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On the Application of the Grad Approximation to Time-Dependent Plasmas

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The Grad 13-moment approximation is applied to a Lorentz-like plasma under the influence of an oscillating electric field. Calculations of the electron diffusion velocity and heat flux and their respective phase lags are compared for a variety of effective interparticle interaction potentials with the results obtained from exact solutions to the first-order kinetic equations. Significant differences appear whenever the force laws correspond to molecules which are much harder or softer than the Maxwellian variety.

INTRODUCTION

A general assumption of many authors[1-7] over the past twelve years is that Grad's 13-moment velocity distribution function[8] permits an accurate description of nonequilibrium plasmas when used to close out the macroscopic equations of change. Since, however, the Grad approximation is an expansion[8]

in the eigenfunctions of Boltzmann's binary elastic collision operator for Maxwellian molecules, convergence for more general interaction potentials is not guaranteed; consequently, verification is desirable at all perturbation orders for most plasmas of practical interest. Previous studies[9,10] of this convergence have shown that Everett-like computations[5] of the residual heat flux, the entropy density, the collisional production rate of entropy, and second-order contributions to the electron pressure tensor can be in error by as much as 26% for very hard or very soft particles, while third-order contributions (proportional to the cube of the applied electric field) to the electron current density are off by factors up to four in the same limits.

The purpose of the present research is to extend the aforementioned convergence studies to collision-dominated plasmas acted upon by an oscillating electric field. Thirteen-moment calculations of the electron diffusion velocity and heat flux and their respective phase lags behind the applied field are compared for a variety of effective interparticle interaction potentials with the results obtained from exact solutions to Lorentz-like kinetic equations. As before, significant differences appear whenever the force laws correspond to particles which are much harder or much softer than the Maxwellian variety.

While the Lorentz-like stipulation of this research may appear highly restrictive because of the implied neglect of electron-electron encounters, such is not the case if the electron-heavy particle potential parameters are generalized semiempirically. Meador[11] has shown, for example, that Lorentz-like distribution functions accurately predict many diverse properties of

real plasmas (including entropy production and tensor conductivities) when the exponent in an electron-heavy particle inverse power interaction potential is chosen properly. In any event, the Lorentz-like collision model is used in both the Grad and the exact calculations so that comparisons between the two should yield a valid assessment of the accuracy of the Grad approximation.

Other simplifications employed in the present investigation include the following assumptions: no magnetic field is applied, all collisions are elastic and obey the rules of classical dynamics, the heavy particles (e.g., ions and neutral atoms) are infinitely massive and at rest relative to the laboratory, the local charge separation is zero, there are no collective oscillations resulting from the long-range coulomb interactions, and the particle pressures and species temperatures are constant through linear terms in the total electric field, which is regarded as spatially homogeneous. The last of these conditions is obviously incompatible with Maxwell's electromagnetic equations unless the induced electric field is arbitrarily ignored. This we shall do in order to avoid unnecessary complications in the essential calculations and comparisons.

EXACT CALCULATIONS

Subject to the conditions outlined in the Introduction, the electronic Boltzmann equation

$$\frac{\partial f_e}{\partial t} + c_e \cdot \nabla f_e - \frac{e}{m_e} (E + c_e \times B) \cdot \frac{\partial f_e}{\partial c_e} = \left(\frac{\partial f_e}{\partial t}\right)_c \tag{1}$$

can be written through first order as

$$\frac{\partial\phi_1}{\partial t} + \frac{2e}{m_e}\left(\frac{m_e}{2kT_e}\right)^{1/2} E\cdot\gamma = - n_h\gamma\left(\frac{2kT_e}{m_e}\right)^{1/2}\int(\phi_1-\phi_1')bdbd\varepsilon \qquad (2)$$

if n_h is the number density for a single species of heavy particles and γ and ϕ_1 are the reduced electron particle velocity and first-order perturbation function defined by

$$\gamma = \left(\frac{m_e}{2kT_e}\right)^{1/2} c_e \qquad (3)$$

and

$$f_e = f_e^{(o)}\ (1 + \phi_1) = n_e\left(\frac{m_e}{2\pi kT_e}\right)^{3/2} e^{-\gamma^2}\ (1+\phi_1), \qquad (4)$$

respectively.

By first order in the present research is meant the retention in f_e of all terms dependent linearly upon the electric field E. Hence, the induced magnetic field is dropped from Eq. (1), but the time derivative of ϕ_1 survives because of the following assumed form of E:

$$E = E_o \exp\ (i\omega t). \qquad (5)$$

One should further note that this appearance of ϕ_1 on the left side of Eq. (2) signifies a different concept of perturbation order from that usually associated with the Chapman-Enskog expansion.[12]

The collisional effects of present interest in the case of inverse ξ-power electron-heavy particle interaction potentials are summarized[11,13]

by the integral

$$\int (\gamma-\gamma')b\,db\,d\varepsilon = \frac{R_{13}}{n_h R_{04}\tau}\left(\frac{m_e}{2kT_e}\right)^{1/2} \gamma^{-4/\xi}\gamma, \tag{6}$$

where

$$R_{ij} = \int_0^\infty x^{\frac{4i}{\xi}+j} e^{-x^2} dx \tag{7}$$

and τ is the collision time defined through the electrical conductivity relation

$$\sigma = e^2 n_e \tau/m_e \tag{8}$$

As previously mentioned, the effective potential parameter ξ may be so chosen[11] as to permit the Lorentz-like collision model to describe the properties of almost any plasma; in particular, $\xi = 5/3$ is the appropriate value for a fully ionized gas with electron-electron encounters included. Similar adjustments can also alleviate the restriction to plasmas with only a single heavy species.

The substitution into Eq. (2) of Eq. (6) and the trial function

$$\phi_1 = g(\gamma)\ E\cdot\gamma \tag{9}$$

yields

$$i\omega g + \frac{2e}{m_e}\left(\frac{m_e}{2kT_e}\right)^{1/2} = -\frac{R_{13}}{R_{04}\tau}\gamma^{1-\frac{4}{\xi}} g, \tag{10}$$

whereupon

$$\phi_1 = -\frac{2R_{04}\sigma}{en_eR_{13}}\left(\frac{m_e}{2kT_e}\right)^{1/2} \gamma^{\frac{4}{\xi}-1}\left(1 + \frac{i\omega\tau R_{04}}{R_{13}}\gamma^{\frac{4}{\xi}-1}\right)^{-1} E\cdot\gamma \tag{11}$$

A particularly convenient representation of Eq. (11) for the purpose of subsequent calculations is obtained by the introduction of the new collision time

$$\tau_s = \frac{R_{04}R_{22}}{R_{13}^2}\tau, \tag{12}$$

which is derived[11] from the following relation between the collisional production rate of entropy density $\dot{s}_c$ and the existing and equilibrium entropy densities s and $s^{(o)}$:

$$\frac{1}{2}\tau_s\dot{s}_c = s^{(o)} - s. \tag{13}$$

Since past applications[11] have shown the Hall conductivity for small magnetic fields to be expressible in its mean-free-path form when τ_s is substituted for τ, one might expect similar simplifications and insight to occur in the present study.

Equation (11) for small $\omega\tau$ thus becomes

$$\phi_1 = -\frac{2R_{04}\sigma}{en_eR_{13}}\left(\frac{m_e}{2kT_e}\right)^{1/2} \gamma^{\frac{4}{\xi}-1}\left(1 - \frac{i\omega\tau_s R_{13}}{R_{22}}\gamma^{\frac{4}{\xi}-1}\right)E\cdot\gamma, \tag{14}$$

the interesting velocity moments of which are the electron current density

$$j = -en_e v_e = -\frac{en_e}{\pi^{3/2}}\left(\frac{2kT_e}{m_e}\right)^{1/2}\int e^{-\gamma^2}\gamma\,\phi_1\,d\gamma = \sigma E\,(1-i\omega\tau_s)$$

$$\approx \sigma E_o \exp\,[i\omega(t-\tau_s)] \tag{15}$$

and the residual heat flux

$$q - \frac{5}{2}p_e v_e = \frac{n_e m_e}{2}\left(\frac{2kT_e}{\pi m_e}\right)^{3/2}\int e^{-\gamma^2}\gamma^2\gamma\phi_1 d\gamma - \frac{5}{2}p_e v_e =$$

$$= \frac{p_e(\xi-4)\sigma}{2en_e\xi}\,E\,(1 - 2\,i\omega\tau_s)$$

$$\approx \frac{p_e(\xi-4)\sigma}{2en_e\xi}\,E_o \exp\,[i\omega(t-2\tau_s)]. \tag{16}$$

The significance of the collision time associated with entropy production is immediately obvious: It is that interval (at the initial applicatio of $E_o \sin \omega t$) during which the macroscopic current density is not a valid concept. In addition, $\omega\tau_s$ and $2\omega\tau_s$ represent the amounts by which the phases of the current density and the residual heat flux lag that of the driving electric field. Although such phase-angle terms as appear in Eqs. (15) and (16) would be labeled second order in the Chapman-Enskog expansion, they can become important at sufficiently high applied frequencies. The present technique permits their evaluation from a much simpler kinetic equation than the second-order one normally considered; consequently, the

many irrelevant (to diffusion velocity and heat flux) second-order terms do not complicate the basic calculations.

THE GRAD APPROXIMATION

Values of the current density and heat flux parameters of Eqs. (15) and (16) are next computed in the Everett manner[5] of closing out the macroscopic equations of change with the Grad 13-moment velocity distribution function

$$f_e = n_e \left(\frac{m_e}{2\pi kT_e}\right)^{3/2} e^{-u^2} \left[1 + \frac{4}{5}\left(u^2 - \frac{5}{2}\right) \beta_1 \cdot u + \frac{1}{p_e} \overset{o}{P}_e : uu\right], \tag{17}$$

where $\overset{o}{P}_e$ is the traceless pressure tensor, u is the reduced electron particle velocity relative to the electron frame of reference and defined by

$$u = \left(\frac{m_e}{2kT_e}\right)^{1/2} \left(c_e - v_e\right) = \gamma - \beta_o, \tag{18}$$

β_o is the reduced electron diffusion velocity, and β_1 is the reduced residual heat flux defined by

$$\beta_1 = \langle u^2 u \rangle. \tag{19}$$

As mentioned earlier, comparisons between the two sets of results should yield valuable information on the accuracy of the Grad approximation.

The first-order form of Eq. (17) can be written

$$f_e = n_e \left(\frac{m_e}{2\pi kT_e}\right)^{3/2} e^{-\gamma^2} \left[1 + 2\beta_o \cdot \gamma + \frac{4}{5}\left(\gamma^2 - \frac{5}{2}\right)\beta_1 \cdot \gamma\right], \tag{20}$$

the application of which to the Lorentz-like collision terms gives

$$\frac{d\beta_o}{dt} + \frac{e}{m_e}\left(\frac{m_e}{2kT_e}\right)^{1/2} E = -\frac{R_{13}R_{-1,5}}{5R_{04}^{\ 2}\ \xi\tau}\left[5\xi\beta_o + (\xi-4)\beta_1\right] \tag{21}$$

and

$$\frac{d}{dt}\left(\beta_1 + \frac{5}{2}\beta_o\right) + \frac{5e}{2m_e}\left(\frac{m_e}{2kT_e}\right)^{1/2} E$$

$$= -\frac{R_{13}R_{-1,5}(3\xi-2)}{5R_{04}^{\ 2}\ \xi^2\tau}\left[5\xi\beta_o + (3\xi-4)\beta_1\right] \tag{22}$$

for the closed-out macroscopic equations of change of β_o and β_1 corresponding to the present problem.

Since the simultaneous solutions of Eqs. (21) and (22) are

$$\beta_o \approx -\frac{R_{04}^{\ 2}(13\xi^2-16\xi+16)\sigma}{4en_eR_{13}R_{-1,5}\xi(3\xi-2)}\left(\frac{m_e}{2kT_e}\right)^{1/2} E_o \exp\left\{i\omega\left[t - \frac{R_{04}R_{13}(179\xi^4-496\xi^3+832\xi^2-512\xi+256)\tau_s}{4R_{22}R_{-1,5}\xi\ (3\xi-2)(13\xi^2-16\xi+16)}\right]\right\} \tag{23}$$

and

$$\beta_1 \approx \frac{5R_{04}^{\ 2}(\xi-4)\sigma}{4en_eR_{13}R_{-1,5}(3\xi-2)}\left(\frac{m_e}{2kT_e}\right)^{1/2} E_o \exp\left\{i\omega\left[t - \frac{R_{04}R_{13}(23\xi^2-16\xi+16)\tau_s}{4R_{22}R_{-1,5}\xi(3\xi-2)}\right]\right\}, \tag{24}$$

the desired current density and residual heat flux can be written as

$$j = a_o\sigma(\text{exact})E_o \exp\left[i\omega(t - \alpha_o\tau_s)\right] \tag{25}$$

and

$$q - \frac{5}{2} p_e v_e = \frac{a_1 p_e \sigma(\text{exact})}{e n_e} E_o \exp\left[i\omega(t-\alpha_1 \tau_s)\right] \tag{26}$$

with the phase angles given in Eqs. (23) and (24) and a_o and a_1 by

$$a_o = \frac{R_{04}^{\ 2}(13\xi^2-16\xi+16)}{4R_{13}R_{-1,5}\xi(3\xi-2)} \tag{27}$$

and

$$a_1 = \frac{5R_{04}^{\ 2}(\xi-4)}{4R_{13}R_{-1,5}(3\xi-2)} . \tag{28}$$

COMPARISON OF RESULTS

Numerical calculations based on Eqs. (15), (16), and (23)-(28) are presented in Tables I and II for a variety of effective interparticle interaction potentials ranging from a Lorentz fully ionized gas ($\xi = 1$), through Maxwellian molecules ($\xi = 4$), and on to a Lorentz gas of rigid spheres ($\xi = \infty$). Only in the neighborhood of $\xi = 4$ does the Grad approximation accurately predict the values of the residual heat flux and the two phase lags, the errors being especially large in the case of α_1. These results, together with those found previously[10] for the third-order contribution to the electron diffusion velocity, would seem to indicate the need for vastly improved distribution functions in the highly nonequilibrium work of Everett[5] and Yen.[6]

A principal reason for the large discrepancies in some transport properties is the fact that the 13-moment function is formally analogous[4]

to only the second Sonine approximation to the first-order distribution function in the Chapman-Enskog perturbation series. Although the general concepts of Eq. (20) need not be so limited, its exact identification with the second Sonine approximation is automatic when the relation between β_1 and β_o obtained from the closing-out procedure is substituted; in particular, the use in Eq. (20) of the strictly first-order contributions to Eqs. (23) and (24) yields the second Sonine expression[11]

$$\phi_1 = \frac{4\sigma(\text{second Sonine})}{en_e(13\xi^2-16\xi+16)} \left(\frac{m_e}{2kT_e}\right)^{1/2} \left[\xi(\xi-4)\gamma^2 - (3\xi-2)(3\xi-4)\right] E\cdot\gamma. \tag{29}$$

This identification also explains the inferiority of the Grad predictions of a_1 compared with a_o because the first Sonine polynomial does not contribute to the residual heat flux arising from applied fields; hence, the 13-moment function does not provide a higher Sonine correction to the first contribution to a_1 as it does in the case of a_o. Such corrections are of far greater importance for plasmas than for neutral gases.

Finally, one should note that if the present use of the Grad 13-moment function <u>is</u> identified with the second Sonine approximation, and if Onsager's reciprocal relation between the residual heat flux and thermal diffusion is employed, the ratio of a_1 (Grad) to a_1 (exact) in Table I can be obtained directly from the work of Chapman and Cowling.[14] The phase parameters, however, cannot be so determined.[15]

SUMMARY

Comparisons between exact and Everett-like calculations of the electrical ~~and thermal conductivities~~ conductivity and residual heat flux and their phase lags behind an oscillating electric field show substantial differences in some of the transport parameters. As indicated by this and previous research, the errors associated with the Grad 13-moment approximation are especially serious in the higher-order terms demanded by strong fields[10] or by significant departures from a stationary state; consequently, much improved electron distribution functions are probably required for highly nonequilibrium plasmas.

TABLE I. Comparison of the electrical ~~and thermal~~ conductivity and heat flux parameters a_o and a_1 as functions of the effective interparticle interaction parameter ξ.

ξ	a_o (Grad)	a_o (exact)	a_1 (Grad)	a_1 (exact)
1	0.957	1.000	-1.105	-1.500
2	0.994	1.000	-0.552	-0.500
4	1.000	1.000	0.000	0.000
∞	0.957	1.000	0.368	0.500

TABLE II. Comparison of the phase lag parameters α_o and α_1 as functions of the effective interparticle interaction parameter ξ.

ξ	α_o (Grad)	α_o (exact)	α_1 (Grad)	α_1 (exact)
1	0.759	1.000	0.876	2.000
2	1.011	1.000	1.900	2.000
4	1.000	1.000	2.000	2.000
∞	0.861	1.000	1.438	2.000

FOOTNOTES

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15. Ibid, pp. 343-5. The magnitude of the oscillating current density given in this reference can be obtained from Eq. (11) of the present text only in the case of Maxwellian molecules. Hence, the modification employed here (and mentioned on p. 345) to the first-order kinetic equation evidently is employed by Chapman and Cowling strictly to the first Sonine approximation.