Modeled kinetic theories of one-component plasmas

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The general kinetic equation for the density-density correlation function $S(\vec{k},\omega)$, derived from projection-operator methods, provides a convenient framework for the modeling of collision processes in plasmas. We present results of the calculation of $S(\vec{k},\omega)$ for the dense one-component plasma utilizing four-collision models. In each case exact static-correlation data available from particle simulations are used as input to the calculation. Numerical results are presented and compared with "exact" results from computer experiments.

I. INTRODUCTION

The one-component plasma (OCP) is a simplified model of a real two-component plasma in which the electrons are assumed to provide a rigid, uniform charge-neutralizing background against ion fluctuations. The ions themselves are considered to be point Coulomb charges. The OCP is a useful model in the study of dense plasmas found in astrophysical environments (white dwarf interiors, neutron-star crustal layers, and the centers of Jovian planets) and the laboratory (the highly compressed plasma generated in inertial confinement fusion experiments, exploding wires, gas puffs, and pinch devices). Because of its simplicity, the OCP provides a useful benchmark model for the study of strongly coupled plasmas since it allows relatively easy access to otherwise unobtainable information.

The one-component plasma consists of N point nuclei of charge Ze and mass m embedded in a charge-neutralizing fluid (NZ points of charge $-e$ and mass m_e smeared into a continuous bath). To further specify the OCP and to relate the model to real physical plasmas, we need to define a few parameters. For an ion fluid of density $n=N/\Omega$ (Ω is the plasma volume), an appropriate scale of length, the ion sphere radius (or mean ion separation distance), is given by

$$a=(\tfrac{4}{3}\pi n)^{-1/3}.$$

Because of the $1/r$ nature of the Coulomb potential, the equilibrium properties of the OCP with temperature T which deviate from ideal gas behavior are governed by

$$\Gamma=(Ze)^2\beta/a,$$

where $\beta=(k_BT)^{-1}$; k_B is Boltzmann's constant. Γ is related to the usual plasma coupling parameter (taken as the inverse of the number of particles in the Debye sphere), ϵ, by

$$\epsilon=\frac{1}{4\pi n\lambda_D^3}=\sqrt{3}\,\Gamma^{3/2},$$

where $\lambda_D^2=(4\pi ne^2Z^2\beta)^{-1}$. Γ is therefore a measure of the amount of correlational (potential) energy in the plasma relative to the amount of kinetic energy present. With this relation we can see that the system will be strongly coupled if Γ is of order one or more. (It should be emphasized that while the distribution functions we use are equilibrium distributions; the $\Gamma\gtrsim 1$ condition can also exist in a dilute turbulent plasma.)

We wish to treat the ions by classical statistical mechanics. This requires that the thermal de Broglie wavelength be much less than the system scale length

$$\lambda_{dB}=(2\pi\hbar^2\beta/m)^{1/2}\ll a.$$

For the OCP model to be realistic, the neutralizing background of electrons must be uniform and rigid; i.e., the background cannot contribute to the dynamics of the ions or screen the ions. These conditions are met if the electrons are degenerate,

$$\frac{\beta^{-1}}{\epsilon_f}=\frac{\beta^{-1}}{(1.84m_ee^4/\hbar^2r_s^2)}\ll 1,$$

and the Thomas-Fermi screening length is large,

$$\frac{\lambda_{TF}}{a}=\frac{(\pi/12Z)^{1/3}}{\sqrt{r_s}}\gg 1.$$

Here $r_s=a/Z^{1/3}a_0$, where a_0 is the Bohr radius, is a measure of the electron density. The ions can still be treated classically because of the large mass difference. The OCP can now be defined by letting r_s go to zero and can be used as a basis for the study of realistic systems where r_s is approximately equal to zero. Since $\Gamma\propto 1/r_s$, this limit soon takes us into the regime of the strongly coupled plasma. An excellent review of the statistical properties of the OCP by Baus and Hansen[1] is available in the literature.

The OCP was first recognized as a viable dense plasma model by Salpeter.[2] The understanding of the system began with the numerical calculation by Brush, Sahlin, and Teller[3] of thermodynamic properties and pair distribution functions over a

wide range of the coupling parameter Γ. More recently, Hansen[4-5] has published much improved evaluations of these properties using Monte Carlo computer simulations. In addition there are available molecular-dynamics simulations of time-dependent properties of the OCP,[6] in particular the dynamic structure factor $S(\vec{k},\omega)$. If we consider the simulation data exact, we can use it to test the range of validity of various kinetic theoretical evaluations of $S(\vec{k},\omega)$.

In Sec. II we define the properties we wish to evaluate and recap the derivation of an exact kinetic equation for the density autocorrelation function. In the kinetic equation, the "collision term" can easily be identified and is modeled by four distinct methods. The results provided by these modeled theories are presented in Sec. III. In Sec. IV we draw some conclusions from these results.

II. THE KINETIC EQUATION

The quantity we wish to investigate in detail for the one-component plasma is the Fourier transformed density-density time correlation function $S(\vec{q},\omega)$ defined by

$$S(\vec{q},\omega)=\int d\vec{p}\,d\vec{p}'\int dt e^{i\omega t}\frac{1}{N}\langle\delta f(\vec{q}\vec{p}t)\delta f(-\vec{q}\vec{p}')\rangle, \tag{2.1}$$

where

$$f(\vec{q}\vec{p}t)=\int d\vec{r}\,e^{-i\vec{q}\cdot\vec{r}/a}f(\vec{r}\vec{p}t) \tag{2.2}$$

is the Fourier transform of the phase-space density for N particles,

$$f(\vec{r}\vec{p}t)=\sum_{i=1}^{N}\delta(\vec{r}-\vec{r}(t))\delta(\vec{p}-\vec{p}_i(t)) \tag{2.3}$$

(here $q=ka$, where a is the ion sphere radius). The fluctuation is defined by

$$\delta f(\vec{q}\vec{p}t)=f(\vec{q}\vec{p}t)-\langle f(\vec{q}\vec{p}t)\rangle. \tag{2.4}$$

In Eqs. (2.1) and (2.4) the equilibrium ensemble average of any function F is represented by

$$\langle F\rangle\equiv\frac{\int d\vec{p}^{N}d\vec{r}^{N}\prod_{i=1}^{N}M(p_i)e^{-\beta V_N(\vec{r}^{N})}F}{\int d\vec{r}^{N}\,e^{-\beta V_N(\vec{r}^{N})}}, \tag{2.5}$$

where $M(p)$ is the Maxwellian,

$$M(p)=(2\pi M/\beta)^{3/2}e^{-\beta p^2/2m}, \tag{2.6}$$

and $V(r)$ is the potential energy appearing in the Hamiltonian. We note that

$$\langle f(\vec{r}\vec{p}t)\rangle=nM(p). \tag{2.7}$$

$S(\vec{q},\omega)$ is directly proportional to the differential cross section ($d\sigma/d\Omega d\epsilon$, over solid angle and energy) for scattering for particles from a system interacting through a potential $V(r)$.[7] The correlation thus contains information about the internal physics of a system and is a measurable quantity. $S(\vec{q},\omega)$ is related to the imaginary part of the linear response function for density fluctuations by the fluctuation-dissipation theorem and is therefore a measure of the density response of a system influenced by an external force and describes the system transport coefficients or dissipation.[8] The mechanism of dissipation is the excitement of modes within the system, and the modes correspond physically to fluctuations. The static structure factor describes thermodynamic fluctuations and is related to the static linear response function.

From the Fourier inverse of Eq. (2.1) the equilibrium fluctuation correlation is found as

$$S(\vec{q},t=0)=S(\vec{q})=\int\frac{d\omega}{2\pi}S(\vec{q},\omega)=1+h(q), \tag{2.8}$$

which defines the total correlation function $h(q)$ in terms of the transformed radial distribution function $g(q)=1+h(q)$. It is this static correlation information available in the literature that we wish to use explicitly in evaluating $S(\vec{q},\omega)$. Until the simulations were performed, only low-density (weak-coupling) approximations to $S(q)$ could be found, and these formulations have been seen to be inadequate for strong coupling.

We will evaluate $S(\vec{q},\omega)$ from the framework of a memory function kinetic equation first derived by Akcasu and Duderstadt[9] using the Mori-Zwanzig projection operator technique.[10] The equation of motion for the phase-space density is written

$$\frac{\partial}{\partial t}\delta f(\vec{r}\vec{p}t)=i\mathcal{L}\delta f(\vec{r}\vec{p}t)=i[\delta f(\vec{r}\vec{p}t),H]_{PB}, \tag{2.9}$$

where the Liouville operator $\mathcal{L}$ is defined in Eq. (2.9) in terms of the system Hamiltonian and Poisson brackets. Fourier transforming in space, Laplace transforming in time via

$$f(\vec{q}\vec{p}z)=\int_0^\infty dt\,e^{izt}f(\vec{q}\vec{p}t), \tag{2.10}$$

multiplying by $f(-\vec{q}\vec{p}')$, and averaging yields the equation for the correlation

$$S(\vec{q}z\vec{p}\vec{p}')=i\left\langle\delta f(\vec{q}\vec{p})\frac{1}{z-\mathcal{L}}\delta f(-\vec{q}\vec{p}')\right\rangle. \tag{2.11}$$

$S(\vec{q},\omega)$ is obtained by integrating out the momenta in Eq. (2.11) and taking twice the real part of $S(\vec{q},z\to\omega+i0)$.

In Ref. 9 an operator $\mathcal{P}$ is defined so that when applied to an arbitrary function F, the part of F that correlates with the static phase-space fluc-

tuation is projected out, i.e.,

$$\mathcal{P}F = \int d\vec{p}\, d\vec{p}'\, \delta f(\vec{q}\vec{p}) S^{-1}(\vec{q}\vec{p}\vec{p}') \langle \delta f(-\vec{q}\vec{p}') F \rangle , \quad (2.12)$$

where $S^{-1}(\vec{q}\vec{p}\vec{p}')$ is defined by

$$\int d\vec{p}'' S(\vec{q}\vec{p}\vec{p}'') S^{-1}(\vec{q}\vec{p}''\vec{p}') = \delta(\vec{p} - \vec{p}') . \quad (2.13)$$

By defining the complementary operator $\mathcal{Q} = I - \mathcal{P}$, multiplying $\mathcal{L}$ in Eq. (2.11) by $\mathcal{P} + \mathcal{Q}$, and twice using the identity

$$\frac{1}{A-B} = \frac{1}{A} + \frac{B}{A}\frac{1}{A-B}, \quad (2.14)$$

one arrives at a (still exact) kinetic equation for the correlation,

$$\left(z - \frac{\vec{q}\cdot\vec{p}}{ma}\right) S(\vec{q}z\vec{p}\vec{p}') + \frac{\vec{q}\cdot\vec{p}}{ma} M(p) c(q) \int d\vec{p}'' S(\vec{q}z\vec{p}''\vec{p}')$$
$$- \int d\vec{p}'' \Phi(\vec{q}z\vec{p}\vec{p}'') S(\vec{q}z\vec{p}''\vec{p}') = iS(\vec{q}\vec{p}\vec{p}') . \quad (2.15)$$

The direct correlation $c(q)$ is defined by $[S(q) - 1]/S(q)$. Here

$$\Phi(\vec{q}z\vec{p}\vec{p}') = \frac{1}{nM(p')} \left\langle \mathcal{Q}\mathcal{L}\delta f(\vec{q}\vec{p}) \frac{1}{z - \mathcal{Q}\mathcal{L}\mathcal{Q}} \mathcal{Q}\mathcal{L}\delta f(-\vec{q}\vec{p}') \right\rangle . \quad (2.16)$$

The "memory function" defined in Eq. (2.16) can be identified as a collision term of the kinetic equation and it is this expression that we will approximate in order to solve Eq. (2.15).

III. THE COLLISION MODELS

In this section we will draw upon previous work in liquid kinetic theory and low-density plasma theory, extending and modifying the results so that the one-component plasma may be studied by these methods. The starting point is the general kinetic equation (2.15) for the Laplace transformed time correlation $S(\vec{q}z\vec{p}\vec{p}')$, where the collision term Φ must be approximated.

The first case we examine is the mean-field approximation corresponding to $\Phi(\vec{q}z\vec{p}\vec{p}') = 0$, that is, neglecting particle collisions altogether. The second case employs a Fokker-Planck-like collision model developed by Lenard and Bernstein.[11] The third model is based on a frequency-dependent collision term suggested by Linnebur and Duderstadt.[12] Our final case is based on an extension of this model due to Jhon and Forster.[13]

All of these models require the introduction of the static structure factor $S(q)$ in the solution. That is, all of the models assume the state structure of the system is known, and then approximate the subsequent dynamic behavior. The three nonzero collision terms also require the introduction of a parameter analogous to a collision frequency. Using these models we will solve the kinetic equation for $S(\vec{q}, \omega)$ and compare these results with those of particle dynamics simulations.[6,14]

A. The collisionless approximation

If $\Phi(\vec{q}z\vec{p}\vec{p}')$ in Eq. (2.15) is set equal to zero, the resulting equation assumes the form of the linearized Vlasov equation with an equilibrium correlation function in place of the bare transformed potential. The solution of this equation for the dynamic structure factor is known in terms of the plasma diepersion function.[15] The direct correlation function $c(q)$ enters as an effective potential, i.e., $V_{\text{eff}}(r) = -(n/\beta)c(r)$. If we let $V_{\text{eff}}(r)$ equal the bare Coulomb potential, we find that

$$c_{\text{DH}}(q) = -k_D^2 a^2/q^2 = -3\Gamma/q^2 ,$$

where $k_D^2 = 1/\lambda_D^2$. In this limit $S(q, \omega)$ becomes just the form given by the familiar linearized Vlasov form. This approximation for $c(q)$ is written here as $c_{\text{DH}}(q)$, since it is just the linearized Debye-Hückel (DH) form of the exact direct correlation. The DH form can also be shown to be the $q \to 0$ limit of the exact $c(q)$.

The form of $c(q)$ to order q^2 is[16]

$$c_{q^2}(q) = \frac{-3\Gamma}{q^2} + (1 + \chi_T^0/\chi_T) , \quad (3.1)$$

where χ_T is the isothermal compressibility and $\chi_T^0 = \beta/n$ is its ideal gas value. If the "exact" equation of state for the one-component plasma is taken from the computer data, $c_{q^2}(q)$ can easily be calculated as a improvement on $c_{\text{DH}}(q)$.

Figure 1 is a plot of the dynamic structure factor calculated from the mean-field approximation with both the $O(q^2)$—designated DH′—and "exact" Monte Carlo (MC) equilibrium values at two values of Γ and $q = ka$ versus the frequency in units of the plasma frequency ω_p. At these high values of Γ the close encounters characteristic of the dynamics of strong coupling are not considered in the approximation. This result is well known and is included here for comparison. See Ref. 6 for further discussion.

B. The Lenard-Bernstein model

It is apparent from the previous section that one has to account for the collisions between particles in a kinetic description of $S(\vec{q}, \omega)$ for strongly coupled OCP. A simple yet nontrivial method of accomplishing this is to apply a model due to Lenard and Bernstein.[11] This model is an approximation to the collision term in the Fokker-

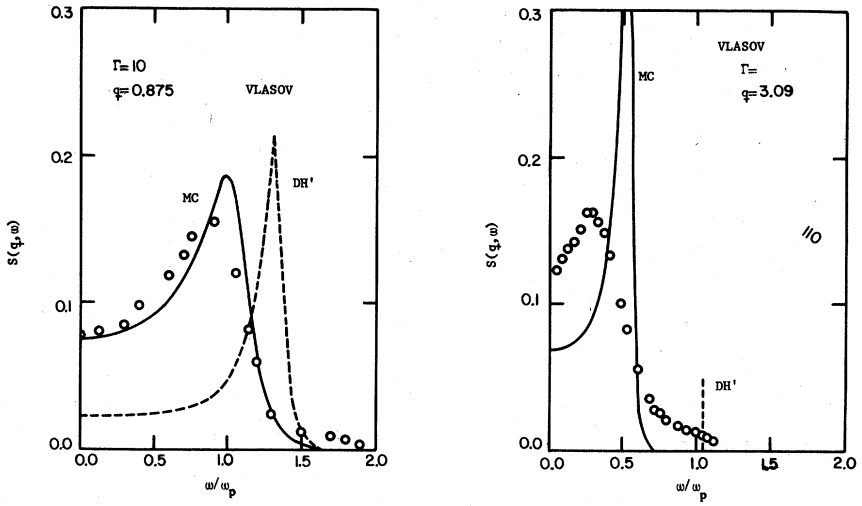

FIG. 1. $S(q,\omega)$ from Vlasov model using DH′ and MC statics at $\Gamma=10$, $q=2.31$ and $\Gamma=110$, $q=3.09$. The circles are the molecular dynamics data of Hansen (Ref. 6).

Planck (FP) equation familiar from conventional plasma physics.

The Fokker-Planck collision term is the result of the rate of change of an expansion of $S(\vec{r}t\vec{p}\vec{p}')$ in momentum transfer truncated after the first two terms. Thus it is a model for systems where small-angle scattering is important. The collision operator is

$$\Phi_{FP}(\vec{q}t\vec{p}\vec{p}') = -\left(\frac{\partial}{\partial\vec{p}}\cdot\vec{D}_1+\frac{\partial}{\partial\vec{p}}\cdot\frac{\partial}{\partial\vec{p}}D_2\right)\delta(\vec{p}-\vec{p}'), \tag{3.2}$$

where D_1 and D_2 are quantities that describe velocity space diffusion and dispersion. These, however, are functionals of the distribution and the kinetic equation is impossible to solve. The Lenard-Bernstein model approximates these terms by the mean collision time approach so that the collision term reads

$$\Phi_{FP}(\vec{q}t\vec{p}\vec{p}') = -\nu\frac{\partial}{\partial\vec{p}}\cdot\left(\frac{\partial}{\partial\vec{p}}+\frac{\beta}{m}\vec{p}\right)\delta(\vec{p}-\vec{p}'), \tag{3.3}$$

where ν is a particle collision frequency. It should be noted that this model can also be derived from the zero-time form of the collision term, $\Phi(\vec{q}\vec{p}\vec{p}'t=0)$. We will refer to this model as the Fokker-Planck (FP), small-angle collision approximation.

The lack of configuration space information in Φ_{FP} implies that the Fokker-Planck dynamic form factor $S_{FP}(\vec{q},\omega)$ cannot satisfy the third-moment sum rule (which is the equivalent of the first-moment sum rule for the collision term). All higher-order moments also remain unsatisfied. In addition, this collision model does not conserve energy and momentum.

The solution to the kinetic equation with Φ_{FP} can be obtained by a Fourier transform in momentum[17]:

$$S_{FP}(q,z)=\frac{S(q)}{2\pi}\frac{(a^2m\beta/q^2)\nu I(\kappa^2,s-1)}{1/S(q)-c(q)(a^2m\beta/q^2)iz\nu I(\kappa^2,s-1)}, \tag{3.4}$$

where $\kappa^2=q^2/m\beta\nu^2a^2$, $s=-iz/\nu$, and

$$I(\kappa^2,s)=e^{\kappa}\kappa^{-2(s+\kappa^2)}\int_0^{\kappa^2}d\mu\,\mu^{s+\kappa^2}e^{-\mu}. \tag{3.5}$$

From Eq. (3.2) it is obvious that letting $\nu\to 0$ returns the kinetic equation to the mean-field approximation. One can show[12] that in the limit of zero-collision frequency, the Vlasov results discussed in Sec. IIIA are recovered. A small-q expansion of Eq. (3.3) exposes a plasmon peak of finite width and intensity, these factors being governed by the collision frequency.

The choice of the collision frequency ν that we have introduced is critical to the appearance of the spectrum of $S_{FP}(q,\omega)$. From a Spitzer-calculated binary collision time, ν has the form

$$\frac{\nu_{sp}}{\omega_p}=\frac{1}{\sqrt{3\pi}}\Gamma^{3/2}\ln\left(\frac{\sqrt{3}}{\Gamma^{3/2}}\right), \tag{3.6}$$

which is evidently invalid when $\Gamma\gtrsim 0.1$. We have available, however,[5] the molecular dynamics calculated self-diffusion coefficient D_s and with an identity

$$\frac{\nu_s}{\omega_p}=(m\beta D_s)^{-1}\cong\frac{1}{8.85}\Gamma^{1/3}. \tag{3.7}$$

If we let $\nu=\nu_s$—an approximation that is certainly good at short times—we now have access to the strong-coupling regime. The results can be seen in Fig. 2.

Figure 2(a) shows that the addition of collisions

has damped and broadened the plasmon peak. The peak position has also shifted closer to the computer results. The damping, however, is excessive. Figure 2(b) reveals the great improvement of the Fokker-Planck approximation over the mean-field approximation in high-Γ plasmas. At lower Γ, the spectra of the FP and Vlasov kinetic equations are quite similar at large q. In more strongly coupled systems the Vlasov spectrum has an increasingly anomalous form out to large-q values. The use of the FP collision term provides a more accurate approximation to the actual spectrum.

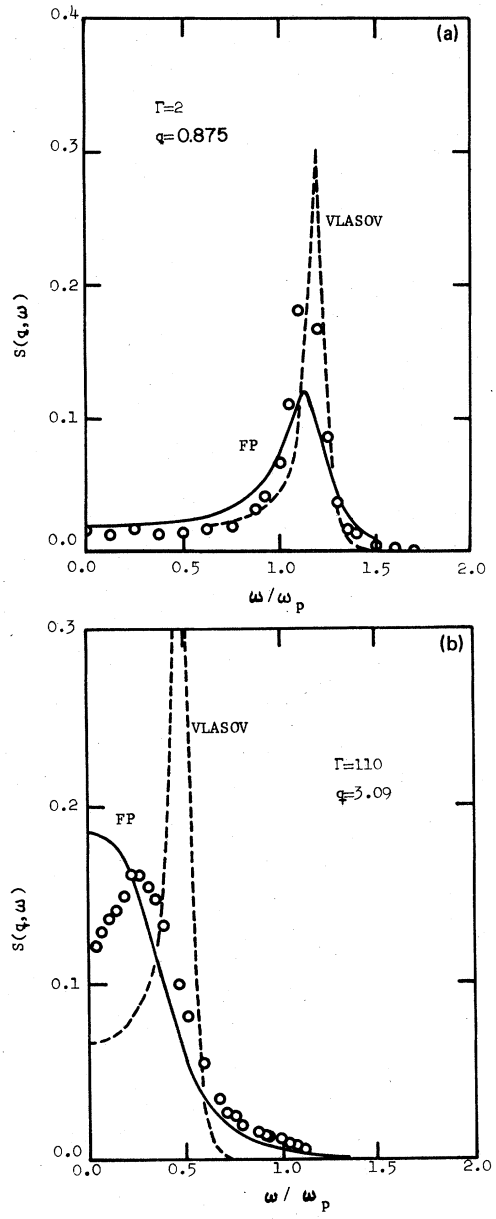

FIG. 2. $S(q,\omega)$ from FP and Vlasov models using MC statics at $\Gamma=2$, $q=0.875$ and $\Gamma=110$, $q=3.09$.

C. The Duderstadt-Akcasu-Linnebur model

The first two models for Φ do not satisfy the third moment sum rule for $S(\vec{q},\omega)$. If we return to the exact expression for $\Phi(\vec{q}z\vec{p}\vec{p}')$, Eq. (2.16), and expand in powers of $1/z$, retaining only the first term, we have

$$\Phi^0(\vec{q}z\vec{p}\vec{p}')\equiv\frac{1}{z}\langle f(\vec{q}\vec{p})\mathcal{L}\mathcal{Q}\mathcal{L}f(-\vec{q}\vec{p}')\rangle\frac{1}{nM(p')}. \quad (3.8)$$

Since Eq. (3.8) is the first nonvanishing term in the correct high-frequency expansion of Φ, it must be the first correct term in the short-time expansion of the collision term. Thus substituting $\Phi^0(\vec{q}z\vec{p}\vec{p}')$ in Eq. (2.15) results in an equation for $S(q,\omega)$ that satisfies the first-, second-, and third-moment sum rules of $S(q,\omega)$. This ensures a more accurate representation of $S(q,\omega)$ at high frequencies.

The quantity in brackets in Eq. (3.8) is related to a force-force correlation function. This time-independent quantity is found to be[9]

$$\Phi^0(\vec{q}z\vec{p}\vec{p}')zM(p')=\left(\frac{\partial}{\partial\vec{p}}\cdot\underline{D}(0)\cdot\frac{\partial}{\partial\vec{p}}\delta(\vec{p}-\vec{p}')+\frac{\partial}{\partial\vec{p}}\cdot\underline{A}(q)\cdot\frac{\partial}{\partial\vec{p}'}M(p)\right)M(p'), \quad (3.9a)$$

where

$$\underline{D}(0)=\frac{n}{\beta}\int dr\ V(r)\vec{\nabla}\vec{\nabla}h(r), \quad (3.9b)$$

and

$$\underline{A}(q)=-\underline{D}(0)+\vec{q}\vec{q}[c(q)/\beta+V(q)]/\beta\times\frac{-n}{\beta}\int d\vec{r}(e^{-i\vec{q}\cdot\vec{r}/a}-1)h(r)\vec{\nabla}\vec{\nabla}V(r). \quad (3.9c)$$

The $z\to 0$ (long time) limit of $\Phi(\vec{q}z\vec{p}\vec{p}')$ cannot be handled by the high-z approximation made to obtain Eq. (3.9). Duderstadt and Akcasu[18] have suggested modeling the time dependence of $\Phi(\vec{q}t\vec{p}\vec{p}')$ with a single relaxation-time exponential, i.e.,

$$\Phi(\vec{q}t\vec{p}\vec{p}')=e^{-\alpha(q)t}\Phi^0(\vec{q}\vec{p}\vec{p}').$$

This idea was extended by Akcasu and Linnebur[19] to a two-relaxation-time approximation—each of the terms in Eq. (3.9) damped in time by an exponential with a distinct damping constant. This model was later applied to two-component plasmas of intermediate density by Linnebur and Duderstadt.[12]

We will define the Duderstadt-Akcasu-Linnebur (DAL) collision term as

$$\Phi_{\mathrm{DAL}}(\vec{q}z\vec{p}\vec{p}')M(p') = \frac{1}{z+i\alpha^s(q)}\frac{\partial}{\partial\vec{p}}\cdot\underline{D}(0)\frac{\partial}{\partial\vec{p}}\delta(\vec{p}-\vec{p}')M(p') + \frac{1}{z+i\alpha^d(q)}\frac{\partial}{\partial\vec{p}}\cdot\underline{A}(q)\cdot\frac{\partial}{\partial\vec{p}}M(p)M(p'), \quad (3.10)$$

where $1/\alpha^s(q)$ is the relaxation time for the "self" term and $1/\alpha^d(q)$ is the relaxation time for the distinct term. Then inserting Φ_{DAL} in Eq. (2.15), we can solve for the dynamic structure factor as

$$S_{\mathrm{DAL}}(q,z) = \frac{S(q)}{2\pi}\frac{(a^2m\beta/q^2)w(q,z)I(\kappa^2,s-1)+(a^2m\beta/q^2)y(q,z)\Delta(q,z)}{1/S(q)-c(q)(a^2m\beta/q^2)izw(q,z)I(\kappa^2,s-1)-(a^2m\beta/q^2)izy(q,z)\Delta(q,z)}, \quad (3.11)$$

where

$$\Delta(q,z) = \frac{a^2m\beta}{q^2}izw(q,z)I(\kappa^2,s-1)-1, \quad (3.12a)$$

$$w(q,z) = \frac{1}{z+i\alpha^s(q)}\frac{\beta}{m}D(0), \quad (3.12b)$$

and

$$y(q,z) = \frac{1}{z+i\alpha^d(q)}A(q). \quad (3.12c)$$

The relaxation parameters appearing in Eqs. (3.10)–(3.12) can be found by comparing limiting results of $S_{\mathrm{DAL}}(q,\omega)$ with known expressions of the exact $S(q,\omega)$. In order that $S_{\mathrm{DAL}}(q,\omega)$ reduce to correct free particle and hydrodynamic forms, the α's are chosen as

$$\alpha^{s,d}(q) = \alpha_0(1+q^2/q_{s,d}^2),$$

where α_0 is known in terms of a transport coefficient involving a collision frequency. The terms q_s and q_d are not independent and q_s is chosen to be the Debye length normalized by the ion sphere radius ($q_s = a\lambda_D$). The details involving these choices can be found in Refs. 12 and 19.

In Eq. (3.11) it is easy to see the $S_{\mathrm{DAL}}(q,\omega)$ goes to $S_{\mathrm{FP}}(q,\omega)$ when $y(q,z)$ goes to zero and $w(q,z)$ is set equal to ν. For large q, $S_{\mathrm{DAL}}(q,\omega)$ and $S_{\mathrm{FP}}(q,\omega)$ will be similar due to damping of $w(q,z)$ and $y(q,z)$. The same is true at very high frequency. At small q, however, the forms of these dynamic structure factors are noticeably different in strongly coupled one-component plasmas. At high Γ, $c(q)$ in $A(q)$ is quite different from $-\beta V(q)$ so that $A(q)$ is non-negligible.

We must choose two transport coefficients as input to the solution of $S_{\mathrm{DAL}}(q,\omega)$. As with the Fokker-Planck operator, this requires the choice of a collision frequency (or a self-diffusion coefficient). In addition, a form for the shear viscosity η_s must be available for the computation of q_d in $\alpha^d(q)$.[20] Here we will follow the same philosophy with η_s as with ν, since for Γ greater than about one, molecular dynamics data for the transverse current correlation provides a fit for $\eta_s(\Gamma)$ in the OCP.[17] For Γ less than about one we will fit from the Spitzer expression

$$\eta_s = \frac{0.96n}{\nu_{sp}}, \quad (3.13)$$

where ν_{sp} is the usual binary collision frequency Eq. (3.6).

The integral appearing in Eq. (3.9c) is easily evaluated in the small-q limit for the Debye-Hückel correlation. The calculation can be rendered accurately at any value of q if the integration is performed numerically. Numerical methods must be employed when the Monte Carlo equilibrium data is used as input.

Figure 3 compares all three models we have examined in the intermediate coupling range for two values of $q = ka$. The similarities of the Fokker-Planck (FP) and Duderstadt-Akcasu-Linnebur (DAL) are apparent in the results as are these models' distinction from the sharper and somewhat ill-positioned Vlasov resonance. For this value of Γ and relatively large values of q ($q \gtrsim 3$), all models predict results nearly identical with the computer simulations. For Γ's of 100 or more, the model results are still distinct at much larger wave numbers ($q \gtrsim 6$) with the mean-field approximation disastrously inaccurate.

Figure 4 shows results at $\Gamma = 155$, very near the liquid-solid transition. At $q = 3.09$, a value at which the mean-field model would give good results for low Γ, the Vlasov model is quite useless. The Fokker-Planck spectrum indicates that it is very near to the ideal gas limit. Only the DAL model manages to reveal evidense of the broadened, shifted plasmon peak.

The Fokker-Planck model conserves particle number only; it does not conserve momentum. The Duderstadt-Akcasu-Linnebur model, however, does conserve momentum. This difference might be expected to show up at small wave numbers. Indeed at $\Gamma = 155$ and $q = 0.875$, the difference in results is tremendous (Fig. 5). The Vlasov equation gives results for these ranges of Γ and q that are essentially delta functions and are not indicated on the plots.

The $S_{\mathrm{FP}}(q,\omega)$ and $S_{\mathrm{DAL}}(q,\omega)$ spectra are not uniformly accurate when compared to the particle

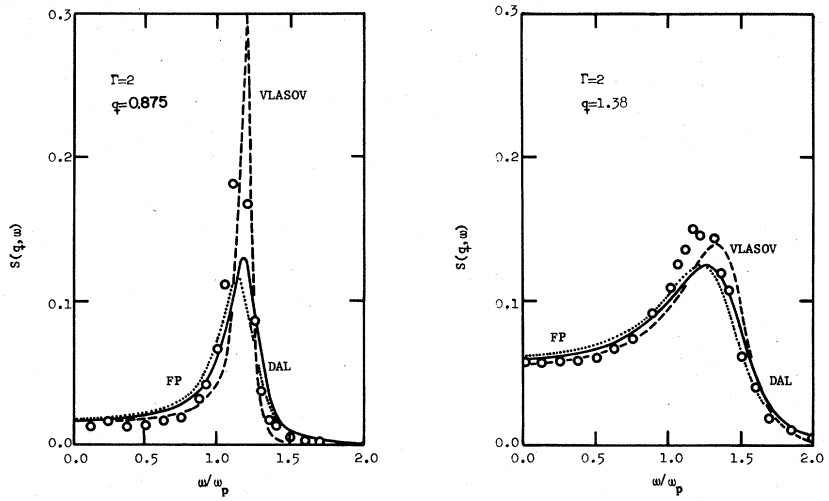

FIG. 3. $S(q,\omega)$ from DAL, FP, and Vlasov models using MC statics at $\Gamma=2$, $q=0.875$, and $q=1.38$.

simulation results. The major influence in this respect is the choice of the collision frequency. The theory behind the derivation of the binary collision frequency breaks down explicitly in the neighborhood of $\Gamma=1$. An examination of the Monte Carlo data shows that the influence of high densities and low temperatures on statistical quantities in the vicinity of $\Gamma=1$ is considerable. Thus ν_{sp} is probably not a good parameter in this region. In addition, $\Gamma=1$ is the lower limit of the usefulness of the fitting formula for D_s.

Another factor to consider is the approximation to a collision frequency appropriate to the full phase-space density by a parameter derived from a coefficient defined for the test-particle case. The collisional part of the kinetic equation for the test-particle fluctuation is similar to Eq. (2.16) with $\delta f(\vec{qp})$ replaced by $\delta f_{\text{self}}(\vec{qp})$ and Φ replaced by Φ_{self}. As far as the dynamics are concerned we can use parameters of the test-particle fluctuation equation in the self part of the phase-space fluctuation equation only at times near zero or in the low-density, weak-coupling limit. Thus the DAL model may be of even greater utility with the presentation of a Monte Carlo calculated full-density collision time.

Alternatively, if we assume the Duderstadt-Akcasu-Linnebur model to be nearly exact, the collision frequency can be found as a fitting parameter to the particle simulation results. Thus it is possible to obtain some information on a transport coefficient through the DAL approximation,

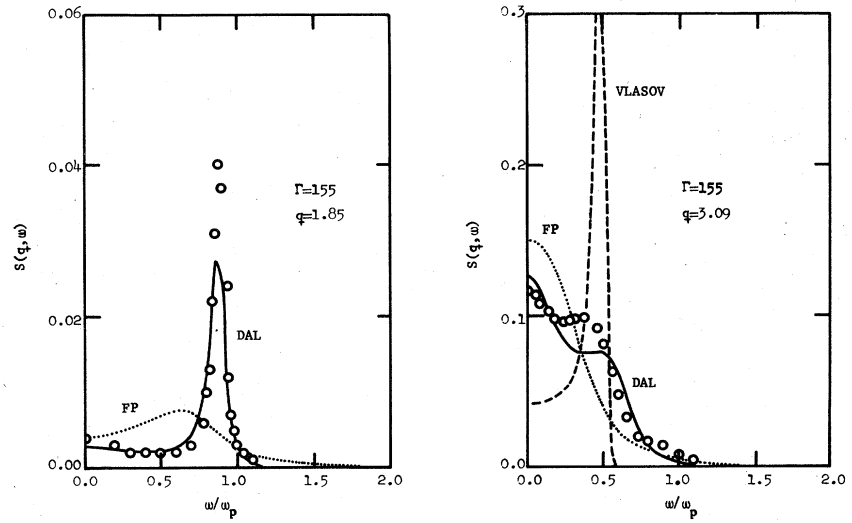

FIG. 4. $S(q,\omega)$ from DAL, FP, and Vlasov models at $\Gamma=155$, $q=1.85$, and $q=3.09$.

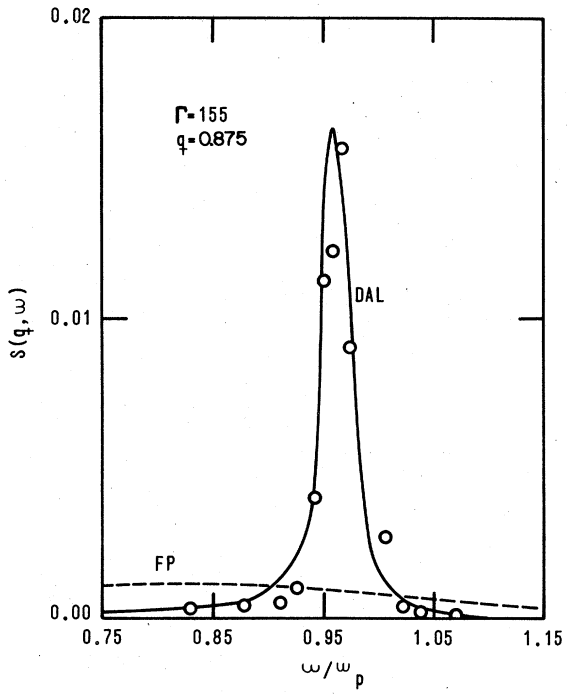

FIG. 5. $S(q,\omega)$ from DAL and FP models at $\Gamma=155$, $q=0.875$.

but the method appears arduous. Since the Fokker-Planck collision term does not conserve momentum, one hardly expects to obtain any information on, for example, the viscosity. The DAL collision term does conserve momentum but does not conserve energy, so one cannot use this approximation to study the thermal conductivity, for example.

D. The Jhon-Forster collision term

The Duderstadt-Akcasu-Linnebur collision term does not conserve energy. However, Jhon and Forster[13] have extended the model by adding a hydrodynamic variable corresponding to energy into the projection operator scheme. More precisely, define the energy density as

$$\epsilon(\vec{r},t)=\int d\vec{p}\,\frac{p^2}{2m}f(\vec{r}\vec{p}t)+\tfrac{1}{2}\sum_{i\neq j}V(|\vec{r}_i(t)-\vec{r}_j(t)|)\delta(\vec{r}-\vec{r}_i(t)) \tag{3.14}$$

and $\delta\epsilon(\vec{r},t)=\epsilon(\vec{r},t)-\langle\epsilon(\vec{r},t)\rangle$. Returning now to Sec. II, we can rederive the kinetic equation for the vector $|\delta f,\delta\epsilon\rangle$ instead of $|\delta f\rangle$ alone. Equation (2.15) then becomes an equation of motion for the correlation matrix of density *and* energy-density fluctuations.

Defining

$$G_{ab}(\vec{r}-\vec{r}',t-t',\vec{p}\vec{p}')=\langle\delta a(\vec{r}\vec{p}t)\delta b(\vec{r}'\vec{p}'t')\rangle, \tag{3.15}$$

we must find a kinetic equation for the correlation matrix

$$\begin{pmatrix} G_{ff}(\vec{r}-\vec{r}',t-t',\vec{p}\vec{p}') & G_{f\epsilon}(\vec{r}-\vec{r}',t-t',\vec{p}) \\ G_{\epsilon f}(\vec{r}-\vec{r}',t-t'\vec{p}') & G_{\epsilon\epsilon}(\vec{r}-\vec{r}',t-t') \end{pmatrix} \tag{3.16}$$

using a projection operator [similar to Eq. (2.12)]

$$\mathcal{P}_{f\epsilon}=(|\delta f\rangle,|\delta\epsilon\rangle)\begin{pmatrix} G_{ff}^{-1}(0) & G_{f\epsilon}^{-1}(0) \\ G_{\epsilon f}^{-1}(0) & G_{\epsilon\epsilon}^{-1}(0)\end{pmatrix}\begin{pmatrix}\langle\delta f| \\ \langle\delta\epsilon|\end{pmatrix}. \tag{3.17}$$

$S(\vec{q},z)$ is the double momentum integral of $i\langle\delta f(z-\mathcal{L})^{-1}\delta f\rangle$ which is now one component $[G_{ff}(\vec{q},z)]$ of the matrix in Eq. (3.16) and depends explicitly on correlations between density and energy as well as energy-energy correlations.

The same operations involved in deriving the kinetic equation (2.15) for $S(\vec{q}z\vec{p}\vec{p}')$ produce an analogous formulation for the correlation matrix. The new high-frequency memory function [see Eq. (3.8)] is

$$\Phi^0_{\mathfrak{J}F}(\vec{q}z\vec{p}\vec{p}')=\frac{1}{z}\langle\delta f(\vec{q}\vec{p})\delta\epsilon(\vec{q})|\mathcal{L}\mathcal{Q}_{f\epsilon}\mathcal{L}|\delta f(-\vec{q}\vec{p}')\delta\epsilon(-\vec{q})\rangle\frac{1}{nM(p')}, \tag{3.18}$$

where $\mathcal{Q}_{f\epsilon}=I-\mathcal{P}_{f\epsilon}$. The terms in Eq. (3.18) can be calculated (in a straightforward if hardly concise manner) by inserting the projector from Eq. (3.17) (see Ref. 13). The terms can then be separated and distinct damping coefficients added in the same manner that led to Eq. (3.10).

The collision term $\Phi(\vec{q}z\vec{p}\vec{p}')$, using the double-relaxation-time approximation for the dynamics (a modification of Ref. 13), becomes

$$\begin{aligned}\Phi_{\mathfrak{J}F}(\vec{q}z\vec{p}\vec{p}')M(p')=&\frac{1}{z+i\alpha^s(q)}\frac{\partial}{\partial\vec{p}}\cdot\underline{D}(0)\cdot\frac{\partial}{\partial\vec{p}'}\delta(\vec{p}-\vec{p}')M(p')+\frac{1}{z+i\alpha^d(q)}\frac{\partial}{\partial\vec{p}}\cdot[\underline{A}(\vec{q})+\underline{A}'(\vec{q})+\underline{B}(\vec{q},z)]\cdot\frac{\partial}{\partial\vec{p}'}M(p)M(p')\\&+B'_{ijlm}(\vec{q},z)(p_ip_j-\delta_{ij})(p'_lp'_m-\delta_{lm})M(p)M(p')\\&+B''_{ij}(\vec{q},z)[\vec{q}\cdot\vec{p}(p'_ip'_j-\delta_{ij})+\vec{q}\cdot\vec{p}'(p_ip_j-\delta_{ij})]M(p)M(p').\end{aligned} \tag{3.19}$$

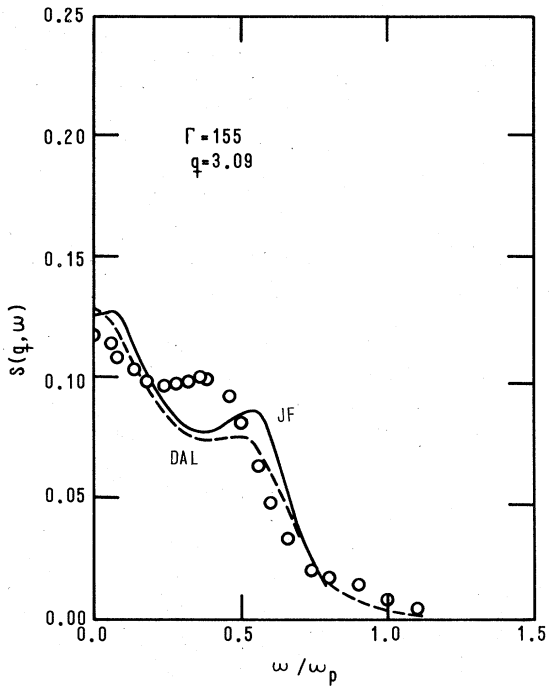

FIG. 6. $S(q,\omega)$ from JF and DAL models at $\Gamma=155$, $q=3.09$.

One can show that

$$\lim_{z\to 0}\lim_{q\to 0}\int d\vec{p}\,\frac{p^2}{2m}\Phi_{JF}(\vec{q}z\vec{p}\vec{p}')\to 0\,.$$

The terms $B(q,z)$, $B'(q,z)$, $B''(q,z)$, and $A'(q)$ contain the energy density fluctuation information not present in the DAL model. This information is provided, however, at a cost. These added terms in Φ_{JF} contain quantities involving static correlations of higher than second order that must be approximated. In addition, another transport coefficient—the thermal conductivity—must be used as input much as the viscosity was used to define unknown parameters in the DAL model. Jhon and Forster did find that $S(\vec{q},\omega)$ calculated using Φ_{JF} was in good agreement with experimental data on liquid argon.

If the unknown equilibrium correlations are approximated by their thermodynamic limits and allowance is made for wavelength dependence, we can use an exact equation of state to determine these quantities. In this case the terms in Eq. (3.18) containing all information incorporating energy-energy, energy-momentum, and energy-number density coupling are found to be small except when the value of Γ is very high. The kinetic equation for $S(\vec{q}z\vec{p}\vec{p}')$ can then be solved by kinetic modeling in the partial basis of the hydrolike Hermite polynomials in momentum.

At small values of the coupling, $S_{JF}(q,\omega)$ $=S_{DAL}(q,\omega)$ to within roughly a percent for all values of q. At larger Γ, $S_{JF}(q,\omega)$ reduced to $S_{DAL}(q,\omega)$ for sufficiently small q, but may be superior to $S_{DAL}(q,\omega)$ for intermediate q ranges. An example of this occurence is given in Fig. 5. For large Γ *and* large wave number, the Jhon-Forster calculated structure factor becomes aberrant at small frequencies. For higher frequencies the energy terms do not provide as significant a contribution—they are damped as $1/z$ or $1/z^2$. At the higher values of q, the approximations we have made to evaluate some of the static correlations are invalid. Thus the $\omega\to 0$ limit of $S_{JF}(q,\omega)$—where the energy terms are significant—is suspect at large q.

The Jhon-Forster model does provide a slight improvement in the spectrum over the Duderstadt-Akcasu-Linnebur model, but at a greatly increased cost in the amount of work that must be done to obtain the result. It has already been demonstrated for a two-component plasma that the extension of a Fokker-Planck-type collision model to a full particle number-, momentum-, and energy-conserving model (the BGK model[21]) provides only slight variances in the spectrum of $S(q,\omega)$ in the collisional domain.[22] This is an indication of the fact that in a plasma—especially a one-component plasma—the high-frequency plasmon oscillations do not couple efficiently with the low-frequency heat modes. That is, the density-energy density fluctuations [and the energy-energy fluctuations via $\delta f(\vec{r}\vec{p}t)-\delta\epsilon(\vec{r}t)$ coupling] contribute little to the dynamic structure factor. At small q, the heat mode intensity is $O(q^2)$ relative to the plasma mode so there is essentially no coupling at very long wavelengths. This point has been nicely illustrated by Baus.[23]

IV. CONCLUSIONS

The collision approximations employed in Sec. III all are capable of using exact computer-evaluated static correlations as input to the solution of $S(\vec{q},\omega)$. This allows the use of the results in the region of strong coupling in plasma.

In the course of this study we found that the mean-field or Vlasov approximation, which completely ignores the dynamics of the memory function, is not adequate for long wavelengths or large coupling. The Fokker-Planck-like Lenard-Bernstein model allows the inclusion of dynamics in the simple form of a collision time. As long as small wave numbers are avoided and the collision frequency is derived from available molecular dynamics data, the spectrum of $S(\vec{q},\omega)$ is improved dramatically. The Fokker-Planck approximation, however, does not satisfy the col-

lisional invariant of momentum, hence the anomalous results at long wavelength.

The exact calculation of the collision term to second order in frequency modified by the inclusion of two unknown relaxation times—a model that does satisfy conservation of momentum—is relatively easy to accomplish. This modified Duderstadt-Akcasu-Linnebur (DAL) model makes use of more known computer information (via the "exact" shear viscosity) and gives results that are in very good agreement with simulation calculations over a wide range of wave number and coupling.

The Jhon-Forster (JF) model is an extension of the DAL interpolation model to include the energy collision invariant. Due to the fact that the OCP is dominated by the plasma oscillations and that charge and mass fluctuations in the OCP are equivalent, the energy modes do not couple efficiently to the mass density modes. The consequence is that the JF model provides only slight improvement over the DAL model except at very large coupling and very small wave number. The amount of calculational effort expended in procuring this slight advantage along with the need to obtain yet another transport coefficient and still unavailable static correlations indicate that the JF solution is more extensively approximated and not as efficient as the DAL calculation. The results can even be worse for shorter wavelengths.

The DAL model solution of $S(\vec{q}, \omega)$ is analytic and easy to compute. The result is dependent on explicitly known (and readily available) static density-density correlations and two transport coefficients, which can be reasonably approximated. We have shown that the model provides a good representation of $S(\vec{q}, \omega)$ over a wide range of wave number, frequency, and coupling.

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[1]M. Baus and J. P. Hansen, Phys. Rep. 59, 1 (1980).
[2]E. E. Salpeter, Astrophys. J. 134, 669 (1961).
[3]S. G. Brush, H. L. Sahlin, and E. Teller, J. Chem. Phys. 45, 2102 (1966).
[4]J. P. Hansen, Phys. Rev. A 8, 3096 (1973).
[5]E. L. Pollock and J. P. Hansen, Phys. Rev. A 8, 3110 (1973).
[6]J. P. Hansen, I. R. McDonald, and E. L. Pollock, Phys. Rev. A 11, 1025 (1975).
[7]L. Van Hove, Phys. Rev. 95, 249 (1954); M. N. Rosenbluth and N. Rostoker, Phys. Fluids 5, 776 (1962).
[8]L. Kadanoff and P. Martin, Ann. Phys. (N.Y.) 24, 419 (1963).
[9]A. Z. Akcasu and J. J. Duderstadt, Phys. Rev. 188, 479 (1969).
[10]R. Zwanzig, *Lectures in Theoretical Physics*, edited by N. W. Brittin (Wiley, New York, 1961).
[11]A. Lenard and I. B. Bernstein, Phys. Rev. 112, 1456 (1958).
[12]E. Linnebur and J. J. Duderstadt, Phys. Fluids 16, 665 (1973).
[13]M. Jhon and D. Forster, Phys. Rev. A 12, 254 (1975).
[14]J. P. Hansen (private communication).
[15]M. Nelkin and S. Ranganathan, Phys. Rev. 164, 222 (1967).
[16]P. Vieillefosse and J. P. Hansen, Phys. Rev. A 12, 1106 (1975).
[17]J. L. Lebowitz, J. K. Percus, and J. Sykes, Phys. Rev. 188, 487 (1969).
[18]A. Z. Akcasu and J. J. Duderstadt, Phys. Rev. A 1, 905 (1970); 2, 1097 (1970).
[19]A. Z. Akcasu and E. Linnebur, *Neutron Inelastic Scattering* (IAEA, Vienna, 1972).
[20]Following the notation (see Ref. 16) that the shear viscosity always dominates the bulk viscosity in the OCP.
[21]P. L. Bhatnager, E. P. Gross, and M. Krook, Phys. Rev. 94, 511 (1954).
[22]E. Leonard, Ph.D. thesis, University of Michigan, 1973 (unpublished).
[23]M. Baus, Physica (Utrecht) 79A, 377 (1975).