

A MICROSCOPIC THEORY OF DENSITY FLUCTUATIONS IN PARTIALLY IONIZED GASES*

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Abstract—This investigation develops a set of exact kinetic equations describing density fluctuations in many body systems with S species. These equations are then applied to the analysis of a partially ionized gas with three species: electrons, ions and neutral atoms. The relationship of this theory to earlier kinetic theory investigations is discussed. A particularly simple approximation for the non-local, non-Markovian collision kernels in these kinetic equations is introduced and used to compute the dynamic structure factors $S(k, \omega)$ characterizing the scattering of electromagnetic radiation (both Thomson and Rayleigh) from partially ionized gases.

1. INTRODUCTION

TIME correlation functions of dynamical variables play an extremely important role in the description of many body systems such as liquids, gases or plasmas. It is well known that transport parameters which characterize the irreversible behavior of such systems can be expressed in terms of time correlation functions calculated under equilibrium conditions (ZWANZIG, 1965). Moreover, the cross sections or emission coefficients for the interaction of radiation with an aggregate of particles can be directly related to the time correlation of density or current fluctuations in the system.

The theoretical significance of time correlation functions, coupled with the ever-increasing use of radiation scattering as a technique for probing the microscopic structure and dynamics of matter, have stimulated the development of a variety of theories of density fluctuations in many particle systems. Most studies of density fluctuations in gases and plasmas (KLIMONTOVICH, 1967; ROSTOKER, 1961) usually begin with a derivation (or postulation) of a kinetic equation describing the time correlation of fluctuations in the microscopic phase space density

$$\mathcal{S}(\mathbf{x}, \mathbf{p}, \mathbf{x}', \mathbf{p}', t) \equiv \langle \delta g(\mathbf{x}, \mathbf{p}, t) \delta g(\mathbf{x}', \mathbf{p}', t) \rangle \quad (1)$$

where

$$g(\mathbf{x}, \mathbf{p}, t) \equiv \sum_{\alpha=1}^N \delta[\mathbf{x} - \mathbf{x}^\alpha(t)] \delta[\mathbf{p} - \mathbf{p}^\alpha(t)] \quad (2)$$

and

$$\delta g(\mathbf{x}, \mathbf{p}, t) \equiv g(\mathbf{x}, \mathbf{p}, t) - \langle g(\mathbf{x}, \mathbf{p}, 0) \rangle. \quad (3)$$

To the lowest order of approximation, the appropriate kinetic equation for neutral gases is just the linearized Boltzmann equation, while for fully ionized plasmas, the corresponding description utilizes the coupled linearized Vlasov equations (MONTGOMERY, 1967).

Of course these simple kinetic equations are inadequate to describe high frequency, short wavelength fluctuations in dense gases or plasmas in which short-range Coulomb

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collisions become important. A number of techniques have been used to derive higher order kinetic equations suitable for the description of density fluctuations in these latter situations. A particularly powerful approach relies upon the use of projection operator algebra to develop an exact, but formal, kinetic equation for $\mathcal{S}(\mathbf{x}, \mathbf{p}, \mathbf{x}', \mathbf{p}', t)$ which can then be approximated using standard perturbation theory or modeling (AKCASU and DUDERSTADT, 1969, 1970). This scheme has recently been applied to the study of density fluctuations in fully ionized plasmas (LINNEBUR and DUDERSTADT, 1973). In this paper, we extend the theory to analyze partially ionized gases in which charged particle-neutral collisions are important.

We begin by deriving a set of exact kinetic equations describing density fluctuations in a many body system containing S species which is assumed to be in thermal equilibrium. This set is then specifically applied to analyze a three species ionized gas (neutrals, ions and electrons). The relation of these coupled kinetic equations to previous theories is discussed, and several standard alternative approximate kinetic equation descriptions of density fluctuations are derived.

A more elaborate modeled kinetic theory of density fluctuations of plasmas of arbitrary ionization is then developed and applied to calculate the electron dynamic form factor $S(k, \omega)$ for a typical partially ionized plasma.

2. KINETIC EQUATION DESCRIPTION OF DENSITY FLUCTUATIONS IN S -SPECIES SYSTEMS

In earlier work (LINNEBUR and DUDERSTADT, 1973) we indicated that the projection operator techniques of ZWANZIG (1961); MORI (1965) can be used to derive an exact equation of motion for a matrix of time correlation functions. In particular, if \mathbf{a} is a column vector whose components are dynamical variables $a_i(x^1, \dots, p^N)$, then Mori has shown that the correlation matrix

$$\tilde{R}(t) \equiv \langle \mathbf{a}(t) \mathbf{a}^* \rangle \cdot \langle \mathbf{a} \mathbf{a}^* \rangle^{-1} \tag{4}$$

satisfies an exact equation of the form

$$\dot{\tilde{R}}(t) - i\tilde{\Omega} \cdot \tilde{R}(t) + \int_0^t d\tau \tilde{\varphi}(\tau) \cdot \tilde{R}(t - \tau) = 0 \tag{5}$$

where the frequency matrix $\tilde{\Omega}$ and the damping matrix $\tilde{\varphi}(\tau)$ are given as

$$i\tilde{\Omega} \equiv \langle \dot{\mathbf{a}} \mathbf{a}^* \rangle \cdot \langle \mathbf{a} \mathbf{a}^* \rangle^{-1} \tag{6}$$

$$\tilde{\varphi}(\tau) \equiv \langle f(\tau) f^*(0) \rangle \cdot \langle \mathbf{a} \mathbf{a}^* \rangle^{-1} \tag{7}$$

where

$$f(\tau) \equiv \exp [i\tau(1 - P)L]i(1 - P)L\mathbf{a}, \tag{8}$$

and the projection operator P is defined by its action on an arbitrary dynamical variable vector \mathbf{G} as

$$P\mathbf{G} \equiv \langle \mathbf{G} \mathbf{a}^* \rangle \cdot \langle \mathbf{a} \mathbf{a}^* \rangle^{-1} \cdot \mathbf{a}. \tag{9}$$

Here \mathbf{a} denotes $\mathbf{a}(0)$, \mathbf{a}^* is the row vector adjoint to \mathbf{a} , and L is the Liouville operator $L = i\{H, \cdot\}$.

This equation can be extended to describe sets of dynamical variables $\mathbf{a}(\mathbf{p}, t) = \text{col } [a_j(\mathbf{p}, t)]$ which depend as well upon a continuous "momentum" parameter \mathbf{p}

$$\frac{\partial \tilde{\mathcal{F}}}{\partial t} - i \int d^3 p' \tilde{\Omega}(\mathbf{p}, \mathbf{p}') \cdot \tilde{\mathcal{F}}(\mathbf{p}', \mathbf{p}'', t) + \int_0^t d\tau \int d^3 p' \tilde{\varphi}(\mathbf{p}, \mathbf{p}', \tau) \cdot \tilde{\mathcal{F}}(\mathbf{p}', \mathbf{p}'', t - \tau) = 0 \quad (10)$$

where

$$\tilde{\mathcal{F}}(\mathbf{p}, \mathbf{p}', t) \equiv \langle \mathbf{a}(\mathbf{p}, t) \mathbf{a}^*(\mathbf{p}') \rangle. \quad (11)$$

The kinetic equations describing density fluctuations in a S -species system can be explicitly derived by choosing

$$\mathbf{a}(\mathbf{p}) = \text{col } [a_1(\mathbf{p}), \dots, a_s(\mathbf{p}), \dots, a_c(\mathbf{p})] \quad (12)$$

where the $a_s(\mathbf{p})$ correspond to the spatial Fourier transform of the fluctuation of $g_s(\mathbf{x}, \mathbf{p}, 0)$ from its equilibrium value

$$a_s(\mathbf{p}) \equiv \sum_{\alpha_s=1}^N e^{i\mathbf{k} \cdot \mathbf{x}^{\alpha_s}} \delta(\mathbf{p} - \mathbf{p}^{\alpha_s}) - n_s \delta(\mathbf{k}) M_s(\mathbf{p}) = \delta g_s(\mathbf{k}, \mathbf{p}, 0) \quad (13)$$

where

$$M_s(\mathbf{p}) \equiv (\beta_s/2\pi m_s)^{3/2} \exp(-\beta_s p^2/2m_s), \quad \beta_s = 1/k_B T_s. \quad (14)$$

In order to explicitly calculate the generalized frequency matrix $\tilde{\Omega}(\mathbf{p}, \mathbf{p}')$ and damping matrix $\tilde{\varphi}(\mathbf{p}, \mathbf{p}', \tau)$, we must first calculate the inverse of the static correlation matrix:

$$\begin{aligned} \phi_{ss'}(\mathbf{p}, \mathbf{p}') &\equiv \langle a_s(\mathbf{p}) a_{s'}^*(\mathbf{p}') \rangle \\ &= n_s M_s(\mathbf{p}) \delta(\mathbf{p} - \mathbf{p}') \delta_{ss'} + n_s n_{s'} M_s(\mathbf{p}) M_{s'}(\mathbf{p}') h_{ss'}(k) \end{aligned} \quad (15)$$

where $h_{ss'}(k)$ is the Fourier transform of $[g_{ss'}(r) - 1]$, $g_{ss'}(r)$ being the static pair correlation function between species s and s' . Here $\tilde{\phi}(\mathbf{p}, \mathbf{p}')$ can be written more concisely as

$$\tilde{\phi}(\mathbf{p}, \mathbf{p}') = \tilde{n} \cdot \tilde{M}(\mathbf{p}) \delta(\mathbf{p} - \mathbf{p}') + \tilde{n} \cdot \tilde{M}(\mathbf{p}) \cdot \tilde{h}(k) \cdot \tilde{n} \cdot \tilde{M}(\mathbf{p}') \quad (16)$$

where

$$[\tilde{n}]_{ss'} = n_s \delta_{ss'}, \quad [\tilde{M}(\mathbf{p})]_{ss'} = M_s(\mathbf{p}) \delta_{ss'}, \quad [\tilde{h}(k)]_{ss'} = h_{ss'}(k). \quad (17)$$

The inverse correlation matrix is defined by

$$\int d^3 p' \tilde{\phi}(\mathbf{p}, \mathbf{p}') \cdot \tilde{\phi}^{-1}(\mathbf{p}', \mathbf{p}'') = \delta(\mathbf{p} - \mathbf{p}'') \tilde{I}. \quad (18)$$

Substituting in equation (16), one finds

$$\tilde{n} \cdot \tilde{M}(\mathbf{p}) \cdot [\tilde{\phi}^{-1}(\mathbf{p}, \mathbf{p}'') + \tilde{h}(k) \cdot \tilde{n} \cdot \tilde{A}(\mathbf{p}'')] = \delta(\mathbf{p} - \mathbf{p}'') \tilde{I} \quad (19)$$

where

$$[\tilde{A}(\mathbf{p}'')]_{ss'} \equiv \int d^3 p' M_s(\mathbf{p}') \phi_{ss'}^{-1}(\mathbf{p}', \mathbf{p}''). \quad (20)$$

But integrating equation (19) over \mathbf{p} yields

$$\tilde{n} \cdot [\tilde{I} + \tilde{h}(k) \cdot \tilde{n}] \cdot \tilde{A}(\mathbf{p}'') = \tilde{I} \quad (21)$$

or

$$\tilde{A}(\mathbf{p}'') = [\tilde{I} + \tilde{h}(k) \cdot \tilde{n}]^{-1} \cdot \tilde{n}^{-1}. \quad (22)$$

We can substitute equation (22) back into equation (19) to find

$$\check{\phi}^{-1}(\mathbf{p}, \mathbf{p}') = [\check{n} \cdot \check{M}(\mathbf{p})]^{-1} \delta(\mathbf{p} - \mathbf{p}') - \check{C}(k) \tag{23}$$

where

$$\check{C}(k) \equiv \check{h}(k) \cdot \check{n} \cdot [\check{I} + \check{h}(k) \cdot \check{n}]^{-1} \cdot \check{n}^{-1}. \tag{24}$$

Thus having evaluated the inverse matrix $\check{\phi}^{-1}(\mathbf{p}, \mathbf{p}')$, we can continue on to calculate the frequency matrix

$$i\check{\Omega}(\mathbf{p}, \mathbf{p}') = \int d^3p'' \langle \hat{\mathbf{a}}(\mathbf{p}) \mathbf{a}^*(\mathbf{p}'') \rangle \cdot \check{\phi}^{-1}(\mathbf{p}'', \mathbf{p}') \tag{25}$$

by first noting that

$$\hat{a}_s(\mathbf{p}) = (i\mathbf{k} \cdot \mathbf{p}/m_s) a_s(\mathbf{p}) + \sigma_s(\mathbf{p}), \quad \sigma_s(\mathbf{p}) \equiv \sum_{\alpha_s=1}^{N_s} e^{i\mathbf{k} \cdot \mathbf{x}^{\alpha_s}} \mathbf{F}^{\alpha_s} \cdot \frac{\partial}{\partial \mathbf{p}^{\alpha_s}} \delta(\mathbf{p} - \mathbf{p}^{\alpha_s}). \tag{26}$$

Hence using equations (23), (25), and (26), one finds

$$i\Omega_{ss'}(\mathbf{p}, \mathbf{p}') = \frac{i\mathbf{k} \cdot \mathbf{p}}{m_s} \delta(\mathbf{p} - \mathbf{p}') \delta_{ss'} - \frac{i\mathbf{k} \cdot \mathbf{p}}{m_s} n_s M_s(\mathbf{p}) C_{ss'}(k). \tag{27}$$

Finally, noting

$$\check{\varphi}(\mathbf{p}, \mathbf{p}', \tau) = \int d^3p'' \langle \mathbf{f}(\mathbf{p}, t) \mathbf{f}^*(\mathbf{p}'', 0) \rangle \cdot \check{\phi}^{-1}(\mathbf{p}'', \mathbf{p}') \tag{28}$$

and $\int d^3p'' \mathbf{f}(\mathbf{p}'', 0) = 0$, one finds

$$\varphi_{ss'}(\mathbf{p}, \mathbf{p}', \tau) = [n_{s'} M_{s'}(\mathbf{p}')]^{-1} \langle f_s(\mathbf{p}, t) f_{s'}^*(\mathbf{p}', 0) \rangle \tag{29}$$

where

$$f_s(\mathbf{p}, 0) = (1 - P) \hat{a}_s(\mathbf{p}) = (1 - P) \sigma_s(\mathbf{p}). \tag{30}$$

Further explicit calculations of the damping matrix $\check{\varphi}(\mathbf{p}, \mathbf{p}', \tau)$ will require approximations.

Hence the coupled set of exact kinetic equations for the time-dependent density correlation functions for an S -species system

$$\mathcal{S}_{rs}(k, \mathbf{p}, \mathbf{p}'', t) \equiv \langle \delta g_r(k, \mathbf{p}, t) \delta g_s^*(k, \mathbf{p}'', 0) \rangle \tag{31}$$

can be explicitly written as

$$\begin{aligned} \frac{\partial \mathcal{S}_{rs}}{\partial t} - \frac{i\mathbf{k} \cdot \mathbf{p}}{m_r} \mathcal{S}_{rs} + \frac{i\mathbf{k} \cdot \mathbf{p}}{m_r} n_r M_r(\mathbf{p}) \left[\sum_{s'=1}^S C_{rs'}(k) \int d^3p' \mathcal{S}_{s's}(k, \mathbf{p}', \mathbf{p}'', t) \right] \\ + \sum_{s'=1}^S \int_0^t d\tau \int d^3p' \varphi_{rs'}(\mathbf{p}, \mathbf{p}', \tau) \mathcal{S}_{s's}(k, \mathbf{p}', \mathbf{p}'', t - \tau) = 0 \quad r, s = 1, \dots, S. \end{aligned} \tag{32}$$

These coupled kinetic equations for the $\mathcal{S}_{rs}(k, \mathbf{p}, \mathbf{p}'', t)$ are still exact, and still quite formal in that the damping kernels $\varphi_{rs}(\mathbf{p}, \mathbf{p}'', \tau)$ remain to be explicitly determined. It should be noted that these equations involve terms which are non-local in space and non-Markovian in time. It is also important to note that these exact kinetic equations for the time correlation functions are linear, unlike kinetic equations for distribution functions such as $\langle g_s(\mathbf{x}, \mathbf{p}, t) \rangle_0$.

3. KINETIC EQUATIONS FOR PARTIALLY IONIZED PLASMAS

We will now consider a classical, partially ionized plasma in thermal equilibrium at a temperature T with neutral density n_n , ion density n_i , and electron density $n_e = Zn_i$, where Z denotes the effective ionization per atom. Since the electron density fluctuations are of most interest in calculating quantities such as the scattering cross section for incident electromagnetic radiation, we will study the coupled kinetic equations for $\mathcal{S}_{ee}(k, \mathbf{p}, \mathbf{p}'', t)$, $\mathcal{S}_{ie}(k, \mathbf{p}, \mathbf{p}'', t)$, and $\mathcal{S}_{ne}(k, \mathbf{p}, \mathbf{p}'', t)$:

$$\begin{aligned} \frac{\partial \mathcal{S}_{se}}{\partial t} - \frac{i\mathbf{k} \cdot \mathbf{p}}{m_s} \mathcal{S}_{se}(k, \mathbf{p}, \mathbf{p}', t) + \frac{i\mathbf{k} \cdot \mathbf{p}}{m_s} n_s M_s(\mathbf{p}) \left[\sum_{s'=e,i,n} C_{ss'}(k) \int d^3 p' \mathcal{S}_{s'e}(k, \mathbf{p}', \mathbf{p}'', t) \right] \\ + \sum_{s'=e,i,n} \int_0^t d\tau \int d^3 p' \varphi_{ss'}(\mathbf{p}, \mathbf{p}', \tau) \mathcal{S}_{s'e}(k, \mathbf{p}', \mathbf{p}'', t - \tau) = 0 \quad s = e, i, n. \end{aligned} \quad (33)$$

To simplify and interpret this set of equations, we first confine our attention to wave-lengths large compared to the range of the charged particle-neutral interaction, but comparable to the much longer range of Coulomb interactions. [Essentially all of the restrictive approximations and assumptions discussed in this section will be removed in the more elaborate alternative theory developed in Section 4.] Hence we can neglect $h_{sn}(k)$ in comparison with $h_{ee}(k)$, $h_{ii}(k)$, and $h_{iz}(k)$. If we furthermore assume that the pair correlation function $g_{ss'}(r)$ for charged particles is given by a simple Debye-Hückel form

$$g_{ss'}(r) = 1 - Z_s Z_{s'} l e^{-r/\lambda_D} / r \quad (34)$$

where $l \equiv e^2/kT$, $\lambda_D \equiv [4\pi\beta n_e e^2(1 + Z)]^{-1/2}$, then

$$h_{ss'}(k) = -4\pi Z_s Z_{s'} l \lambda_D^2 / (1 + k^2 \lambda_D^2). \quad (35)$$

Under these two assumptions, one then finds that

$$C_{ss'}(k) = 0 \quad \text{if } s \text{ or } s' = n$$

and

$$C_{ss'}(k) = -4\pi Z_s Z_{s'} l / k^2 \equiv \beta V_{ss'} \quad \text{for } s, s' = e, i. \quad (36)$$

The coupled kinetic equations (33) then reduce to the more familiar form:

$$\begin{aligned} \frac{\partial \mathcal{S}_{ee}}{\partial t} - \frac{i\mathbf{k} \cdot \mathbf{p}}{m_e} \mathcal{S}_{ee} + \frac{i\mathbf{k} \cdot \mathbf{p}}{m_e} n_e M_e(\mathbf{p}) \left(\frac{4\pi e^2 \beta}{k^2} \right) \int d^3 p' [Z \mathcal{S}_{ie}(k, \mathbf{p}', \mathbf{p}'', t) - \mathcal{S}_{ee}(k, \mathbf{p}', \mathbf{p}'', t)] \\ = \sum_{s=e,i,n} \int_0^t d\tau \int d^3 p' \varphi_{es}(\mathbf{p}, \mathbf{p}', \tau) \mathcal{S}_{se}(k, \mathbf{p}', \mathbf{p}'', t - \tau) \\ \frac{\partial \mathcal{S}_{ie}}{\partial t} - \frac{i\mathbf{k} \cdot \mathbf{p}}{m_i} \mathcal{S}_{ie} + \frac{i\mathbf{k} \cdot \mathbf{p}}{m_i} n_e M_i(\mathbf{p}) \left(\frac{4\pi e^2 \beta}{k^2} \right) \int d^3 p' [\mathcal{S}_{ee}(k, \mathbf{p}', \mathbf{p}'', t) - Z \mathcal{S}_{ie}(k, \mathbf{p}', \mathbf{p}'', t)] \\ = \sum_{s=e,i,n} \int_0^t d\tau \int d^3 p' \varphi_{is}(\mathbf{p}, \mathbf{p}', \tau) \mathcal{S}_{se}(k, \mathbf{p}', \mathbf{p}'', t - \tau) \\ \frac{\partial \mathcal{S}_{ne}}{\partial t} - \frac{i\mathbf{k} \cdot \mathbf{p}}{m_n} \mathcal{S}_{ne} = \sum_{s=e,i,n} \int_0^t d\tau \int d^3 p' \varphi_{ns}(\mathbf{p}, \mathbf{p}', \tau) \mathcal{S}_{se}(k, \mathbf{p}', \mathbf{p}'', t - \tau) \end{aligned} \quad (37)$$

where the self-consistent field terms characterizing charged particle density fluctuations can readily be identified, while the damping terms can now be seen to play the role of generalized, nonlocal collision terms.

To proceed further, one must now introduce approximations in order to obtain explicit expressions for the damping kernels $\varphi_{ss'}(\mathbf{p}, \mathbf{p}', \tau)$. Of course, one could proceed by using perturbation theory to calculate $\varphi_{ss'}(\mathbf{p}, \mathbf{p}', \tau)$ to lowest order in some suitable parameter. Earlier investigations (AKCASU and DUDERSTADT, 1969, 1970; ZWANZIG, 1961) have indicated that $\varphi_{ss'}(\mathbf{p}, \mathbf{p}', \tau)$ yields the more familiar collision operators in the appropriate limits. For example, in the low density limit (MAZENKO, 1971)

$$\lim_{\substack{n \rightarrow 0 \\ t \rightarrow \infty}} \int_0^t d\tau \int d^3 p' \varphi(\mathbf{p}, \mathbf{p}', \tau) f(\mathbf{p}', t - \tau) = J_B[f(\mathbf{p}, t)]$$

where $J_B[\]$ is the usual linearized Boltzmann operator. Similarly, the weak coupling limit yields the linearized Fokker-Planck operator, while an expansion in the plasma parameter $(n_e \lambda_D^3)^{-1}$ yields the Balescu-Lenard collision operator to lowest order.

With these facts in mind, we can now easily make contact with earlier theories of electron fluctuations in ionized gases. For example, if all short range collisions were neglected entirely, one would arrive immediately at the coupled Vlasov description of SALPETER (1960); FEJER (1960); DOUGHERTY and FARLEY (1960); ROSTOKER and ROSENBLUTH (1962). For weakly ionized gases, one can essentially neglect charged particle (Coulomb) collisions in comparison to charged-particle-neutral collisions. Furthermore, for weak ionization, the neutral density fluctuations decouple from the electron and ion fluctuations. Finally, for low frequency, large wavelength processes in low density ionized gases, a density expansion of the $\varphi_{ee}(\mathbf{p}, \mathbf{p}', t)$ and $\varphi_{ii}(\mathbf{p}, \mathbf{p}', t)$ kernels is appropriate, yielding the linearized Boltzmann operator characterizing electron- and ion-neutral collisions

$$\begin{aligned} \frac{\partial \mathcal{S}_{ee}}{\partial t} - \frac{i\mathbf{k} \cdot \mathbf{p}}{m_e} \mathcal{S}_{ee} + \frac{i\mathbf{k} \cdot \mathbf{p}}{m_e} n_e M_e(\mathbf{p}) \left(\frac{4\pi e^2 \beta}{k^2} \right) \int d^3 p' [Z \mathcal{S}_{ie} - \mathcal{S}_{ee}] &= J_B^{en}[\mathcal{S}_{ee}] \\ \frac{\partial \mathcal{S}_{ie}}{\partial t} - \frac{i\mathbf{k} \cdot \mathbf{p}}{m_i} \mathcal{S}_{ie} + \frac{i\mathbf{k} \cdot \mathbf{p}}{m_i} n_e M_i(\mathbf{p}) \left(\frac{4\pi e^2 \beta}{k^2} \right) \int d^3 p' [\mathcal{S}_{ee} - Z \mathcal{S}_{ie}] &= J_B^{in}[\mathcal{S}_{ie}]. \end{aligned} \quad (38)$$

Such approximate kinetic equations were recently derived by WILLIAMS and CHAPPELL (1971) to describe electron density fluctuations in weakly ionized plasmas. These authors then approximated the Boltzmann operator $J_B[\]$ by a simple BGK collision model in order to obtain an explicit analytic solution for $\mathcal{S}_{ee}(k, \mathbf{p}, \mathbf{p}', t)$, and hence for the electron dynamic form factor

$$S(k, \omega) = \frac{1}{\pi} \operatorname{Re} \left\{ \lim_{s \rightarrow i\omega} G_{ee}(k, s) \right\} \quad (39)$$

where

$$G_{ee}(k, s) \equiv \frac{1}{n_e} \int d^3 p \int d^3 p'' \mathcal{S}_{ee}(k, \mathbf{p}, \mathbf{p}'', s) \quad (40)$$

is the Laplace transform of the time correlation function of electron density fluctuations (s being the transform variable).

Such a BGK model was used earlier by GOROG (1969) to investigate the effect of charged particle-neutral collisions on the Thomson scattering of electromagnetic radiation from weakly ionized plasmas. Our exact set of kinetic equations (32) clearly indicates the sequence of approximations necessary to derive such kinetic models for partially ionized plasmas, and furthermore indicates how such a model can be improved—for instance, by including neutral dynamics or charged particle collisions. In the next section, we will develop a much more sophisticated kinetic equation description valid for arbitrary k and ω and degree of ionization by utilizing a simple model of the time dependence of the non-Markovian damping kernels $\varphi_{ss'}(\mathbf{p}, \mathbf{p}', t)$ which has proven extremely effective in describing high k , ω density fluctuations in liquids, gases, and plasmas.

It should be mentioned that Williams and Chappel also derived an equation analogous to (38) for the “self” part of the density correlation function which characterizes test particle motions (self-diffusion). A more general (indeed, exact) kinetic equation for test particle motions can easily be derived using the projection operator formalism. This equation is presented and discussed in Appendix A.

4. A MODELED KINETIC EQUATION DESCRIPTION

As in earlier studies (LINNEBUR and AKCASU, 1972) we will model the time dependence of the damping kernel in the following fashion:

$$\varphi_{ss'}(\mathbf{p}, \mathbf{p}', t) = \varphi_{ss'}^s(\mathbf{p}, \mathbf{p}', 0) \exp(-\alpha_{ss'}^s(k)t) + \varphi_{ss'}^d(\mathbf{p}, \mathbf{p}', 0) \exp(-\alpha_{ss'}^d(k)t) \quad (41)$$

where $\varphi_{ss'}^s$ and $\varphi_{ss'}^d$ refer to the self- and distinct parts of the damping kernel which can be explicitly calculated at $t = 0$:

$$\varphi_{ss'}^s(\mathbf{p}, \mathbf{p}', 0) = -\delta_{ss'} D_s(0) \left[\frac{\partial}{\partial \mathbf{p}} \cdot \frac{\partial}{\partial \mathbf{p}} + \frac{\beta_s}{m_s} \frac{\partial}{\partial \mathbf{p}} \cdot \mathbf{p} \right] \delta(\mathbf{p} - \mathbf{p}') \quad (42)$$

$$\varphi_{ss'}^d(\mathbf{p}, \mathbf{p}', 0) = M_s(\mathbf{p}) \mathbf{p} \cdot \left[\frac{\mathbf{k}\mathbf{k}}{m_s m_{s'}} n_s C_{ss'}(k) - \frac{\beta_s \beta_{s'} n_s}{m_s m_{s'} n_{s'}} \tilde{D}_{ss'}(k) \right] \cdot \mathbf{p}' \quad (43)$$

where

$$D_s(0) = \sum_{s'} D_{ss'}(0), \quad D_{ss'}(0) = -\frac{n_{s'}}{3\beta_s} \int d^3R \frac{\partial g_{ss'}}{\partial \mathbf{R}} \cdot \frac{\partial V^{ss'}}{\partial \mathbf{R}}, \quad (44)$$

$$\tilde{D}_{ss'}(k) = D_{ss'}(0) \tilde{I} - \frac{n_{s'}}{\beta_s} \int d^3R g_{ss'}(R) \frac{\partial^2 V^{ss'}}{\partial \mathbf{R} \partial \mathbf{R}} (1 - \cos \mathbf{k} \cdot \mathbf{R}).$$

The exponential relaxation parameters $\alpha_{ss'}(k)$ can be specified by applying various known constraints (LINNEBUR and AKCASU, 1972) to the small and large k behavior of the solutions to the corresponding modeled kinetic equations (substituting equations (41–43) into equation (32) and Laplace transforming in time):

$$\begin{aligned} & \left(s - \frac{\mathbf{i}\mathbf{k} \cdot \mathbf{p}}{m_r} \right) \mathcal{S}_{re} - \frac{\mathbf{i}\mathbf{k} \cdot \mathbf{p}}{m_r} M_r(\mathbf{p}) n_r \left[\sum_{s=1}^S C_{rs}(k) \int d^3p' \mathcal{S}_{se}(\mathbf{k}, \mathbf{p}', \mathbf{p}'', s) \right] \\ &= \mathcal{S}_{re}(\mathbf{k}, \mathbf{p}, \mathbf{p}'', 0) + \frac{D_r(0)}{s + \alpha_{rr}^s(k)} \left[\frac{\partial}{\partial \mathbf{p}} \cdot \frac{\partial}{\partial \mathbf{p}} + \frac{\beta_r}{m_r} \frac{\partial}{\partial \mathbf{p}} \cdot \mathbf{p} \right] \mathcal{S}_{re} - \sum_{s=1}^S \frac{\mathbf{p} M_r(\mathbf{p})}{s + \alpha_{rs}^d(\mathbf{k})} \\ & \quad \times \left[\frac{\mathbf{k}\mathbf{k}}{m_r m_s} n_r C_{rs}(k) - \frac{\beta_r \beta_s n_r}{m_r m_s n_s} \tilde{D}_{rs}(k) \right] \cdot \int d^3p' \mathcal{S}_{se}(\mathbf{k}, \mathbf{p}', \mathbf{p}'', s). \quad (45) \end{aligned}$$

These constraints require that we choose (LINNEBUR and DUDERSTADT, 1972)

$$\begin{aligned}\alpha_{rr}^s(k) &= \alpha_{rr}^s(0)[1 + (k/k_{rr}^s)^2] \\ \alpha_{rr}^d(k) &= \alpha_{rr}^d(0)[1 + (k/k_{rr}^d)^2] \\ \alpha_{rs}^d(k) &= [\alpha_{rr}^d(k)\alpha_{ss}^d(k)]^{1/2} = \alpha_{sr}^d(k)\end{aligned}\quad (46)$$

where

$$\begin{aligned}\alpha_{rr}^s(0) &= \left[\frac{\beta_r}{m_r} D_r(0) \right] [m_r \beta_r D_{sr}] = \frac{\beta_r}{m_r} \frac{D_r(0)}{\nu_{rr}} \\ \alpha_{rr}^d(0) &= \alpha_{rr}^s(0)\end{aligned}\quad (47)$$

where ν_{rr} is the self-collision frequency for the r th species, while

$$\begin{aligned}k_{ee}^s &= k_{ii}^s = \lambda_D^{-1}, & k_{nn}^s &\cong 2\pi n^{1/3} \\ k_{ee}^d &= 1.08 \left(\frac{\nu_{ee}}{\omega_{pe}} \right) \lambda_D^{-1}, & k_{ii}^d &= 1.08 \left(\frac{\nu_{ii}}{\omega_{pi}} \right) \lambda_D^{-1}\end{aligned}\quad (48)$$

and k_{nn}^d is given in terms of the shear viscosity η_{sn} as

$$\left(\frac{1}{k_{nn}^d} \right)^2 = \left(\frac{1}{k_{nn}^s} \right)^2 + \frac{\alpha_{nn}^s(0)}{n_n \beta_n D_n(0)} \left[\eta_{sn} - \frac{C_{nn}^{44}(0) - n_n / \beta_n}{\alpha_{nn}^s(0)} - \frac{\alpha_{nn}^s(0) n_n m_n}{2\beta_n^2 D_n(0)} \right] \quad (49)$$

where

$$C_{nn}^{44}(k) \equiv \frac{n_n}{\beta_n} + n_n^2 \int d^3R g_{nn}(\mathbf{R}) \frac{\partial^2 V_{nn}}{\partial X^2} \left(\frac{1 - \cos kZ}{k^2} \right). \quad (50)$$

The solution of the set of coupled kinetic equations (45) for

$$G_{rs}(k, s) = \int d^3p \int d^3p'' \mathcal{S}_{rs}(\mathbf{k}, \mathbf{p}, \mathbf{p}'', s) \quad (51)$$

is straightforward and yields (in matrix notation)

$$\begin{pmatrix} G_{ee} \\ G_{ie} \\ G_{ne} \end{pmatrix} = \begin{pmatrix} 1 + a_{ee} & a_{ei} & a_{en} \\ a_{ie} & 1 + a_{ii} & a_{in} \\ a_{ne} & a_{ni} & 1 + a_{nn} \end{pmatrix}^{-1} \begin{pmatrix} \mathcal{S}_{ee} \\ \mathcal{S}_{ie} \\ \mathcal{S}_{ne} \end{pmatrix}, \quad (52)$$

where

$$a_{rs} \equiv \left[\frac{Z_r}{\kappa_r} I(\kappa_r^2, Z_r) - \kappa_r \right] \left[\frac{kn_r}{\sqrt{m_r \beta_r}} C_{rs}(k) - \sqrt{\frac{m_s \beta_r}{m_r \beta_s}} \frac{Z_s}{\kappa_s} f_{rs}(k, s) \right], \quad (53)$$

$$\begin{aligned}S_{re} &\equiv n_e [\delta_{re} + n_r h_{re}(k)] \left[\frac{m_r \beta_r}{k^2} g_{rr}(k, s) I(\kappa_r^2, Z_r - 1) \right], \\ &- \left[\frac{m_r \beta_r s}{k^2} g_{rr}(k, s) I(\kappa_r^2, Z_r - 1) - 1 \right] \left[\sum_{s=e, i, n} \frac{m_s \beta_r}{k^2} n_e [\delta_{re} + n_s h_{se}(k)] f_{rs}(k, s) \right], \quad (54)\end{aligned}$$

and

$$Z_r = s/g_{rr}(k, s), \quad \kappa_r^2 = k^2/m_r\beta_r g_{rr}^2(k, s), \quad (55)$$

$$g_{rr}(k, s) \equiv \frac{(\beta_r/m_r)D_r(0)}{s + \alpha_{rr}^s(k)}, \quad (56)$$

$$f_{rs}(k, s) \equiv \frac{1}{s + \alpha_{rs}^s(k)} \left[\frac{k^2}{m_r\beta_r} n_r C_{rs}(k) - \frac{\beta_s n_r}{m_s n_s} D_{rs}^{33}(k) \right], \quad (57)$$

$$I(\kappa^2, z) \equiv e^{\kappa^2} \kappa^{-2(z+\kappa^2)} \int_0^{\kappa^2} du e^{-u} u^{z+\kappa^2}. \quad (58)$$

Although rather formidable in appearance, this model lends itself quite readily to explicit calculations of the dynamic form factor $S_{rs}(k, \omega)$ characterizing density fluctuations, primarily since the $t = 0$ form of the damping kernels yield kinetic equations which can be solved analytically. It furthermore yields the exact large frequency behavior (i.e. $\omega \rightarrow \infty$ or $t \rightarrow 0$) in contrast to other more phenomenological kinetic models such as the Boltzmann–Vlasov–BGK model. The non-local and non-Markovian character of the modeled damping or collision terms is frequently significant in analyzing scattering experiments at large k and ω .

One particularly interesting application of these results is to the study of light scattering from partially ionized gases. Since ionized as well as neutral atoms are present, both Thomson and Rayleigh scattering will occur, the first being characterized by the electron dynamic structure factor $S_{ee}(k, \omega)$ while the second is characterized by the neutral factor $S_{nn}(k, \omega)$. The relative significance of these two mechanisms depends upon the ionization of the plasma. Since the total cross section characterizing Rayleigh scattering from neutral atoms is of order 10^{-28} cm², while the Thomson scattering cross section from free electrons is 6.65×10^{-25} cm², it is evident that for ionizations $n_e/n_n > 0.01$, the Thomson scattering will dominate Rayleigh scattering, and hence the primary role played by the neutral atoms will be to perturb the electron dynamic structure factor from its behavior for a fully ionized plasma.

As a specific application, we have applied this theory to study the influence of neutral collisions on $S_{ee}(k, \omega)$ characterizing Thomson scattering from a singly-ionized, lithium-like plasma. The neutral-neutral and neutral-charged particle collisions were crudely modeled using a Maxwell force law (see Appendix B) with force constants

$$K_{en} = K_{ne} = 5.87 \times 10^{-44} \text{ erg cm}^4$$

$$K_{in} = K_{ni} = 9.36 \times 10^{-43} \text{ erg cm}^4$$

$$K_{nn} = 9.36 \times 10^{-43} \text{ erg cm}^4.$$

The plasma was taken to have an electron and ion density of $n_e = n_i = 10^{19}$ cm⁻³ and a temperature $T_e = T_i = T_n = 5.0$ eV. The neutral density was varied from $n_n = 10^{20}$ cm⁻³ to $n_n = 10^{18}$ cm⁻³ (corresponding to ionizations of from 10 to 90 per cent). The predictions of the kinetic model equations (46–58) for both the ion and electron resonances in $S_{ee}(k, \omega)$ are shown in Figs. 1 and 2. As one would expect, the effect of neutrals is to broaden (and lower) these resonances.

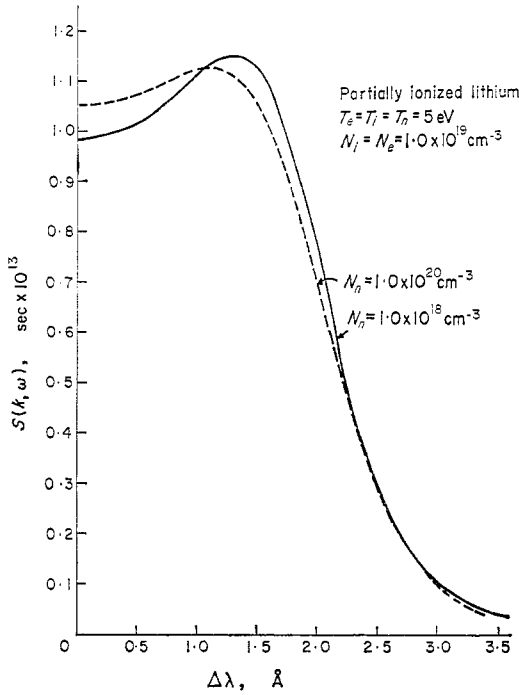


FIG. 1.—The ion feature of $S_{ee}(k, \omega)$ for a partially ionized lithium-like plasma with neutral density 10^{18} cm^{-3} (solid curve) and 10^{20} cm^{-3} (dashed curve). Here, $n_e = 10^{19} \text{ cm}^{-3}$, $T = 5 \text{ eV}$.

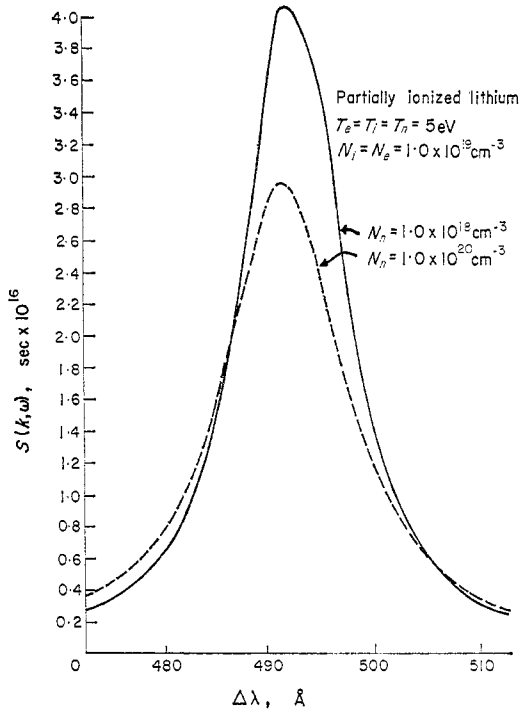


FIG. 2.—The electron satellite peak of $S_{ee}(k, \omega)$ for a partially ionized lithium-like plasma with neutral density 10^{20} cm^{-3} (solid curve) and 10^{18} cm^{-3} (dashed curve).

We have chosen this calculation as only one illustration of the utility of the model. It is a trivial extension to calculate other quantities such as the high frequency electrical conductivity $\sigma(k, \omega)$ for partially ionized plasmas (since this is closely related to the longitudinal current correlation and hence to $S(k, \omega)$), and to study such quantities for arbitrary k and ω as well as arbitrary degree of ionization.

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APPENDIX A: TEST PARTICLE MOTIONS

Define the test particle correlation function for species r as

$$\mathcal{G}_r^{(s)}(\mathbf{k}, \mathbf{p}, \mathbf{p}'', t) \equiv \langle \delta f_{1r}(\mathbf{k}, \mathbf{p}, t) \delta f^{*}_{1r}(\mathbf{k}, \mathbf{p}, 0) \rangle \tag{A.1}$$

where

$$\delta f_{1r}(\mathbf{k}, \mathbf{p}, t) \equiv \exp[i\mathbf{k} \cdot \mathbf{x}^{1r}(t)] \delta[\mathbf{p} - \mathbf{p}^{1r}(t)] - \frac{1}{V} \delta(\mathbf{k}) M_r(\mathbf{p}). \tag{A.2}$$

If we choose our dynamical variable $a(\mathbf{p}) = \delta f_{1r}(\mathbf{k}, \mathbf{p})$, then repeating the analysis of Section 2 yields an exact kinetic equation for $\mathcal{G}_r^{(s)}(\mathbf{k}, \mathbf{p}, \mathbf{p}'', t)$:

$$\left(\frac{\partial}{\partial t} - i \frac{\mathbf{k} \cdot \mathbf{p}}{M_r} \right) \mathcal{G}_r^{(s)} + \int_0^t d\tau \int d^3p' \varphi_r^{(s)}(\mathbf{p}, \mathbf{p}', \tau) \mathcal{G}_r^{(s)}(\mathbf{k}, \mathbf{p}', \mathbf{p}'', t - \tau) = 0 \tag{A.3}$$

where

$$\varphi_r^{(s)}(\mathbf{p}, \mathbf{p}', \tau) \equiv [M_r(\mathbf{p}')]^{-1} \langle e^{-i\mathbf{k} \cdot \mathbf{x}^{1r} \mathbf{F}^{1r}} \cdot \frac{\partial}{\partial \mathbf{p}^{1r}} \delta(\mathbf{p}' - \mathbf{p}^{1r}) e^{i\tau(1-P)} e^{i\mathbf{k} \cdot \mathbf{x}^{1r} \mathbf{F}^{1r}} \cdot \frac{\partial}{\partial \mathbf{p}^{1r}} \delta(\mathbf{p} - \mathbf{p}^{1r}) \rangle \tag{A.4}$$

and the projection operator P_r is defined by

$$P_r G(\mathbf{p}) \equiv \int d^3p' [M_r(\mathbf{p}')]^{-1} \langle G(\mathbf{p}) \delta f^{*}_{1r}(\mathbf{k}, \mathbf{p}', 0) \rangle \delta(\mathbf{p}' - \mathbf{p}^{1r}). \tag{A.5}$$

It should be noted that the "self-consistent field" terms do not arise in this equation since it characterizes single particle motions. Furthermore, the test particle density fluctuation does not couple directly to the collective density fluctuations $\delta g_s(\mathbf{k}, \mathbf{p}, t)$. [Such coupling terms are of order $1/N$ and vanish in the thermodynamic limit as $N \rightarrow \infty$, $V \rightarrow \infty$ such that $N/V = n$.] Hence choosing additional dynamical variables, e.g.

$$\mathbf{a}(\mathbf{p}) \equiv \text{col} \{ \delta f_{1r}, \delta g_s, \dots \} \tag{A.6}$$

will merely reproduce the test particle equation (A.3) decoupled from a set of collective kinetic equations for the correlation functions of $\delta g_s(\mathbf{k}, \mathbf{p}, t)$.

APPENDIX B: STATIC CORRELATION FUNCTIONS FOR MAXWELL FORCE LAWS

If one chooses a Maxwell force law such that

$$V_{rs}(r) = \frac{K_{rs}}{4r^4} \quad (\text{B.1})$$

then equations (44) and (50) become

$$D_{rs}(0) = 4\pi\Gamma\left(\frac{3}{2}\right)n_s K_{rs}^{1/4} / \sqrt{2}\beta^{7/4} \quad (\text{B.2})$$

$$D_{rs}^{33}(k) \cong D_{rs}(0) - \frac{13\pi\Gamma\left(\frac{3}{2}\right)n_s K_{rs}^{3/4} k^2}{15\sqrt{2}\beta^{5/4}} \quad (\text{B.3})$$

$$C_r^{44}(k) - n_s/\beta \cong \frac{\pi\Gamma\left(\frac{3}{2}\right) K_{rs}^{3/4} n_r n_s}{15\sqrt{2} \beta^{1/4}}. \quad (\text{B.4})$$