frac{2}{\sqrt{\pi}} N\mu e^{-\mu^2\tilde{v}^2}, \tag{71}$$

then in terms of Langmuir's variables ξ^+, ξ^-, and η

$$N = \left(\frac{\xi^+ + \xi^-}{2\mu}\right)^2 e^{\eta}. \tag{72}$$

ξ^- is the normalized distance from the cathode to the potential minimum, ξ^+ is the normalized distance from the potential minimum to the anode, and η is the normalized potential of the minimum referred to the cathode potential. The parameter μ is chosen so that the expansion in Laguerre polynomials of Eq. (71) yields the exact value at $\tilde{v} = 0$ (e.g., if the order of the approximation is n and $n = 4$, $\mu = 0.58016$; if $n = 5$, $\mu = 0.68739$: see Appendix C). In the test run, the choice $\eta = 0.564$ was made and the anode and cathode were taken to be at the same potential ($V_d = 0$). It then follows that $\xi^+ = 1.704$ and $\xi^- = 1.279$. N was calculated from Eq. (72) and a fourth-order approximation was used. The circuit field was taken to be zero. Figure 4 shows the current density plotted as a function of time at the anode and cathode planes. The diode is initially void of electrons, current begins to flow at $\tilde{t} = 0$ and a steady state is reached at $\tilde{t} \simeq 3$. The agreement with the

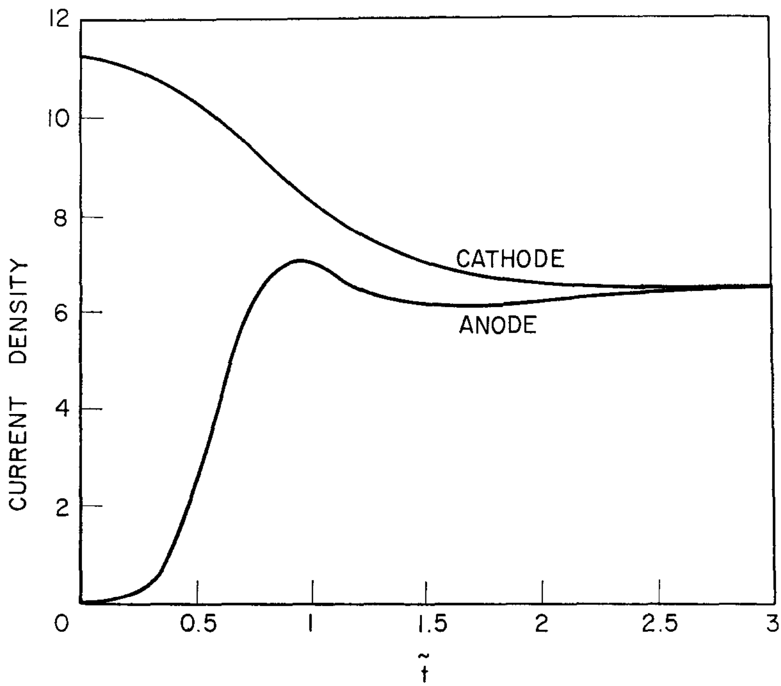

FIG. 4. Current density at the cathode and anode *vs.* time for the short circuited Langmuir diode

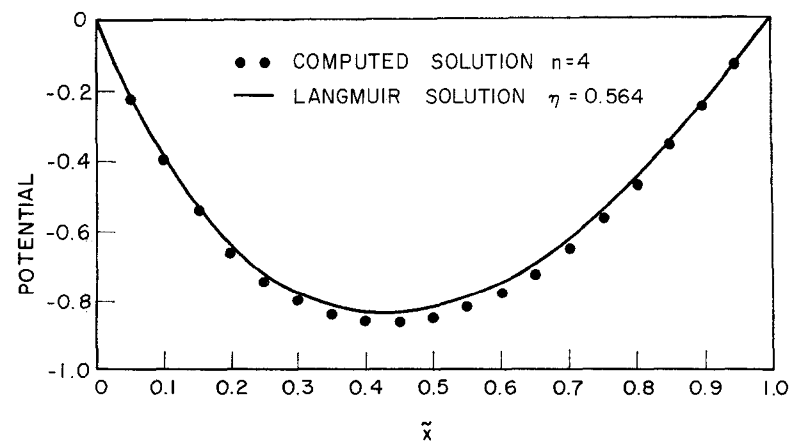

FIG. 5. Potential distribution in the equilibrium state for the short circuited Langmuir diode

Langmuir solution is to within the accuracy that the curves can be plotted. Figure 5 shows the final potential distribution compared with the Langmuir solution. Good agreement is seen to be obtained.

It should be re-emphasized that the result obtained required less than one minute computing time on an IBM 7090 Computer and that the transient solution converged to the known steady-state solution within less than three electron transit times.

7. Future Work

The main body of this paper will be concluded by a few brief remarks concerning work currently in progress and a statement of future plans. At the moment, a diode problem involving the interaction of electrons emitted from the cathode, and ions of a single species emitted from the anode, is under investigation by the appropriate modification and generalization of the methods presented here. This same problem is also being treated from the ballistic point of view (the Lagrangian formulation) by J. E. Rowe. While some encouraging preliminary results have been obtained by both methods, it would be premature to present them here. In fact, a comparison of the results of the velocity distribution method and the ballistic method and their physical significance will be published elsewhere in a joint work by Lomax and Rowe. Future plans include the investigation of the nonlinear traveling-wave tube theory in the above formulation both for the one-dimensional case and, hopefully, at least for the two-dimensional axially symmetric case.

Appendix A. The c-Unitary Equivalence of Operators Occurring in the Full-Rance Hermitian Expansion of the Velocity Distribution

The consideration of Section 2 can be specialized to the full-range Hermitian case. The substitution

$$f = ge^{-v^2/2} \tag{A.1}$$

in Eq. (1) yields

$$\frac{\partial g}{\partial t} + v\frac{\partial g}{\partial x} + a\left(\frac{\partial g}{\partial v} - vg\right) = 0. \tag{A.2}$$

If it is assumed that

$$g(x, v, t) = \sum_{k=0}^{\infty} q_k(x, t)\, \varphi_k(v), \tag{A.3}$$

where the functions $\varphi_k(v)$ are defined by

$$\varphi_k(v) = \frac{e^{-v^2/2}\, H_k(v)}{\pi^{1/4} 2^{k/2} (k!)^{1/2}} \tag{A.4}$$

and $H_k(v)$ is the kth Hermite polynomial, the procedure of Section 2 leads to the infinite system of equations

$$\frac{\partial g_k}{\partial t} + \left(\frac{k+1}{2}\right)^{1/2} \frac{\partial g_{k+1}}{\partial x} + \left(\frac{k}{2}\right)^{1/2} \frac{\partial g_{k-1}}{\partial x} = 2a\left(\frac{k}{2}\right)^{1/2} g_{k-1}, \qquad k = 0, 1, 2 \cdots. \tag{A.5}$$

If the one parameter family of Jacobi matrices

$$A(\theta) \triangleq \{a_{mn}(\theta)\}; \qquad m, n = 0, 1, 2, \cdots \tag{A.6}$$

is defined by

$$a_{mn}(\theta) \triangleq e^{i\theta}\left(\frac{n}{2}\right)^{1/2} \delta_{m+1,n} + e^{-i\theta}\left(\frac{n+1}{2}\right)^{1/2} \delta_{m-1,n} \tag{A.7}$$

and in addition

$$\mathbf{g} \triangleq (g_0, g_1, g_2, \cdots), \tag{A.8}$$

the system Eq. (A.5) can be written as

$$i\frac{\partial \mathbf{g}}{\partial t} + i\frac{\partial}{\partial x}[A(0)\,\mathbf{g}] = -a\left[A\left(\frac{\pi}{2}\right) - iA(0)\right]\mathbf{g}. \tag{A.9}$$

In an Nth order truncation obtained by putting

$$g_k = 0, \qquad a_{mn}(\theta) = 0 \qquad \text{for} \qquad k, m, n \geqslant N \tag{A.10}$$

a fictitious source term appears as in Section 2, Eq. (29). In this case the approximating equation is

$$\frac{\partial f_N}{\partial t} + v\frac{\partial f_N}{\partial x} + a\frac{\partial f_N}{\partial v} = \left(\frac{N}{2}\right)^{1/2}\left(\frac{\partial g_{N-1}}{\partial x} - a g_{N-1}\right) e^{-v^2/2}\varphi_N(v). \tag{A.11}$$

Then the real problem is to prove that Eq. (A.11) converges to Eq. (1). Here, only the matrices $A(\theta)$ as defined above will be dealt with. Let

$$V(\theta) \triangleq \{v_{mn}\}, \qquad v_{mn} \triangleq e^{im\theta}\,\delta_{mn} \tag{A.12}$$

$$V^{-1}(\theta) = \{v_{mn}^{-1}\}, \qquad v_{mn}^{-1} = e^{-im\theta}\,\delta_{mn} \tag{A.13}$$

Then

$$V(\theta)\,A(\theta)\,V^{-1}(\theta) = A(0) \tag{A.14}$$

as the following element calculation shows:

$$A(\theta)\, V^{-1}(\theta) = \sum_{p=0}^{\infty} \left[e^{i\theta} \left(\frac{p}{2}\right)^{1/2} \delta_{m+1,p} + e^{-i\theta} \left(\frac{p+1}{2}\right)^{1/2} \delta_{m-1,p} \right] e^{-ip\theta}\, \delta_{pn}$$

$$= e^{i(1-n)\theta} \left(\frac{n}{2}\right)^{1/2} \delta_{m+1,n} + e^{-i(1+n)\theta} \left(\frac{n+1}{2}\right)^{1/2} \delta_{m-1,n}\,, \tag{A.15}$$

$$V(\theta)\, A(\theta)\, V^{-1}(\theta) = \sum_{p=0}^{\infty} e^{im\theta}\, \delta_{mp} \left[e^{i(1-n)\theta} \left(\frac{n}{2}\right)^{1/2} \delta_{p+1,n} + e^{-i(1+n)\theta} \left(\frac{n+1}{2}\right)^{1/2} \delta_{p-1,n} \right]$$

$$= \left(\frac{n}{2}\right)^{1/2} \delta_{m+1,n} + \left(\frac{n+1}{2}\right)^{1/2} \delta_{m-1,n}$$

$$= a_{mn}(0). \tag{A.16}$$

(At the moment, questions of convergence are left aside.) Thus if

$$A_N(0)\, \psi = \lambda \psi = V_N(\theta)\, A_N(\theta)\, V_N^{-1}(\theta)\, \psi, \tag{A.17}$$

it follows that, for the truncated system, $V_N^{-1}(\theta)\, \psi$ is an eigenvector of $A_N(\theta)$ corresponding to the same value of λ. The eigenvalues are the roots of

$$H_N(\lambda) = 0. \tag{A.18}$$

The eigenvector is

$$\psi = \begin{bmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-1} \end{bmatrix}, \tag{A.19}$$

where

$$\psi_k = e^{-ik\theta} \left(\frac{2^{N+1} N!}{2^k k!}\right)^{1/2} \frac{H_k(\lambda)}{H_{N+1}(\lambda)}\,. \tag{A.20}$$

Recall that if

$$y_i \triangleq \sum_{k=1}^{\infty} a_{ik} x_k\,, \qquad a_{ik} = \tilde{a}_{ki} \tag{A.21}$$

is subject to

$$d_k^2 = \sum_{i=1}^{\infty} |\, a_{ik} \,|^2, \tag{A.22}$$

then $y_i \in l_2$ since the series defining it will converge absolutely for each $\bar{x} = \{x_1, x_2, \cdots\} \in l_2$. However, the series

$$\sum_{i=1}^{\infty} | y_i |^2 \tag{A.23}$$

need not converge and hence $\bar{y} = \{y_1, y_2, \cdots\}$ need not be in l_2. Let A_0 denote the operator with a matrix representation $\{a_{ik}\}$ with domain $\mathscr{D}(A_0)$ consisting of the linear manifold of all x_i, $x \in l_2$, such that

$$\sum_{k=1}^{\infty} d_k | x_k | < \infty. \tag{A.24}$$

Let B be the operator whose domain $\mathscr{D}(B)$ is the linear manifold of all x_i, $x \in l_2$, such that

$$\bar{y} = \{y, y_2, \cdots\} \in l_2. \tag{A.25}$$

Then it is known that $\mathscr{D}(A_0)$ is dense in l_2, and that $\mathscr{D}(A_0) \subseteq \mathscr{D}(B)$. If $\tilde{A}$ denotes the closure of A_0, then $\tilde{A}$ has a domain $\mathscr{D}(\tilde{A})$ consisting of the linear manifold of all $x \in \mathscr{D}(B)$ such that

$$\langle Bx, y \rangle = \langle x, By \rangle \qquad \text{for} \qquad y \in \mathscr{D}(B). \tag{A.26}$$

Moreover, it is known (cf. e.g., Smirnov [21, vol. V, p. 553]) that $A(\theta)$ for $\theta = 0$, i.e., $A(0) = A_0$, is self-adjoint, and that it possesses a simple continuous spectrum covering the entire real axis $(-\infty, \infty)$.

If $P_k(\lambda)$ denotes the normalized Hermite polynomial

$$P_k = \frac{H_k(\lambda)}{\pi^{1/4}(2^k k!)^{1/2}}, \tag{A.27}$$

then

$$\lambda P_k(\lambda) = \left(\frac{k+1}{2}\right)^{1/2} P_{k+1}(\lambda) + \left(\frac{k}{2}\right)^{1/2} P_{k+1}(\lambda), \tag{A.28}$$

$$P_0(\lambda) = 1, \tag{A.29}$$

$$\frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} e^{-\lambda^2} P_k(\lambda) P_l(\lambda) \, d\lambda = \delta_{kl}, \tag{A.30}$$

$$\begin{aligned} a_{ij}(0) &= \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} e^{-\lambda^2} \lambda P_i(\lambda) P_j(\lambda) \, d\lambda \\ &= \left(\frac{j}{2}\right)^{1/2} \delta_{i+1,j} + \left(\frac{j+1}{2}\right)^{1/2} \delta_{i-1,j}. \end{aligned} \tag{A.31}$$

The second half of Stone's [22] Theorem 7.2 implies that there exists an orthonormal set $\{w_n\}$ in the Hilbert space and a generating element f such that $\{f, A^n f; n = 0, 1, 2, \cdots\}$ span the Hilbert space and such that

$$\rho(\lambda) = \| E(\lambda) f \|^2 = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\lambda} e^{-\mu^2} d\mu, \tag{A.32}$$

where $E(\lambda)$ in the spectral resolution of the identity corresponding to $A(0)$, and moreover that

$$\begin{aligned} a_{ij}(0) &= \langle \tilde{A}(0) w_i , w_j \rangle \\ &= \int_{-\infty}^{\infty} \lambda P_i(\lambda) P_j(\lambda) d\rho(\lambda). \end{aligned} \tag{A.33}$$

Now let the reduced Jacobi matrices of $A(0)$ be defined by the relations

$$A_p(0) = \{a_{mn}^{(p)}(0)\}, \tag{A.34}$$

where

$$a_{mn}^{(p)} \triangleq a_{mn}(0) \qquad \text{for} \qquad m \leqslant p, \quad n \leqslant p, \tag{A.35}$$

$$a_{mn}^{(p)} \triangleq 0 \qquad \text{for} \qquad m > p, \quad n > p. \tag{A.36}$$

Further, let $T[A_p]$ be the linear transformation associated with the reduced matrix A_p and the orthonormal set $\{w_i\}$ introduced above when a_{mn} is replaced by $a_{mn}^{(p)}$. Theorem 10.23 of Stone [22] guarantees that $T[A_p]$ is an essentially self-adjoint transformation, that its closure, denoted by $\tilde{T}[A_p]$, is bounded and self-adjoint if $E^{(p)}(\lambda)$ is the resolution of the identity associated with $T[\tilde{A}_p]$, and, if

$$\rho^{(p)}(\lambda) = \| E^{(p)}(\lambda) w_1 \|^2, \tag{A.37}$$

then $\rho^{(p)}(\lambda)$ is a real monotonic increasing function of λ which assumes exactly $p + 1$ distinct values, namely, at the roots of $P_{p+1}(\lambda) = 0$. (Here the indices, as in Stone, run $p = 1, 2, 3, \cdots$ instead of $0, 1, 2, \cdots$ as has been used formerly.) Moreover,

$$\int_{-\infty}^{\infty} d\rho^{(p)}(\lambda) = 1, \tag{A.38}$$

$$\int_{-\infty}^{\infty} P_i(\lambda) P_j(\lambda) d\rho^{(p)}(\lambda) = \delta_{ij} , \tag{A.39}$$

$$\int_{-\infty}^{\infty} \lambda P_i(\lambda) P_j(\lambda) d\rho^{(p)}(\lambda) = a_{mn}^{(p)}; \qquad m, n = 1, 2, \cdots p. \tag{A.40}$$

Theorem 10.28 of Stone [22] implies that $T[\tilde{A}_p(0)]$ is an approximating sequence of self-adjoint transformations for the self-adjoint transformation $\tilde{T}[A(0)]$ in the sense of his definition (9.9), namely

$$\lim_{p\to\infty} T[\tilde{A}_p(0)] = \tilde{A}(0) \tag{A.41}$$

and

$$\tilde{A}(0) \subseteq \text{closure of } A(0). \tag{A.42}$$

(Of course actually equality occurs in the last relation.) In addition

$$\lim_{p\to\infty} \rho^{(p)}(\lambda) = \rho(\lambda). \tag{A.43}$$

It is easy to see that

$$A(\theta_1)\, A(\theta_2) \neq A(\theta_2)\, A(\theta_1) \tag{A.44}$$

and by direct calculation it will be shown that $A(\theta)$ and $A(0)$ are unitary equivalent c-matrices in the sense of von-Neumann [20], cf., Smirnov [21].

If $\{w_i\}$ is the orthonormal set associated with $A(0)$ and if the definition

$$\zeta_p \triangleq \{e^{ip\theta} w_p\} \tag{A.45}$$

is made, the unitary matrix $V(\theta)$ is given simply by

$$v_{pq}(\theta) = \langle \zeta_q , w_p \rangle = e^{ip\theta} \delta_{pq} . \tag{A.46}$$

To show that $A(\theta)$ is unitary c-equivalent to $A(0)$ it is necessary to verify that

$$\sum_{s=1}^{\infty} \left| \sum_{t=1}^{\infty} a_{st} v_{tk} \right|^2 < \infty, \tag{A.47}$$

$$\sum_{t=1}^{\infty} \left| \sum_{s=1}^{\infty} \bar{v}_{sn} a_{st} \right|^2 < \infty, \tag{A.48}$$

$$\begin{aligned} a_{nk}(0) &= \sum_{t=1}^{\infty} v_{tk} \sum_{s=1}^{\infty} \bar{v}_{sn} a_{st} \\ &= \sum_{s=1}^{\infty} \bar{v}_{sn} \sum_{t=1}^{\infty} a_{st} v_{tk} . \end{aligned} \tag{A.49}$$

The calculations follow.

$$a_{mn} = e^{i\theta} \left(\frac{n}{2}\right)^{1/2} \delta_{m+1,n} + e^{-i\theta} \left(\frac{n+1}{2}\right)^{1/2} \delta_{m-1,n} , \tag{A.50}$$

$$\bar{a}_{mn} = e^{-i\theta} \left(\frac{n}{2}\right)^{1/2} \delta_{m+1,n} + e^{i\theta} \left(\frac{n+1}{2}\right)^{1/2} \delta_{m-1,n} . \tag{A.51}$$

Thus

$$\sum_{m=1}^{\infty} a_{mn}\bar{a}_{mn} = \sum_{m=1}^{\infty} | a_{mn} |^2$$

$$= \sum_{m=1}^{\infty} \Big\{ \frac{n}{2} \delta_{m+1,n}\delta_{m+1,n} + \frac{n+1}{2} \delta_{m-1,n}\delta_{m-1,n}$$

$$+ \frac{[n(n+1)]^{1/2}}{2} (e^{-2i\theta} \delta_{m-1,n}\delta_{m+1,n} + e^{2i\theta} \delta_{m+1,n}\delta_{m-1,n} \Big\}$$

$$= \frac{2n+1}{2}. \tag{A.52}$$

Equation (A.46) is now used and the following definition is made.

$$c_{sk} \triangleq \sum_{t=1}^{\infty} a_{st} v_{tk}$$

$$= \sum_{t=1}^{\infty} \left[e^{i\theta} \left(\frac{t}{2}\right)^{1/2} \delta_{s+1,t} + e^{-i\theta} \left(\frac{t+1}{2}\right)^{1/2} \delta_{s-1,t} \right] \delta_{tk}\, e^{ik\theta}$$

$$= e^{i(k+1)\theta} \left(\frac{s+1}{2}\right)^{1/2} \delta_{s+1,k} + e^{i(k-1)\theta} \left(\frac{s}{2}\right)^{1/2} \delta_{s-1,k} \tag{A.53}$$

and

$$d_{nt} \triangleq \sum_{s=1}^{\infty} \bar{v}_{sn} a_{st}$$

$$= e^{i(1-n)\theta} \left(\frac{t}{2}\right)^{1/2} \delta_{n+1,t} + e^{i(1+n)\theta} \left(\frac{t+1}{2}\right)^{1/2} \delta_{n-1,t}\,. \tag{A.54}$$

Therefore

$$\sum_{s=1}^{\infty} \left| \sum_{t=1}^{\infty} a_{st} v_{tk} \right|^2 = \sum_{s=1}^{\infty} | c_{sk} |^2$$

$$= \frac{2k+1}{2} \tag{A.55}$$

and

$$\sum_{t=1}^{\infty} \left| \sum_{s=1}^{\infty} \bar{v}_{sn} a_{st} \right|^2 = \sum_{t=1}^{\infty} | d_{nt} |^2$$

$$= \frac{2n+1}{2}\,. \tag{A.56}$$

Moreover,

$$\sum_{t=1}^{\infty} v_{tk} \sum_{s=1}^{\infty} \bar{v}_{sn} a_{st} = \sum_{t=1}^{\infty} v_{tk} d_{nt}$$

$$= \sum_{t=1}^{\infty} \delta_{tk}\, e^{ik\theta} \left[e^{i(1-n)\theta} \left(\frac{t}{2}\right)^{1/2} \delta_{n+1,t} \right.$$

$$\left. + e^{-i(1+n)\theta} \left(\frac{t+1}{2}\right)^{1/2} \delta_{n-1,t} \right]$$

$$= \left(\frac{k}{2}\right)^{1/2} \delta_{n+1,k}\, e^{i(k+1-n)\theta} + \left(\frac{k+1}{2}\right)^{1/2} \delta_{n-1,k}\, e^{i(k-1-n)\theta}$$

$$= \left(\frac{k}{2}\right)^{1/2} \delta_{n+1,k} + \left(\frac{k+1}{2}\right)^{1/2} \delta_{n-1,k}$$

$$= a_{mn}(0), \tag{A.57}$$

and similarly

$$\sum_{s=1}^{\infty} \bar{v}_{sn} \sum_{t=1}^{\infty} a_{st} v_{tk} = \sum_{s=1}^{\infty} \bar{v}_{sn} c_{sk}$$

$$= a_{nk}(0). \tag{A.58}$$

Thus the conditions of von-Neumann are satisfied and the matrices $V(\theta)$ are applicable. In particular then, the two systems $\{a_{nk}(0), w_p\}$, $\{a_{nk}(\theta), \zeta_q\}$ are unitary equivalent c-matrices under the unitary transformation $v_{pq} = (\zeta_q\,, w_p)$. A further theorem of von-Neumann now implies that the closed linear self-adjoint operator associated with the extensions of these operators must be *identical.* In particular, then, the closed linear extension of $A(\pi/2)$ must tend to the same linear extension of $A(0)$ whose properties were given above. Moreover, since $A_p(\pi/2)$, the truncated Jacobi matrix, is obviously unitary equivalent to $A_p(0)$ for every p, it follows that $A_p(\pi/2)$ must be an approximating sequence to the same operator for which $A_p(0)$ is known to be an approximating sequence.

The fact that $A(0)$ and $iB = A(\pi/2)$ have a common self-adjoint closed linear operator for their closed extension is intimately connected with the simple harmonic oscillator problem in quantum mechanics. The operator $A(0)$ is associated with multiplication by v, while $A(\pi/2)$ is obviously associated with the operator $i(\partial/\partial v)$. Not only are v and $i(\partial/\partial v)$ Fourier transforms of each other but, for the problem of the simple harmonic oscillator, they satisfy the same differential equation since Hermite expansions in velocity space were used.

Appendix B. Transformation to Characteristic Form for a General Orthogonal Polynomial Expansion

The evaluation of the matrices $(\alpha_{ij}^{\pm})$ given in Section 2 is carried out as follows.

Equation (4) is multiplied by $\alpha_{jk}^{\pm}$ and summed over k to obtain

$$\sum_{k=0}^{n-1} \left[\frac{\partial}{\partial t}(\alpha_{jk}^{\pm}M_k^{\pm}) + \frac{\partial}{\partial x}(\alpha_{jk}^{\pm}M_{k+1}^{\pm}) - ka\alpha_{jk}^{\pm}M_{k-1}^{\pm}\right] = \pm\, a\alpha_{j0}^{\pm}f(x, 0, t). \quad \text{(B.1)}$$

Equation (B.1) is in canonical form if the operands of the space and time derivatives are the same within a multiplicative constant, i.e., omitting the $\pm$ for the time being,

$$\sum_{k=0}^{n-1} \alpha_{jk}M_{k+1} = \lambda_j \sum_{k=0}^{k-1} \alpha_{jk}M_k . \quad \text{(B.2)}$$

M_n is interpreted from Eq. (15) giving

$$\sum_{k=1}^{n-1} \alpha_{j,k-1}M_k - \frac{\alpha_{j,n-1}}{C_{n,n}} \sum_{k=0}^{n-1} C_{n,k}M_k \equiv \lambda_j \sum_{k=0}^{n-1} \alpha_{jk}M_k . \quad \text{(B.3)}$$

Thus

$$\lambda_j\alpha_{jk} = -\frac{C_{n,k}}{C_{k,k}}\alpha_{j,n-1} + \alpha_{j,k-1}; \qquad k = 0, 1, 2 \cdots n-1 \quad \text{(B.4)}$$

provided

$$\alpha_{j,-1} \triangleq 0. \quad \text{(B.5)}$$

This recurrence relation, which is easily solved recursively, is satisfied by

$$\alpha_{j,k} = -\frac{\alpha_{j,n-1}}{C_{n,n}\lambda_j^{k+1}} \sum_{s=0}^{k} \lambda_j^s C_{n,s} . \quad \text{(B.6)}$$

For this equation to be compatible when $k = n - 1$, it is necessary that

$$\sum_{s=0}^{n} \lambda_j^s C_{n,s} = 0. \quad \text{(B.7)}$$

By definition of $C_{n,s}$, Eq. (11), this is stated equivalently

$$p_n(\lambda_j) = 0. \quad \text{(B.8)}$$

Thus the λ_j are identified as the zeroes of the nth degree polynomial. On renaming $\alpha_{j,n-1} = \Gamma_j$, the form Eq. (17) is obtained. The inverse matrix

(β_{ij}) can be obtained most simply by reversing the above argument. The result is given in Eq. (18).

It remains to evaluate the third term on the left of Eq. (B.1). From the definition of $\beta_{i,j}$, Eq. (16), it follows that

$$\sum_{k=0}^{n-1} \alpha_{ik}(-kM_{k-1}) \doteq \sum_{j,k=0}^{n-1} (-k\alpha_{ik}\beta_{k-1,j}m_j) \triangleq \sum_{j=0}^{n-1} G_{ij}m_j . \tag{B.9}$$

Attention will be confined to the coefficient of m_j:

$$G_{ij} = \frac{\Gamma_i}{\Gamma_j} \frac{1}{p_n'(\lambda_j)} \sum_{k=0}^{n-1} \sum_{l=0}^{k} C_{n,l}\lambda_i^{l-2}k \left(\frac{\lambda_j}{\lambda_i}\right)^{k-1}. \tag{B.10}$$

The following identity is used to evaluate Eq. (B.10) when $i \neq j$.

$$\sum_{k=l}^{n-1} kx^{k-1} \equiv \frac{d}{dx}\left[\sum_{k=l}^{n-1} x^k\right] \equiv \frac{d}{dx}\left[x^l\left(\frac{1-x^{n-l}}{1-x}\right)\right]$$

$$= \frac{lx^{l-1} - nx^{n-1} - (l-1)\,x^l + (n-1)\,x^n}{(1-x)^2}. \tag{B.11}$$

Thus

$$G_{ij} = \frac{\Gamma_i/\Gamma_j}{p_n'(\lambda_j)\,(\lambda_i-\lambda_j)^2} \sum_{l=0}^{n-1} C_{n,l}\lambda_i^l \left[l\left(\frac{\lambda_j}{\lambda_i}\right)^{l-1} - n\left(\frac{\lambda_j}{\lambda_i}\right)^{n-1} \right.$$

$$\left. - (l-1)\left(\frac{\lambda_j}{\lambda_i}\right)^l + (n-1)\left(\frac{\lambda_j}{\lambda_i}\right)^n\right]. \tag{B.12}$$

The following identities are now used.

$$p_n(\lambda_j) \equiv \sum_{l=0}^{n} C_{n,l}\lambda_j^l = 0, \tag{B.13}$$

$$p_n'(\lambda_j) \equiv \sum_{l=1}^{n} lC_{n,l}\lambda_j^{l-1} . \tag{B.14}$$

The former is true because λ_j is a zero of p_n. The four terms in Eq. (B.12) simplify radically after summation to $(\lambda_i - \lambda_j)\,p_n'(\lambda_j)$, and so finally

$$G_{ij} = \frac{\Gamma_i}{\Gamma_j} \cdot \frac{1}{\lambda_i - \lambda_j}; \qquad i \neq j. \tag{B.15}$$

When $i = j$, Eq. (B.10) becomes

$$G_{ii} = \frac{1}{p_n'(\lambda_i)} \sum_{k=0}^{n-1} \sum_{l=0}^{k} kC_{n,l}\lambda_i^{l-2}$$

$$= \frac{1}{p_n'(\lambda_i)} \sum_{l=0}^{n-1} C_{n,l}\lambda_i^{l-2} \frac{(n-l)(n+l-1)}{2}$$

$$= \frac{1}{2p_n'(\lambda_j)} \sum_{l=0}^{n-1} \left[\frac{n(n-1)\, C_{n,l}\lambda_i^{l}}{\lambda_i^2} - l(l-1)\, C_{n,l}\lambda_i^{l-2}\right]$$

$$= -\frac{p_n''(\lambda_i)}{2p_n'(\lambda_i)}, \tag{B.16}$$

where the series expansion for the second derivative has been used.

The right-hand side of Eq. (B.1), given explicitly in Eq. (20), is derived as follows from Eq. (12).

$$\alpha_{j0}^{\pm} f_n^{\operatorname{sgn}(-a)}(x, 0, t) = -\left[\frac{\Gamma_j C_{n,0}}{\lambda_j}\right]^{\pm} \left[\frac{C_{n-1,n-1}}{C_{n,n}} \sum_{k=0}^{n-1} (C_{n,k+1}C_{n-1,0} - C_{n-1,k+1}C_{n,0})M_k\right]^{\operatorname{sgn}(-a)}$$

$$= -\left[\frac{\Gamma_j C_{n,0}}{\lambda_j}\right]^{\pm} \left[\frac{C_{n-1,n-1}}{C_{n,n}} \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} (C_{n,k+1}C_{n-1,0} - C_{n-1,k+1}C_{n,0}) \frac{\lambda_l^k m_l}{\Gamma_l p_n'(\lambda_l)}\right]^{\operatorname{sgn}(-a)}. \tag{B.17}$$

Summation over k may be performed using Eq. (B.14) yielding

$$\alpha_{j0}^{\pm} f_n^{\operatorname{sgn}(-a)}(x, 0, t) = \left[\frac{\Gamma_j C_{n,0}}{\lambda_j}\right]^{\pm} \left[\frac{C_{n,0}C_{n-1,n-1}}{C_{n,n}} \sum_{l=0}^{n-1} \frac{p_{n-1}(\lambda_l)}{\Gamma_l \lambda_l p_n'(\lambda_l)}\, m_l\right]^{\operatorname{sgn}(-a)}. \tag{B.18}$$

The collected results Eqs. (B.2), (B.15), (B.16), and (B.18) give the general form of Eq. (20) of the main text.

Appendix C. The Finite-Difference Analysis of the Hyperbolic System Resulting from the Half-Range Expansions of the Velocity Distribution Function in Laguerre Polynomials

C.1. *The Difference Equations*

Although originally an adaptation of the method of Keller and Wendroff [15] was used to obtain a set of difference equations suitable for computer integration, a modification which has been described by Thomée [30] appears to be more suitable. Equations based on this approach will be presented.

The following definitions of the values of the dependent variables at grid points of the finite difference net.

$$m_l^{\pm}(x, t) = m_l^{\pm}(ih, jk) \triangleq m_l^{\pm}(i, j). \tag{C.1}$$

In the subsequent development it will be assumed that the equations are stepped forward in time (j becoming $j + 1$) meanwhile solved for all values of i. In order to integrate along the characteristic directions as closely as possible, the positive moments are integrated in the positive direction and the negative moments in the opposite direction. The equation is approximated at $(x + 1/2h, y + 1/2k)$ in terms of the moment values at (i, j), $(i + 1, j)$, $(i, j + 1)$, and $(i + 1, j + 1)$. An iterative method is used for solution. The following notation is used for the approximation to the value of any variable Q at the νth iteration.

$$\langle Q\rangle \triangleq \tfrac{1}{4}[Q(i,j) + Q(i \pm 1, j) + Q^{\nu}(i, j + 1) + Q^{\nu}(i \pm 1, j + 1)]. \tag{C.2}$$

With this notation and the definition

$$R^{\nu}(m_l^{\pm}) \triangleq \langle a\rangle \left\{\frac{\lambda_l - 1}{2\lambda_l}\langle m_l^{\pm}\rangle - \sum_{\substack{s=0\\ s\neq l}}^{n-1} \frac{\langle m_s^{\pm}\rangle}{\lambda_l - \lambda_s}\right\}$$
$$- \mid \langle a\rangle \mid \sum_{j=0}^{n-1} \langle m_j^{\operatorname{sgn}[-\langle a\rangle]}\rangle, \tag{C.3}$$

the difference equations are

$$m_l^{(\nu+1)\pm}(i \pm 1, j + 1) = m_l^{\pm}(i, j) + \left(\frac{h - \lambda_l k}{h + \lambda_l k}\right) \cdot$$
$$[m_l^{\pm}(i \pm 1, j) - m_l^{(\nu+1)\pm}(i, j + 1)] + \left(\frac{2hk}{h + \lambda_l k}\right) R^{\nu}(m_l^{\pm}). \tag{C.4}$$

It should be noted that these equations are nonlinear since $a(i, j)$ is calculated from the moments. Their stability and convergence to the differential equations for sufficiently small h and bounded h/k has been shown by Thomée [30].

C. 2. *Boundary Conditions*

A typical problem will have boundary conditions for positive velocities (f^+) specified, say, on the left-hand boundary, and for negative velocities (f^-) on the right-hand boundary. Suppose these boundaries are normalized to $x = 0$, $x = 1$ respectively. Then for example

$$f^+(x, v, t) = f_0(v, t) \quad \text{on} \quad x = 0, \tag{C.5}$$

$$f^-(x, v, t) = f_1(v, t) \quad \text{on} \quad x = 1. \tag{C.6}$$

In addition, the initial distribution must be specified:

$$f^+(x, v, t) = h^+(x, v), \; t = 0, \tag{C.7}$$

$$f^-(x, v, t) = h^-(x, v), \; t = 0. \tag{C.8}$$

Because f^+ and f^- are finite series, the boundary conditions can be satisfied only approximately, thus if $f_0(v, t)$ is to be approximated it can be required that the velocity moments of order 0, 1, 2, ... $n - 1$ of f_0 and its approximating function agree. In addition, because of the critical role played by $f(x, 0, t)$, it is reasonable to require that the agreement is exact for $v = 0$. This additional condition can be imposed by making a scale change in v. The expansion is carried out in terms of v/μ where μ is a constant, or, what amounts to the same thing, $f_0(\mu v, t)$ is expanded in terms of v. It is therefore required, for instance, that

$$f_0(\mu v, t) \sim w^+(v) \sum_{k=0}^{n-1} b_k{}^+(0, t) p_k{}^+(v). \tag{C.9}$$

The agreement at $v = 0$ yields

$$f_0(0, t) = w^+(0) \sum_{k=0}^{n-1} b_k{}^+(0, t) p_n{}^+(0). \tag{C.10}$$

If the velocity moments of order 0, 1, 2 ... $n - 1$ agree, then so do moments of f_0 with p_0, p_1, ... p_{n-1}, and consequently, on using the orthogonal properties of the polynomials

$$b_k{}^+(0, t) = \int_0^\infty f_0(\mu v, t) p_k(v) \, dv. \tag{C.11}$$

For this to be possible, it is sufficient that $f_0(v, t)$ be a separable function of v and t. When Eq. C.11 is substituted into Eq. C.10, a polynomial equation of degree n in μ is obtained—the value of μ giving the "best" representation may be used. The actual choice remains somewhat arbitrary. The other boundary conditions can be applied similarly.

It can be seen that a considerable arbitrariness is present in the choice of boundary conditions. The ones chosen may depend on the particular problem.

Appendix D. Transformation of the Distribution Function Coefficients to Characteristic Form

An alternative approach to the use of the moment equations is a direct calculation of the coefficients $b_k^{\pm}(x, t)$ which appear in the definition of the nth order approximating function $f_n^{\pm}$ (Eq. (7)). These satisfy Eq. (27) and the corresponding functions $b_{ijk}(x_1, x_2, x_3, t)$ satisfy Eq. (46) in the three-dimensional case. In this case also it is necessary to put the partial differential equations in characteristic form. Thus the transformation T is sought such that

$$W_i = \sum_{j=0}^{n-1} T_{ij} b_j, \tag{D.1}$$

where T diagonalizes the Jacobi matrix Z whose elements are (cf. Eqs. (25) and (27))

$$\begin{aligned} Z_{k,k-1} &= A_{k-1}, && k = 1, 2, \cdots n-1, \\ Z_{k,k} &= B_k, && k = 0, 1, \cdots n-1, \\ Z_{k,k+1} &= C_{k+1}, && k = 0, 1, \cdots n-2, \\ Z_{ij} &= 0, && \text{otherwise}, \end{aligned} \tag{D.2}$$

in the sense that TZT^{-1} is a diagonal matrix. In matrix notation, Eq. (27) can be written

$$\frac{\partial \mathbf{b}^{\pm}}{\partial t} \pm \left(Z \frac{\partial \mathbf{b}^{\pm}}{\partial x} + aY\mathbf{b}^{\pm} \right) = \pm\, a[\mathbf{Ip}(0) \cdot \mathbf{b}]^{\operatorname{sgn}(-a)}, \tag{D.3}$$

where $\mathbf{b}^{\pm}$ is a column vector $(b_0^{\pm}, b_1^{\pm}, \cdots b_{n-1}^{\pm})$, $\mathbf{I}$ is the n dimensional column vector $(1, 1, \cdots 1)$, and $\mathbf{p}(0)$ is the vector $(p_0(0), p_1(0), \cdots)$. The matrix Y has elements

$$\begin{aligned} Y_{ij} &= 0, && j \geqslant i, \\ Y_{ij} &= -D_j^i, && j < i. \end{aligned} \tag{D.4}$$

Under the transformation Eq. (D.1) and Eq. (D.3) becomes

$$\frac{\partial \mathbf{W}^{\pm}}{\partial t} \pm \left(\hat{Z}\frac{\partial \mathbf{W}^{\pm}}{\partial x} + a\hat{Y}\mathbf{W}^{\pm}\right) = \pm\, a(\hat{X}\mathbf{W})^{\operatorname{sgn}(-a)}, \tag{D.5}$$

where

$$\hat{X} = T\mathbf{Ip}(0)\, T^{-1}, \tag{D.6}$$

$$\hat{Y} = TYT^{-1}, \tag{D.7}$$

$$\hat{Z} = TZT^{-1}. \tag{D.8}$$

By definition, $\hat{Z}$ is diagonal with diagonal elements λ_n say, therefore Eq. (D.8) which is equivalent to

$$\hat{Z}T = TZ \tag{D.9}$$

can be written in component form using Eq. (D.2)

$$\lambda_k T_{k,j} = T_{k,j+1}A_j + T_{k,j}B_j + T_{k,j-1}C_j\,, \qquad j = 0, 1, 2 \cdots n-2 \tag{D.10}$$

$$\lambda_k T_{k,n-1} = T_{k,n-1}B_{n-1} + T_{k,n-2}C_{n-1}\,. \tag{D.11}$$

It follows immediately from Eq. (25) that Eq. (D.10) is satisfied by

$$T_{kj} = Q_k p_j(\lambda_k) \tag{D.12}$$

where Q_k is independent of j. In addition, Eq. (D.11) is satisfied by Eq. (D.12) if $T_k = 0$, i.e., if

$$p_n(\lambda_k) = 0. \tag{D.13}$$

Thus the λ_k are the zeros of the nth degree polynomial. By choosing Q_k suitably, T becomes an orthogonal transformation. To see this it is simplest to evaluate

$$\sum_{j=0}^{n-1} T_{kj}T_{ij} = \sum_{j=0}^{n-1} Q_k Q_i p_j(\lambda_k)\, p_j(\lambda_i). \tag{D.14}$$

The Christoffel-Darboux formulas (Szegö [28]) are satisfied by orthogonal polynomials. These are:

$$\sum_{k=0}^{n-1} p_k(x)\, p_k(y) = \frac{C_{n-1,n-1}}{C_{n,n}} \frac{p_n(x)\, p_{n-1}(y) - p_{n-1}(x)\, p_n(y)}{x-y}, \tag{D.15}$$

$$\sum_{k=0}^{n-1} [p_k(x)]^2 = \frac{C_{n-1,n-1}}{C_{n,n}} [p_n'(x)\, p_{n-1}(x) - p_{n-1}'(x)\, p_n(x)]. \tag{D.16}$$

If Eq. (D.15) is used in Eq. (D.14) when $i \neq k$, it follows from Eq. (D.13) that

$$\sum_{j=0}^{n-1} T_{kj} T_{ij} = 0, \qquad i \neq k. \tag{D.17}$$

On the other hand, when $i = k$, Eq. (D.16) and Eq. (D.13) used in Eq. (D.14) show that

$$\sum_{j=0}^{n-1} T_{ij} T_{ij} = \frac{C_{n-1,n-1}}{C_{n,n}} Q_i^2 p_n'(\lambda_i)\, p_{n-1}(\lambda_i). \tag{D.18}$$

This is equal to unity, and thus the matrix T, Eq. (D.12), is orthogonal provided

$$Q_i = \sqrt{\frac{C_{n,n}}{C_{n-1,n-1}} \frac{1}{p_n'(\lambda_i)\, p_{n-1}(\lambda_i)}}. \tag{D.19}$$

The evaluation of $\hat{X}$ and $\hat{Y}$ cannot be carried very far in general, so at this stage the discussion will be confined to the Laguerre polynomials. The Eq. (52) to (55) can be used to evaluate T, the elements of which are

$$T_{kj} = \frac{L_j(\lambda_k)}{\sqrt{\lambda_k}\, L_n'(\lambda_k)}. \tag{D.20}$$

Thus

$$\begin{aligned}
\hat{Y}_{ij} &= \sum_{k=0}^{n-1} \frac{L_k(\lambda_i)}{\sqrt{\lambda_i}\, L_n'(\lambda_i)} \sum_{l=0}^{k-1} \frac{L_l(\lambda_j)}{\sqrt{\lambda_j}\, L_n'(\lambda_j)} \\
&= \frac{1}{\sqrt{\lambda_i \lambda_j}\, L_n'(\lambda_i)\, L_n'(\lambda_j)} \sum_{k=0}^{n-1} \sum_{l=0}^{k-1} L_k(\lambda_i)\, L_l(\lambda_j) \\
&= \frac{1}{\sqrt{\lambda_i \lambda_j}\, L_n'(\lambda_i)\, L_n'(\lambda_j)} \sum_{k=0}^{n-1} L_k(\lambda_i) \cdot \sum_{l=0}^{k-1} L_l(\lambda_j) \\
&= \frac{1}{\sqrt{\lambda_i \lambda_j}\, L_n'(\lambda_i)\, L_n'(\lambda_j)} \sum_{k=0}^{n-1} - L_k(\lambda_i)\, L_k'(\lambda_j).
\end{aligned} \tag{D.21}$$

In the last line, the identity

$$L_n'(v) = - \sum_{k=0}^{n-1} L_k(v) \tag{D.22}$$

has been used, in addition, it is easily proved by differentiating the Christoffel-Darboux formula that

$$\sum_{k=0}^{n-1} L_k(\lambda_i) L_k'(\lambda_j) = -\left(\frac{\lambda_i}{\lambda_i - \lambda_j}\right) L_n'(\lambda_i) L_n'(\lambda_j), \qquad i \neq j \tag{D.23}$$

and that

$$\sum_{k=0}^{n-1} L_k(\lambda_i) L_k'(\lambda_i) = \tfrac{1}{2} (\lambda_i - 1) [L_n'(\lambda_i)]^2. \tag{D.24}$$

Thus when $i \neq j$,

$$\hat{Y}_{ij} = \left(\frac{\lambda_i}{\lambda_j}\right)^{1/2} \frac{1}{\lambda_i - \lambda_j} \tag{D.25}$$

and when $i = j$

$$\hat{Y}_{ij} = \tfrac{1}{2}\left(\frac{1}{\lambda_i} - 1\right). \tag{D.26}$$

Finally

$$\hat{X}_{ij} = \frac{1}{(\lambda_i \lambda_j)^{1/2}}, \tag{D.27}$$

where again Eq. (D.22) has been used.

Appendix E. Closed-Form Solution for the Constant Retarding Field Diode

E.1. *Separation into an Initial Value and a Boundary Value Problems*

A closed-form solution can be obtained for a diode in which the particles experience a constant retarding field and in which there is no interaction. A heuristic derivation of the solution is given which is then verified to be a weak solution. The problem may be stated as follows. The solution of the equation

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + a \frac{\partial f}{\partial v} = 0 \tag{E.1}$$

is required subject to the boundary conditions.

$$\text{At } t = 0, \quad \begin{aligned} f &= e^{-v^2}, & v > 0 \\ f &= 0 \;\;, & v < 0 \end{aligned} \Big\} \; 0 \leqslant x \leqslant 1. \tag{E.2}$$

$$\begin{aligned} \text{At } x = 0, \quad f &= e^{-v^2}, & v > 0 \\ \text{At } x = 1, \quad f &= 0 \;\;, & v < 0 \end{aligned} \Big\} \; t \geqslant 0. \tag{E.3}$$

The acceleration is constant and retarding. Therefore let

$$a = -g, \qquad g > 0.$$

Because the acceleration is constant and the particles do not interact, those which were present initially (described by Eq. (E.2)) can be treated independently from those introduced at later times (described by Eq. (E.3)).

The motion will be solved in Lagrangian coordinates. To this end Eq. (E.1) will be replaced by the equivalent pair of ordinary differential equations:

$$\frac{dx}{dt} = v, \qquad \frac{dv}{dt} = a = -g. \tag{E.4}$$

E.2. *Particles Already Present at $t = 0$*

Consider the motion of those particles present at $t = 0$ and inquire how particles at x with velocity v at time t arrived there, and from where. Let x_0, v_0 be the velocity and position at $t = 0$, then from Eq. E.4

$$x = x_0 + v_0 t - \tfrac{1}{2} g t^2, \qquad v = v_0 - gt. \tag{E.5}$$

Thus the particles with velocity v at t, at the initial instant, must have had

$$v_0 = v + gt. \tag{E.6}$$

Since from Eq. (E.2), $v_0 \geqslant 0$, it follows that it is necessary that

$$v + gt \geqslant 0. \tag{E.7}$$

Also it is necessary that $0 \leqslant x_0 \leqslant 1$, i.e.,

$$0 \leqslant x - vt - \tfrac{1}{2} g t^2 \leqslant 1. \tag{E.8}$$

It is further required that particles with negative velocities at time t must have turned round before reaching $x = 1$, otherwise they would have been collected. The maximum value of x is obtained from Eq. (E.5) and is

$$x_{\max} = x_0 + \frac{{v_0}^2}{2g}. \tag{E.9}$$

The condition that this is less than unity can be expressed (again using Eq. (E.5)) in the form

$$x + \frac{v^2}{2g} < 1, \qquad \text{if} \qquad v < 0, \tag{E.10}$$

or equivalently

$$v + \sqrt{2g(1 - x)} > 0. \tag{E.11}$$

The density of particles with velocity v_0 at $t = 0$ was $\exp(-v_0^2)$, therefore from Eq. (E.6) and the conservation of the number of particles, at time t these particles have density

$$f = e^{-(v+gt)^2}. \tag{E.12}$$

When the restrictions Eqs. (E.7), (E.8), and (E.11) are taken into account it follows that the particles present at $t = 0$ have subsequently a density given by

$$f_a = e^{-(v+gt)^2} H[v + gt] H[x - vt - \tfrac{1}{2}gt^2] \\ H[1 - x + vt + \tfrac{1}{2}gt^2] H[v + \sqrt{2g(1 - x)}], \tag{E.13}$$

where $H[\ ]$ is the Heaviside step function. It is straightforward to show that the third Heaviside function is always unity when the fourth is nonzero, which allows the simplification

$$f_a = e^{-(v+gt)^2} H[v + gt] H[x - vt - \tfrac{1}{2}gt^2] H[v + \sqrt{2g(1 - x)}]. \tag{E.14}$$

E.3. *Particles Injected Subsequently to $t = 0$*

Let t_0 be the time of injection of particles with velocity v_0 at $x = 0$, and let their position and velocity at t be x, v. Then on integrating the equations of motion the position and velocities may be expressed as

$$x = v_0(t - t_0) - \tfrac{1}{2}g(t - t_0)^2, \qquad v = v_0 - g(t - t_0). \tag{E.15}$$

Therefore

$$v_0 = v + g(t - t_0) \tag{E.16}$$

and again it is required that (cf. Eq. (E.7))

$$v + g(t - t_0) > 0. \tag{E.17}$$

Equation (E.15) can be rearranged as follows:

$$v_0^2 = v^2 + 2gx, \tag{E.18}$$

$$t - t_0 = \frac{\sqrt{v^2 + 2gx} - v}{g}. \tag{E.19}$$

The positive root is taken since $t - t_0 > 0$ for particles to be present. It then follows that Eq. (E.17) is automatically satisfied. Since by definition $t_0 \geqslant 0$, Eq. (E.19) implies the condition

$$v + gt - \sqrt{v^2 + 2gx} \geqslant 0. \tag{E.20}$$

As before, if v is negative, the maximum excursion of the particle before arriving at its current position must be less than unity. Therefore, from Eq. (E.15)

$$x_{\max} = \frac{v_0^2}{2g} < 1 \tag{E.21}$$

and by making further use of Eq. (E.15) this can be put equivalently as

$$v + \sqrt{2g(1 - x)} > 0. \tag{E.22}$$

The particle density $e^{-v_0^2}$ at $x = 0$ becomes $\exp[-(v^2 + 2gx)]$ at a general position (see Eq. (E.18)). When the restrictions (Eqs. (E.20) and (E.22)) are included, the part of the distribution function arising from the particles injected subsequently to $t = 0$ becomes

$$f_b = e^{-(v^2+2gx)} H[v + gt - \sqrt{v^2 + 2gx}]\, H[v + \sqrt{2g(1 - x)}]. \tag{E.23}$$

Thus the complete solution, valid for $0 \leqslant x \leqslant 1$, all v, and $t \geqslant 0$ is

$$\begin{aligned} f = {} & e^{-(v+gt)^2} H[v + gt]\, H[x - vt - \tfrac{1}{2}gt^2]\, H[v + \sqrt{2g(1 - x)}] \\ & + e^{-(v^2+2g)} H[v + gt - \sqrt{v^2 + 2gx}]\, H[v + \sqrt{2g(1 - x)}]. \end{aligned} \tag{E.24}$$

E.4. *Verification of the Weak Solution*

That Eq. (E.24) is a solution of the problem may be verified by substitution. The boundary conditions, Eqs. (E.2) and (E.3), are seen by inspection to be satisfied. In addition, the characteristics of Eq. (E.1) are

$$C_1 = v + gt \tag{E.25}$$

and

$$C_2 = v^2 + 2gx, \tag{E.26}$$

thus Eq. (E.24) can be expressed as

$$f = H[v + \sqrt{2g(1 - x)}]\, F(C_1, C_2). \tag{E.27}$$

This will therefore be a weak solution of the problem if $H[v + \sqrt{2g(1-x)}]$ satisfies Eq. (E.1) in the sense of the theory of distributions. Since

$$\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial x} - g\frac{\partial}{\partial v}\right) H[v + \sqrt{2g(1-x)}]$$

$$= -\frac{g[v + \sqrt{2g(1-x)}]\,\delta[v + \sqrt{2g(1-x)}]}{\sqrt{2g(1-x)}} \tag{E.28}$$

and

$$x\delta[x] = 0 \tag{E.29}$$

in the sense of the theory of distributions, the verification is completed.

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