Ion-transport theory for a slightly ionized rarefied gas in a strong electric field

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A moment solution to the Boltzmann equation is considered for the initial-value problem of a weakly ionized rarefied gas, or gas mixture, in a uniform electric field. No restrictions are placed on the smoothness of the initial data or the mass ratio between the ions and the neutrals although the theory converges fastest for heavy ions in a light gas. A principal result of this theory is the prediction of shock-wave phenomena in pulsed drift tubes. The result is most persistent for heavy ions in a light gas. For instance U^+ ions in He can be significantly affected by sharp initial conditions for 10^4 collisions. Comparison is made with the results of asymptotic theories to smooth initial data.

I. INTRODUCTION

The diffusion equation is frequently used to describe the motion of a weakly ionized gas under the influence of a uniform electric field.¹⁻⁴⁹ Such a theory may be viewed as an asymptotic solution to the Boltzmann equation in the limits of smooth initial data and high gas density^{50,51} (but still in the binary-collision region). Corrections to the diffusion equation (still for smooth initial data) in an asymptotic series in inverse powers of the neutral-gas density are standard in the kinetic theory of neutral gases 50-53 and more recently in the case of sparse electrons 54-56 and ions 57-60 in a relatively dense neutral gas under an applied uniform electric field. Convergent theories of the Boltzmann equation exist^{51,61-68} but such theories have apparently not been applied to the case of a weakly ionized gas in a strong uniform electric field. There are some miscellaneous theories concerning deviations from the diffusion equation for ionized gases⁶⁹⁻⁷¹ but they are suspect since they do not reduce to the asymptotic theory. There also exist some numerical studies.⁷²⁻⁷⁴ The ion density is assumed so low that both ion-ion collisions and the effect that the ions have on the gas can be neglected. Equilibrium conditions are assumed for the neutral gas and collisions are assumed elastic.

The subject herein is basic in the sense that some penetration can easily be made in a doubly nonlinear transport theory. That is, fluxes due to both electric fields and density inhomogeneities are not strictly proportional to gradients. The simplicity lies in the fact that the theory is mathematically linear to all orders since we take the neutral gas to be totally unaffected by the chargedparticle motion.

II. GENERAL FORMULATION

The method employed is simply a different truncation of an extension⁵⁸ of a theory due to Kihara.^{75,76} Under the assumptions mentioned, a linear Boltzmann equation suffices to describe the motion of the ions.⁷⁵⁻⁷⁷ Taking moments of the Boltzmann equation as in Ref. 75, and extending them to mixtures of neutral gases,⁵⁸ one obtains

$$\frac{\partial}{\partial t} \langle n\psi \rangle + \vec{\nabla} \cdot \langle n\vec{\nabla}\psi \rangle - (q\vec{\mathbf{E}}/m) \cdot \langle n\nabla_{v}\psi \rangle + nN \sum_{j} X_{j} \langle J_{j}\psi \rangle = 0, \qquad (1)$$

where q, m, v, n are the ion charge, mass, velocity, and density, respectively; ψ is an arbitrary function of velocity, N is the neutral-gas density, and X_j is the fraction of neutral-gas species j in the total mixture; E is the applied electric field. The angular brackets stand for averages over the ionvelocity distribution function; J_j is a collision operator which for elastic collisions is defined as

$$NX_{j}J_{j}\psi \equiv \int d\Omega_{j}d\vec{\nabla}_{j}F_{j}[\psi(\vec{\nabla}) - \psi(\vec{\nabla}')]g_{j}\sigma_{j}, \quad (2)$$

where F_j is the equilibrium distribution function for neutral-gas species j, V_j is the *j*th-species neutral-gas velocity, $g_j \equiv |\vec{\nabla} - \vec{\nabla}_j|$, σ_j is the differential scattering cross section between the ions and the neutral-gas species j, and $\vec{\nabla}'$ is the ion velocity just after a collision. If

$$\psi(\vec{\mathbf{v}}) = \psi_{lm}^{(r)}(\vec{\mathbf{v}}) = |c|^{l} S_{l+1/2}^{(r)}(c^{2}) P_{l}^{|m|}(c_{z}/c) e^{im\phi}, \quad (3)$$

where $\vec{c} \equiv (m/2kT)^{1/2} \vec{v}$, k is Boltzmann's constant, T is the neutral-gas temperature, S are Sonine polynomials, P are Legendre polynomials, and ϕ is the azimuthal angle of the ion-velocity vector about the field direction, then for the Maxwell model of constant mean free time, these functions are eigenfunctions for the collision operator^{76,78} so that

$$J_{j} \psi_{lm}^{(r)} = \lambda_{lmj}^{(r)} \psi_{lm}^{(r)} \,. \tag{4}$$

The Maxwell model corresponds to an ion neutral potential varying as r^{-4} . For other potentials the

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collision operator may be expanded in a series 62,76 which, extended to neutral-gas mixtures, 58 reads

$$J_{j}\psi_{lm}^{(r)} = \sum_{s=0}^{\infty} \left[a_{rs}(lm) \right]_{j}\psi_{lm}^{(s)},$$
(5)

where the expansion coefficients are

$$[a_{rs}(lm)]_{j} = \frac{(2l+1)s!(l-|m|)!}{2\pi\xi^{3/2}(l+r+\frac{3}{2})(l+|m|)!} \times \int e^{-(v/\xi)^{2}}\psi_{lm}^{(s)}J_{j}\psi_{lm}^{(r)}d\vec{v}.$$
 (6)

The evaluation of $[a_{rs}(lm)]_j$ from the cross sections or potentials is indicated elsewhere.^{58,76,79–81} The following notation will be defined for convenience:

$$b_{rs}(lm) \equiv \sum_{j} X_{j}[a_{rs}(lm)]_{j},$$

$$\xi_{rlm} \equiv \frac{b_{00}(10)}{b_{rr}(lm)} \equiv \frac{1}{\mu_{rlm}}, \quad \eta_{rslm} \equiv \frac{b_{rs}(lm)}{b_{00}(10)}.$$
 (7)

Values of ξ and η are given in the Appendix for a few low-order values of the indices.

The thermal speed of the ions is defined as

$$\zeta = (2kT/m)^{1/2} \,. \tag{8}$$

A collision frequency ν is defined as

$$\nu \equiv Nb_{00}(10), \tag{9}$$

which is equal to a momentum-transfer collision frequency in the zero-field limit. For the Maxwell

model⁷⁶

$$\nu = qE/mv_d, \tag{10}$$

for all values of the field.

A dimensionless field is defined as

$$\hat{\boldsymbol{\mathcal{S}}} = q \, \vec{\mathbf{E}} / m \, \zeta \, \boldsymbol{\nu} \, . \tag{11}$$

For $m \approx M$ (*M* is the mass of the neutral gas) at about room temperature the ion energy gained by the field is about equal to the thermal energy when $\mathcal{S} \sim 1$.

Dimensionless coordinates are introduced,

$$\tau \equiv \nu t, \quad \rho \equiv \nu z / \zeta \mathcal{E} \,, \tag{12}$$

so that $\tau \sim 1$ for times on the order of a mean free time between collisions and $\rho \sim 1$ for distances corresponding to how far an ion drifts on the average in one mean free time. Derivatives of high order with respect to the dimensionless coordinates are expected to be relatively unimportant for long times *t*, or large distances *z*, compared with derivatives of low order.

Restricting ourselves to one spatial dimension, Eq. (1) reads

$$\frac{\partial}{\partial \tau} \langle n\psi_{lm}^{(r)} \rangle + \mu_{rlm} \langle n\psi_{lm}^{(r)} \rangle - \vec{\mathcal{E}} \cdot \langle n\vec{\nabla}_{c}\psi_{lm}^{(r)} \rangle + \sum_{s \neq r} \eta_{rslm} \langle n\psi_{lm}^{(s)} \rangle + \frac{1}{\mathcal{E}} \frac{\partial}{\partial \rho} \langle c_{s}n\psi_{lm}^{(r)} \rangle = 0.$$
(13)

Making use of some of the properties of Burnett functions,^{58,76} Eq. (13) becomes

$$\frac{\partial \phi_{l}^{r}}{\partial \tau} + \mu_{rl} \phi_{l}^{r} - \mathcal{S} \left(\frac{l(2l+2r+1)}{2l+1} \phi_{l-1}^{r} - \frac{2l+2}{2l+1} \phi_{l+1}^{r-1} \right) + \sum_{s \neq r} \eta_{rsl} \phi_{l}^{s} + \frac{1}{\mathcal{S}} \frac{\partial}{\partial \rho} \left(\frac{l+1}{2l+1} \phi_{l+1}^{r} - \frac{l+1}{2l+1} \phi_{l+1}^{r-1} - \frac{l(r+1)}{2l+1} \phi_{l-1}^{r+1} + \frac{l(2r+2l+1)}{2(2l+1)} \phi_{l-1}^{r} \right) = 0 \quad (14)$$

where $\phi_l^r \equiv \langle n\psi_l^{(r)} \rangle$ and the index *m*, which can be taken to be zero for the one-dimensional problem, is deleted.

Equation (14) is the basic equation considered. The essential assumption implicit in it is that the collisions are elastic. There is no assumption about smooth initial data so that a judicious truncation could yield a convergent theory in which sharp initial conditions and boundaries can be dealt with. The previous theories for ions^{57, 58} treat the last two terms in Eq. (14) to a lower order than the remaining terms which has as a result:

$$\zeta^{2r+l}\langle n\psi_{lm}^{(r)}\rangle = \sum_{i=0}^{\infty} \omega_{lm}^{ri} \nabla^{i} n, \qquad (15)$$

which is an asymptotic series.^{52,53} Here ω_i is a tensor of rank *i* whose components are called

asymptotic transport coefficients. Previous theories for electrons^{55, 56} assume that the electron distribution function can be expanded in a spherical-harmonic expansion which is truncated at the second term. In addition, the time variation of the second term in the spherical-harmonic expansion is neglected. These assumptions in effect assume that the initial data are smooth which puts into suspicion results claiming to account for large density gradients. All these asymptotic theories make worse a fault already exhibited by the diffusion equation, namely, for the sharpest possible initial distribution

$$f(t=0,\,\mathbf{\ddot{r}},\,\mathbf{\ddot{v}}) \propto \,\delta(\,\mathbf{\ddot{r}})\,\delta(\,\mathbf{\ddot{v}})\,,\tag{16}$$

the diffusion equation predicts that

$$\frac{\partial}{\partial t}f(t=0^+) > 0 \tag{17}$$

everywhere, which of course is not correct. Corrections to this result using the asymptotic theories, if anything, make the result worse⁵⁷⁻⁶⁰ which is not unexpected since these theories are not up to dealing with (16). In Sec. VI we will see result (17) modified.

III. TRUNCATION

There are two separate things to be truncated in Eq. (14), both of them having to do with high-order averages appearing on the right-hand side $(\phi_{l}^{s}, \phi_{l+1}^{r}, \phi_{l-1}^{r+1})$. The first term ϕ_{l}^{s} deals with departures from the Maxwell model of constant mean free time. For the Maxwell model, $\eta = 0$, and for heavy ions in a light gas, $\eta \propto M/m$, ^{76,79-81} and the collision operator is diagonal. Cases for which η is not negligible can be considered by simply putting the resulting transport coefficients in terms of the ω 's appearing in Eq. (15), obtainable from the asymptotic theory,⁵⁸ which should work so long as the phenomena to be studied do not depend on the details of the spectra of the collision operator. As an alternative, terms in η can be treated to a lower-order approximation and asymptotic deviations to the diagonal J will result.⁵⁸ As another alternative a two-temperature Kihara-like theory⁸² can be employed which results in moment equations of similar form as Eq. (13), but which promise convergence instead of asymptopia for other than Maxwell-model ion-neutral interactions at high fields.

The system of moment equations (14) is truncated at the number of equations desired. The averages $\phi_{l+1}^{r}, \phi_{l-1}^{r+1}$ in the highest retained equation are approximated in order to decouple the retained equations from the deleted ones. A reasonable way to decouple these moments is by letting

$$\frac{\partial}{\partial \rho}\phi \approx \frac{\phi}{n}\frac{\partial n}{\partial \rho},\tag{18}$$

where the ϕ on the right-hand side of Eq. (18) is evaluated from Eq. (13) or (14) neglecting derivative terms. Since Eq. (18) is only used for some of the terms in only the highest-order equation considered, I will conjecture that the approximation scheme is convergent.

IV. EQUATIONS FOR THE ION DENSITY

The first approximation starts with the lowest possible moment, $\langle v^0 \rangle$. Higher-order approximations include accurately the higher moments in the preceding approximation. The first few approximations are considered for the diagonal collision operator ($\eta = 0$). The complete first ten approximations may be obtained from the determinant in

Table I which shows the dispersion relations of the first ten moment equations resulting from application of Eq. (14). This also visually indicates the approximate scheme which consists of considering for the *j*th approximation only a $j \times j$ square matrix starting at the upper left-hand corner as indicated, and approximating the nonzero elements lying to the right of the square matrix as indicated by Eq. (18).

The first approximation yields the well-known Euler result

$$\frac{\partial n}{\partial \tau} + \frac{1}{\mathcal{S}} \frac{\partial \phi_1^0}{\partial \rho} = 0, \qquad (19)$$

where we approximate

$$\frac{1}{\mathcal{S}}\frac{\partial\phi_1^0}{\partial\rho}\approx\frac{\partial n}{\partial\rho},\tag{20}$$

which yields

$$\frac{\partial n}{\partial \tau} + \frac{\partial n}{\partial \rho} = 0, \qquad (21)$$

which simply propagates the initial condition, unchanged in shape, with the drift velocity.

The second approximation (Navier-Stokes) is the simultaneous solution of Eq. (19) and

$$\frac{\partial \phi_1^0}{\partial \tau} + \phi_1^0 - \mathcal{E}n + \frac{1}{2\mathcal{E}} \frac{\partial n}{\partial \rho} - \frac{1}{3\mathcal{E}} \frac{\partial \phi_0^0}{\partial \rho} + \frac{2}{3\mathcal{E}} \frac{\partial \phi_2^0}{\partial \rho} = 0, \quad (22)$$

where we approximate [using Eq. (14) neglecting derivative terms]

$$\frac{1}{3\mathcal{S}}\left(\frac{\partial}{\partial\rho}\left(2\phi_{2}^{0}-\phi_{0}^{1}\right)\right)\approx\mathcal{S}\left(\alpha-\frac{1}{2\mathcal{S}^{2}}\right)\frac{\partial n}{\partial\rho},\qquad(23)$$

where

$$\alpha \equiv \frac{2}{3}\xi_{10} + \frac{4}{3}\xi_{02} + 1/2\mathcal{E}^2 \,. \tag{24}$$

In order for a nontrivial solution of Eqs. (19), (22), and (23) to exist,

$$\frac{\partial n}{\partial \tau} + \frac{\partial n}{\partial \rho} + \frac{\partial^2 n}{\partial \tau^2} - \alpha \frac{\partial^2 n}{\partial \rho^2} = 0, \qquad (25)$$

or the same equation for ϕ_1° . We will consider this equation further in Sec. VI.

The third approximation (incomplete Burnett) is the simultaneous solution of Eqs. (19), (22), and

$$\frac{\partial \phi_0^1}{\partial \tau} + \mu_{10} \phi_0^1 + 2\mathcal{E} \phi_1^0 - \frac{1}{\mathcal{E}} \frac{\partial \phi_1^0}{\partial \rho} + \frac{1}{\mathcal{E}} \frac{\partial \phi_1^1}{\partial \rho} = 0, \qquad (26)$$

where we approximate

$$\frac{1}{g} \frac{\partial \phi_1^1}{\partial \rho} \approx -\frac{2}{3} \xi_{11} (5\xi_{10} + 4\xi_{02}) \mathcal{S}^2 \frac{\partial n}{\partial \rho} .$$
(27)

In order for a nontrivial solution of Eqs. (19), (22), (26), and (27) to exist,

3	0	0
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			TABL	E I. Dispers	tion relations	of the first t	ten moment e	equations.		· · · ·				. ···	
2r +l ·	0	1	2	5	ę	က	4	4	4	5	5	5	9	9	
1	0	1	0	2	1	က	0	7	4	Ч	က	5	0	67	
r	0	0		0	1	0	7	1	0	67	Ч	0	ŝ	63	
0 0 0	ь	2 40	0	0	0	0	0	0	0	0	0	0	0	0	1
1 1 0	$\frac{k}{2\mathcal{E}} - \mathcal{E}$	σ +1	- 3 6	<u>36</u> 3	η_{011}	0	0	0	0	η_{011}	0	0	0	0	
2 0 1	0	$2\mathcal{E} - \frac{k}{\mathcal{E}}$	$\sigma + \mu_{10}$	0	2 CO	0	η_{120}	0	0	0	0	0	η_{130}	0	
2 2 0	0	$\frac{k}{\mathcal{S}} - 2\mathcal{S}$	0	σ +µ ₀₂	$-\frac{2k}{5\delta}$	<u>3</u> <i>k</i>	0	η_{012}	0	0	0	0	0	η_{022}	
311	0	η_{101}	$\frac{5k}{6\mathcal{S}} - 5\mathcal{S}$	$\frac{4\mathcal{E}}{3} - \frac{2k}{3\mathcal{E}}$	$\sigma + \mu_{11}$	0	$-\frac{2k}{56}$	3 <u>6</u> 3	0	η_{121}	0	0	0	0	
3 3 0	0	0	0	$\frac{2k}{3\mathcal{E}} - 3\mathcal{E}$	0	$\sigma + \mu_{03}$	0	$-\frac{3k}{7\mathcal{E}}$	$\frac{4k}{7\mathcal{E}}$	0	η_{013}	0	0	0	
4 0 2	0	0	η_{210}	0	$2\mathcal{E} - \frac{k}{\mathcal{E}}$	0	σ + μ_{20}	0	0	20	0	0	η_{230}	0	
421	0	0	0	η_{102}	$\frac{7k}{5\mathcal{E}} - \frac{14\mathcal{E}}{5}$	$\frac{6\mathcal{S}}{5} - \frac{3k}{5\mathcal{S}}$	0	$\sigma + \mu_{12}$	0	$-\frac{4k}{5\mathcal{S}}$	$\frac{3k}{5\delta}$	0	0	η_{122}	
440	0	0	0	0	0	$\frac{2k}{\mathcal{E}} - 4\mathcal{E}$	0	0	$\sigma + \mu_{04}$	0	0	<u>96</u>	0	0	
512	0	η_{201}	0	0	η_{211}	0	$\frac{7k}{6\delta} - \frac{7\delta}{3}$	$\frac{4\mathcal{E}}{3} - \frac{2k}{3\mathcal{E}}$	0	$\sigma + \mu_{21}$	0	0	२ <mark>१</mark> २० ।	$\frac{2k}{3c}$	

$$\frac{\partial n}{\partial \tau} + \frac{\partial n}{\partial \rho} + (1 + \xi_{10}) \frac{\partial^2 n}{\partial \tau^2} + \frac{5}{3} \xi_{10} \frac{\partial^2 n}{\partial \rho \partial \tau} - \left(\frac{1}{2\mathcal{B}^2} + \frac{4}{3} \xi_{02}\right) \frac{\partial^2 n}{\partial \rho^2} + \xi_{10} \frac{\partial^3 n}{\partial \tau^3} - \left(\frac{5}{6\mathcal{B}^2} \xi_{10} + \frac{4}{3} \xi_{10} \xi_{02}\right) \frac{\partial^3 n}{\partial \rho^2 \partial \tau} + \frac{2}{9} \xi_{11} \xi_{10} (5\xi_{10} + 4\xi_{02}) \frac{\partial^3 n}{\partial \rho^3} = 0.$$
(28)

The same equation is satisfied by both ϕ_1^0 and ϕ_0^1 .

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The fourth approximation (complete Burnett) is the simultaneous solution of Eqs. (19), (22), (26) and

 $\frac{\partial \phi_2^0}{\partial \tau} + \mu_{02} \phi_2^0 - 2 \mathcal{E} \phi_1^0 + \frac{1}{\mathcal{E}} \frac{\partial \phi_1^0}{\partial \rho} - \frac{2}{5\mathcal{E}} \frac{\partial \phi_1^1}{\partial \rho} + \frac{3}{5\mathcal{E}} \frac{\partial \phi_3^0}{\partial \rho} = 0,$ (29)

$$\frac{1}{\mathcal{S}} \frac{\partial \phi_3^0}{\partial \rho} \approx 6\xi_{03} \xi_{02} \mathcal{S}^2 \frac{\partial n}{\partial \rho}.$$
(30)

In order for nontrivial solutions of Eqs. (19), (22), (26), (29), (30) to exist,

$$\frac{\partial n}{\partial \tau} + \frac{\partial n}{\partial \rho} + (1 + \xi_{10} + \xi_{02}) \frac{\partial^2 n}{\partial \tau^2} + (\frac{5}{3} \xi_{10} + \frac{7}{3} \xi_{02}) \frac{\partial^2 n}{\partial \rho \partial \tau} - \frac{1}{2 \mathcal{S}^2} \frac{\partial^2 n}{\partial \rho^2} + (\xi_{10} + \xi_{02} + \xi_{02} \xi_{10}) \frac{\partial^3 n}{\partial \tau^3} + 3\xi_{10} \xi_{02} \frac{\partial^3 n}{\partial \rho \partial \tau^2} \\ - \frac{1}{\mathcal{S}^2} (\frac{5}{6} \xi_{10} + \frac{7}{6} \xi_{02}) \frac{\partial^3 n}{\partial \rho^2 \partial \tau} + [\frac{2}{9} \xi_{11} (\xi_{10} + \frac{4}{5} \xi_{02}) (5\xi_{10} + 4\xi_{02}) + \frac{12}{5} \xi_{02}^2 \xi_{03}] \frac{\partial^3 n}{\partial \rho^3} + \xi_{10} \xi_{02} \frac{\partial^4 n}{\partial \tau^4} - \frac{3}{2 \mathcal{S}^2} \xi_{02} \xi_{10} \frac{\partial^4 n}{\partial \rho^2 \partial \tau^2} \\ + [\frac{38}{45} (5\xi_{10} + 4\xi_{02}) - \frac{12}{5} \xi_{10} \xi_{02}^2 \xi_{03}] \frac{\partial^4 n}{\partial \rho^3 \partial \tau} = 0.$$
(31)

The effect of higher approximations is to change the coefficients of the second- and higher-order derivative terms, and to add derivative terms of order equal to the order of approximation. The meaning of incomplete Burnett and complete Burnett approximation will become clear in Sec. V.

V. REDUCTION TO THE ASYMPTOTIC THEORY

In the asymptotic theory, the ion flux j is computed from the Boltzmann equation, with the timederivative term put in terms of space derivatives via the continuity equation, which results in⁵⁸

$$j = nv_d - D_{ZZ} \frac{\partial n}{\partial z} + Q_{ZZZ} \frac{\partial^2 n}{\partial z^2} - \cdots, \qquad (32)$$

where v_d , D, and Q are the ion drift velocity, diffusion coefficients, and higher-order transport coefficients, respectively.

If dimensionless transport coefficients are defined,

$$v_0 \equiv v_d / \zeta \, \mathcal{S} \approx 1 \,, \tag{33}$$

$$d_0 \equiv (\nu/\zeta^2 \mathcal{E}^2) D_{ZZ} , \qquad (34)$$

$$q_{0} \equiv (\nu^{2} / \mathcal{S}^{3} \zeta^{3}) Q_{ZZZ} , \qquad (35)$$

$$r_{0} \equiv (\nu^{3} / \mathcal{E}^{4} \zeta^{4}) R_{ZZZZ}, \qquad (36)$$

$$s_{0} \equiv (\nu^{4} / \mathcal{E}^{5} \zeta^{5}) S_{ZZZZZ}, \qquad (37)$$

then the approximation scheme described in Sec. IV reduces to the asymptotic theory as follows: to sixth order,

$$\frac{\partial^{2} n}{\partial \tau^{2}} - \frac{\partial^{2} n}{\partial \rho^{2}} - 2d_{0}\frac{\partial^{3} n}{\partial \rho^{3}} + (2q_{0} + d_{0}^{2})\frac{\partial^{4} n}{\partial \rho^{4}} - 2(r_{0} + d_{0}q_{0})\frac{\partial^{5} n}{\partial \rho^{5}} + (2s_{0} + 2d_{0}r_{0} + q_{0}^{2})\frac{\partial^{6} n}{\partial \rho^{6}} + O(7), \qquad (38)$$

$$\frac{\partial^{3}n}{\partial\tau^{3}} - \frac{\partial^{3}n}{\partial\rho^{3}} + 3d_{0}\frac{\partial^{4}n}{\partial\rho^{4}} - 3(q_{0} + d_{0}^{2})\frac{\partial^{5}n}{\partial\rho^{5}} + (3r_{0} + 6d_{0}q_{0} + d_{0}^{4})\frac{\partial^{6}n}{\partial\rho^{6}} + O(7), \qquad (39)$$

$$\frac{\partial^4 n}{\partial \tau^4} \rightarrow \frac{\partial^4 n}{\partial \rho^4} - 4d_0 \frac{\partial^5 n}{\partial \rho^5} + 2(q_0 + 2d_0^2) \frac{\partial^6 n}{\partial \rho^6} + O(7), \qquad (40)$$

$$\frac{\partial^5 n}{\partial \tau^5} \rightarrow -\frac{\partial^5 n}{\partial \rho^5} + 5d_0 \frac{\partial^6 n}{\partial \rho^6} + O(7), \qquad (41)$$

$$\frac{\partial^6 n}{\partial \tau^6} + \frac{\partial^6 n}{\partial \rho^6} + O(7) \,. \tag{42}$$

The general equation in any approximation for n to second order is

$$\frac{\partial n}{\partial \tau} + \frac{\partial n}{\partial \rho} + d_1 \frac{\partial^2 n}{\partial \tau^2} - d_2 \frac{\partial^2 n}{\partial \rho^2} + d_3 \frac{\partial^2 n}{\partial \rho \partial \tau} = 0, \qquad (43)$$

which reduces to the diffusion equation

$$\frac{\partial n}{\partial t} + \frac{\partial n}{\partial \rho} - d_0 \frac{\partial^2 n}{\partial \rho^2} = 0, \qquad (44)$$

asymptotically in all orders of approximation. Table II shows how the coefficients d_1 , d_2 , and d_3 change in the first five approximations.

In the analogous case of a single monotonic neu-

tral gas, the acceleration term in the Boltzmann equation is zero resulting in $d_1 = 0$, $d_2 = \frac{1}{2}$, $d_3 = 0$ in any approximation higher than the Euler approximation. Thus the convergence of the coefficients is no problem and the sequence of approximations should have at least a finite radius of convergence.^{65,67} Pekeris *et al.*⁶⁵ have tested this for the Maxwell model for the first 483 moment equations and for rigid spheres for 105. The speculation of a finite radius of convergence is reasonably well

The third approximation has terms of third order (i.e., third-order derivatives) in it but does not reduce to the asymptotic theory. However, the fourth approximation does reduce to the asymptotic theory to third order

founded at least in neutral gases.

$$\frac{\partial n}{\partial \tau} + \frac{\partial n}{\partial \rho} - d_0 \frac{\partial^2 n}{\partial \rho^2} + q_0 \frac{\partial^3 n}{\partial \rho^3} = 0, \qquad (45)$$

which suggests, as in the case of neutral gases,⁵⁰ that suitable truncation points should include 1, 2, 4, 6, 9, etc. numbers of moment equations (as is shown in Table I). That is, the complete Navier-Stokes approximation has all of the moment equations included up to 2r + l = 1, the complete Burnett approximation has all of the moment equations included up to 2r + l = 2, etc. Therefore the third approximation, resulting in Eq. (28), is called the incomplete Burnett approximation because it does not include all the 2r + l = 2 moment equations. A natural suggestion is that the complete super-Burnett approximation (six moment equations) reduces to asymptotic theory of fourth order

$$\frac{\partial n}{\partial \tau} + \frac{\partial n}{\partial \rho} - d_0 \frac{\partial^2 n}{\partial \rho^2} + q_0 \frac{\partial^3 n}{\partial \rho^3} - r_0 \frac{\partial^4 n}{\partial \rho^4} = 0, \qquad (46)$$

and the nine-moment-equation approximation reduces to the asymptotic theory of the fifth order

$$\frac{\partial n}{\partial \tau} + \frac{\partial n}{\partial \rho} - d_0 \frac{\partial^2 n}{\partial \rho^2} + q_0 \frac{\partial^3 n}{\partial \rho^3} - r_0 \frac{\partial^4 n}{\partial \rho^4} + s_0 \frac{\partial^5 n}{\partial \rho^5} = 0.$$
(47)

The important fact to be gleaned from all this is that higher complete approximations do not alter the asymptotic theory to lower order which leads one to conjecture that to the extent $\tau \gg 1$, terms higher than the Navier-Stokes approximation do not contribute significantly.

VI. SOLUTIONS FOR THE NAVIER-STOKES APPROXIMATION

We consider Eq. (25) for the density in unbounded space,

$$\frac{\partial^2 n}{\partial \tau^2} + \frac{\partial n}{\partial \tau} + \frac{\partial n}{\partial \rho} - \alpha \frac{\partial^2 n}{\partial \rho^2} = 0, \qquad (48)$$

where

$$\alpha = \frac{1}{2\mathcal{E}^2} + \frac{2}{3}\xi_{10} + \frac{4}{3}\xi_{02} = \frac{\langle v_z^2 \rangle}{\langle v_z \rangle^2} - 1 \cong \frac{qD_{ZZ}}{mKv_d},$$
(49)

where K is the ion mobility. Apart from the scaling of z and t, Eq. (48) depends on only one parameter, α . In Fig. 1 is shown a contour plot of α in a plane whose axes are \mathscr{E} and m/M.

Under the transformation

$$\psi(\rho,\tau) = n(\rho,\tau) \exp\left(\frac{1}{2}\tau - \rho/2\alpha\right),\tag{50}$$

Eq. (48) becomes

$$\frac{\partial^2 \psi}{\partial \tau^2} = \alpha \, \frac{\partial^2 \psi}{\partial \rho^2} + \beta^2 \psi \,, \tag{51}$$

where

$$\beta^2 = (\alpha - 1)/4\alpha . \tag{52}$$

Equation (51) is a telegraphers equation on which there is much literature. $^{83-86}$

The solution to (51) transformed back to n, is

$$n(\rho,\tau) = \int_{-\infty}^{+\infty} \left(G_1(\rho',\tau)n(\rho-\rho',0) + G_2(\rho',\tau)\frac{\partial}{\partial\tau}n(\rho-\rho',0) \right) d\rho', \qquad (53)$$

Order of approximation	d_1	<i>d</i> ₂	d_3
1	0	0	0
2	1	$1/2\mathcal{E}^2 + (\frac{4}{3}\xi_{02} + \frac{2}{3}\xi_{10})$	0
3	$1 + \xi_{10}$	$1/2\mathcal{E}^2 + \frac{4}{3}\xi_{02}$	$\frac{5}{3} \xi_{10}$
4	$1 + \xi_{10} + \xi_{02}$	$1/2 \mathcal{E}^{2}$	$\frac{5}{3}\xi_{10} + \frac{7}{3}\xi_{02}$
5	$1 + \xi_{10} + \xi_{02} + \xi_{11}$	$1/2\mathcal{E}^2 - (\frac{8}{15}\xi_{02} + \frac{5}{3}\xi_{10})\xi_{11}$	$\frac{5}{3}\xi_{10} + \frac{7}{3}\xi_{02} + \xi_{11}\left(1 + \frac{5}{3}\xi_{10} + \frac{8}{15}\xi_{02}\right)$
Asymptotic theory	0	$1/2\mathcal{E}^2 + (\frac{4}{3}\xi_{02} + \frac{2}{3}\xi_{10} - 1)$	0

TABLE II. Divergence of second-order coefficients.



FIG. 1. Contour map of α , a shock parameter in the ion-neutral mass ratio-electric field strength plane.

where the Green's functions are, for $\rho^2 \leq \alpha \tau^2$

$$G_{1}(\rho, \tau) = \frac{1}{2}e^{-\tau/2} [\delta(\rho + a\tau)e^{-a\tau/2\alpha} + \delta(\rho - a\tau)e^{a\tau/2\alpha}]$$

$$+\frac{1}{4a}\exp\left(-\frac{\tau}{2}+\frac{\rho}{2\alpha}\right)\left(I_{0}(\mu)+\frac{2\beta^{2}\tau}{\mu}I_{1}(\mu)\right),\quad(54)$$

 $G_{2}(\rho, \tau) = (1/2a) \exp(-\frac{1}{2}\tau + \rho/2\alpha) I_{0}(\mu), \qquad (55)$

where

$$\mu = \beta (\tau^2 - \rho^2 / \alpha)^{1/2}, \quad a^2 = \alpha .$$
 (56)

Notice that more initial data need to be supplied to Eq. (48) than the diffusion equation [Eq. (44)] because of the higher-order time derivative.

In order to illustrate the nature of the solution, Eq. (53), we will assume that the initial ion distribution is a δ function, Eq. (16), which means that

$$\frac{\partial n(\rho, 0)}{\partial \rho} = 0, \qquad (57)$$

so that the G_2 term can be neglected. In this case

$$n(\rho, \tau) = G_1(\rho, \tau).$$
 (58)

Equation (54) is plotted for several values of α (α = 10 000, 100, 3, 1.1, 1.01) in Figs. 2-6, respectively. It is convenient to compare with the results predicted by the diffusion equation. Therefore the vertical coordinate is multiplied by

$$(4D_{zz}t)^{1/2} = [4(\alpha - 1)\mathcal{E}^2\tau]^{1/2}, \tag{59}$$

which expands in time, and the horizontal coordinate is transformed to

$$y = \frac{z - v_d t}{(4D_{ZZ}t)^{1/2}} = \frac{\rho - \tau}{[4(\alpha - 1)\tau]^{1/2}},$$
(60)

so that the diffusion-equation Green's function in unbounded space for this coordinate system is

$$n_D(\rho,\tau) = (\pi)^{-1/2} e^{-y^2} \tag{61}$$

for all time.



FIG. 2. Navier-Stokes-level ion density vs y at various times for $\alpha = 10000$. The horizontal coordinate is moving in the field direction and compressing in time and the vertical coordinate is expanding in time so that the diffusion-equation solution to this case $(\tau = \infty)$ remains stationary.

The function, equation (54) [which represents the ion density under initial conditions equation (16) in unbounded space] is plotted for extremely low fields or low mass ratios in Figs. 2 and 3. In the limit of large α , Eq. (54) becomes more symmetric about y = 0, but otherwise remains very much like Fig. 2. The height of the thick lines in the shock front and rear indicate the fraction of ions contained in the shock. The ion-density evolution corresponding to electrons in a neutral gas at any fields or ions in a neutral gas at extremely low fields is shown in Fig. 2. For ions at low fields but slightly higher than those shown in Fig. 2, Fig. 3 typifies the density evolution. As can be seen from Figs. 2 or 3, it only takes a dozen or so collisions for the density to evolve to the diffusionequation solution $(\tau = \infty)$. See Eq. (62).

In Fig. 4 is considered a case typical of light ions $(m/M \approx 0.2)$ at high fields or heavier ions at medium fields (see the contour of $\alpha = 3$ in Fig. 1). The principal difference between Fig. 4 and the previous two figures is that the density distribution



FIG. 3. Navier-Stokes-level ion density vs y at various times for α =100.



FIG. 4. Navier-Stokes-level ion density vs y at various times for $\alpha = 3$.

is more skewed for short times. As opposed to the cases where $\alpha \gg 1$, it takes about 250 collisions to relax to the diffusion-equation solution.

In Figs. 5 and 6 is shown the extreme case of heavy ions and very heavy ions at high fields. For the regions where $\alpha = 1.1$ and 1.01, see Fig. 1. Here the distributions are yet more skewed and deviations from the diffusion-equation solution persist for 4000 and 65 000 collisions, respectively.

The prominent feature of these curves, the shock wave, depends for its existence on a discontinuous initial ion-density distribution. Since such a density discontinuity is not readily produced in the laboratory the shock wave would be smoothed out in experiment, though not as smooth as the diffusion equation would have it.

Such effects could conceivably be measurable for heavy ions at high fields in experimental situations^{87,88} possibly hampering at least the interpretation of the mobility due to the peak shift. As an example, for Xe⁺ in He $(m/M \approx 33)$ shock effects could be present for ~30 000 collisions, and for U⁺ in He $(m/M \approx 60)$ shock effects could be present for 45 000 collisions.



FIG. 5. Navier-Stokes-level ion density vs y at various times for $\alpha = 1.1$.



FIG. 6. Navier-Stokes-level ion density vs y at various times for $\alpha = 1.01$.

The asymptotic form of Eq. (54) for long time is

$$G_{I}(\rho,\tau) \approx \frac{1}{[4\pi(\alpha-1)\mathcal{S}^{2}\tau]^{1/2}} e^{-y^{2}} \times \left(1 + \frac{2(y-y^{3})}{[\tau(\alpha-1)]^{1/2}} + O(1/\tau)\right)$$
(62)

which is valid as long as $[\tau(\alpha - 1)]^{1/2} \gg 1$ and $|\rho| \ll a\tau$ (i.e., not near a shock front).

The correction terms in the large parentheses of Eq. (62) should not be taken too seriously however because competing terms of the same order should arise from the Burnett theory [Eqs. (31) or (45)]. For instance, solving Eq. (45) in unbounded space in the long-time limit yields^{59,60}

$$G(\rho,\tau) \approx \frac{1}{[4\pi(\alpha-1)\mathcal{S}^{2}\tau]^{1/2}} e^{-y^{2}} [1 - \frac{1}{2}C(y - \frac{2}{3}y^{3}) + O(C^{2})], \quad (63)$$

where

$$C = 3q_0 / (d_0^{3/2} \tau^{1/2}).$$
(64)

Normally C > 0 so that the correction terms in Eq. (63) are of the opposite sign to those in Eq. (62) (corresponding to a density distribution skewed in the opposite direction in Figs. 2-6). However for the Maxwell model at high fields with m/M > 20, $q_0 < 0$ and the correction terms in Eqs. (62) and (63) have the same sign.

VII. CONCLUSION

A number of theories have been discussed in this paper. I shall indicate in this section the scope of each, what physical phenomena are encompassed in each, in what cases each is liable to be important, and what outstanding problems can be considered. The theories considered are at the Eulerlevel hydrodynamics, Eq. (21), Navier-Stokes – level hydrodynamics, Eq. (25) convergent or Eq. (44) asymptotic, and Burnett-level hydrodynamics Eq. (31) convergent or Eq. (45) asymptotic. These are shown in Fig. 7 indicating their accuracy and scope.

The Navier-Stokes-level hydrodynamics for a weakly ionized gas considers that momentum is a function of position within a pulse. The convergent theory allows for stationization of momentum where the asymptotic theory (diffusion equation) does not. Since stationization of momentum happens very quickly for electrons, Eqs. (25) and (44) give almost identical results for electrons as soon as the shocks wear off.

Burnett-level hydrodynamics take into account that energy is also a function of position in a pulse. The convergent theory takes into account energy stationization as well. At least the asymptotic theory suggests that this level of hydrodynamics may be especially important for electrons⁵⁹ where the higher-order transport coefficient, Q, is very large at high fields.⁵⁸ Thus solution of Eq. (31), or the equivalent set of moment equations, is necessary for a good electron-transport theory if electron inhomogeneities are significant on the scale of an energy relaxation distance. Burnett-level hydrodynamics should also yield a good back diffusion theory where none now exists^{73,89-100} and can take care of transport near boundaries. Burnettlevel hydrodynamics may also be important in various types of gaseous discharges where certain types of constrictions or instabilities develop which are preceded by large density gradients.

The asymptotic theory at the Burnett level has little useful to say except to suggest when the diffusion equation should break down.

Analysis of higher-order effects might best be carried out by considering the dispersion relations contained in Table I as has been done extensively in neutral gases.^{62, 64–68,101,102}

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APPENDIX

Values of low order ξ_{rl_m} , η_{rsl} , and a few ξ 's are as follows:

$$\xi_{01} = 1$$
, $\xi_{10} = (m + M)/2m$

$$\xi_{02} = (m+M)/(2m+M),$$

regardless of the force law. A few are

$$\xi_{11} = \frac{3(m+M)^2}{9m^2 + 3M^2 + 4mM} ,$$





$$\xi_{20} = \frac{3(m+M)^3}{24m^3 + 16m^2M + 24mM^2} ,$$

$$\xi_{03} = \frac{(m+M)^2}{3m^2 + M^2 + 3mM} ,$$

for the Maxwell model with isotropic scattering, or

$$\xi_{11} = \frac{5(m+M)^2}{15m^2 + 5m^2 + 8mM} ,$$

$$\xi_{20} = \frac{5(m+M)^3}{20m^3 + 16m^2M + 20M^2m} ,$$

$$\xi_{03} = \frac{70(m+M)^2}{210m^2 + 252mM + 135M^2} ,$$

for rigid spheres. (See the literature for more details.^{76,79,80,81}) The main point is that the above two sets are weak functions of the force law.⁸⁰ However, η is a strong function of the force law. It vanishes identically for the Maxwell model and thermal diffusion depends for its existence on $\eta \neq 0$. Gaseous diffusion plants require $\eta \neq 0$ for their operation. A useful ploy is to equate η_{011} to $\partial \ln K/\partial \ln \epsilon$, a measurable quantity:

$$\eta_{011} = \frac{3}{4\xi_{11}(5\xi_{10} + 4\xi_{02})\mathcal{B}^2} \frac{\partial \ln K}{\partial \ln \epsilon} ,$$

$$\eta_{srl} = \eta_{rsl} \frac{[r!\Gamma(l+s+\frac{3}{2})]}{[s!\Gamma(l+r+\frac{3}{2})]} ,$$

where a convenient formula for ${\mathcal S}$ is

$$\mathcal{E} = 0.020837(m/T)^{1/2}KE/N,$$

where m is in amu, T in $^{\circ}$ K, K—the reduced mo-

bility—in cm^2/V sec, and E/N in Townsends. (For more detailed information on these collision integrals see Ref. 80.)

For a Rayleigh mixture $(m \gg M)$ the matrix elements of the collision operator have a particularly

simple form,

 $\xi_{rl} = 1/(2r+l), \ \eta_{rsl} \propto (M/m)^{|r-s|},$

so that the η_{rsl} are negligible.

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