Dynamic structure factors in two-component plasmas

R. Cauble
Berkeley Research Associates, P.O. Box 582, Springfield, Virginia 22151

D. B. Boercker
Lawrence Livermore National Laboratory, University of California, Livermore, Livermore, California 94550
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The general kinetic equation for the charge-charge structure factor of a fully ionized strongly coupled hydrogen plasma is solved in three distinct collision approximations. The equilibrium correlation functions necessary to these solutions are provided by solution of the hypernetted-chain integral equation in which an effective pair potential has been used to take into account short-range quantum effects. The results are compared with molecular-dynamics simulations of the plasma using the effective pair potential and with a hierarchical approach involving known sum rules.

I. INTRODUCTION

Theoretical investigations into the properties of dense plasmas have benefited greatly from the results of computer simultations of model systems. The simplest of these models is the classical one-component plasma (OCP), which is a system of classical ions embedded in a uniform neutralizing background. Monte Carlo[1,2] and molecular-dynamics[3] simulations of the OCP have guided theoretical pursuits and have provided benchmarks for analytic calculations of its properties, which are now well understood.[4,5]

The OCP is, however, a very simplified model of a real plasma and is applicable only to systems which are so dense that the electrons are completely degenerate. When the electrons are nondegenerate, they can no longer be pictured as a uniform, rigid background, and the OCP becomes an inappropriate model. Under these conditions, one must treat both the electrons and ions as particles. A reasonable model which does this is the two-component plasma (TCP).

In the TCP the electrons and ions are treated as classical (quasi) particles that interact through effective potentials which deviate from pure Coulombic behavior at short distances in a way that simulates the essential quantum diffraction effects. A specific form for such a potential is the one suggested by Deutsch.[6] If α and β are species labels, and if

$$\lambda\!\!\!^{-}_{\alpha\beta}\equiv\hbar/(2\pi\mu_{\alpha\beta}k_BT)^{1/2}\ ,$$

where $\mu_{\alpha\beta}$ is the reduced mass of this interacting pair, then Deutsch's potential is

$$v_{\alpha\beta}(r)=\frac{Z_\alpha Z_\beta e^2}{r}\left[1-\exp\left[-\frac{r}{\lambda\!\!\!^{-}_{\alpha\beta}}\right]\right]\ . \tag{1}$$

This potential remains finite at the origin, and, therefore, prevents the collapse of the system. It is expected to give reasonable results for nondegenerate plasmas with temperatures above the ionization potential and coupling parameters less than about 2, or

$$\Gamma=\beta e^2/a\lesssim 2\ ,$$

where $a^3=3/4\pi n=r_s^3a_0^3$ and a_0 is the Bohr radius.

The TCP is more difficult to simulate than the OCP, but recently Hansen and McDonald[7,8] have published results of molecular-dynamics (MD) analyses of a fully ionized hydrogen TCP using the effective potential in Eq. (1). Among the properties calculated from the simulation data is the dynamic charge-charge structure factor $S_{QQ}(k,\omega)$. As the Fourier transform of the charge-density–charge-density time-correlation function, $S_{QQ}(k,\omega)$ reflects in its shape the spectrum of longitudinal modes in the plasma. The motivation of this paper is to use the simulation data of Ref. 8 as a reference against which various kinetic theoretical calculations of $S_{QQ}(k,\omega)$ can be tested. A similar study[9] has already been made for the OCP; the intention here is to generalize that work to two components.

The type of theories of interest here are microscopic theories based upon formally exact kinetic equations derived from the projection operator[10–12] or other techniques.[13–16] A general characteristic of such theories is the separation of the so-called "memory" operator into a static mean field or Vlasov term and a frequency-dependent collision term. Calculations of density fluctuations in dense plasmas, using just such a theory, were performed several years ago by Linnebur and Duderstadt.[17] Unfortunately, they were unable to estimate the short-range part of the direct correlation functions appearing in the memory operator and had to approximate those correlations by their Debye-Hückel limits. We are now able to calculate the direct correlation functions using the potential in Eq. (1) in the so-called hypernetted-chain (HNC) equation.[18,19] This is an approximate integral equation method for calculating static correlation functions which has proven to be accurate for plasmas in which the coupling parameter is of order unity,[4] and produces excellent agreement with the static properties calculated by computer simulations in Ref. 8. The proposal here, then, is to generate the HNC direct correlation functions and use them in the model kinetic theories described in Ref. 17.

In Sec. II, we define the quantities of interest and review the basic kinetic-theory concepts involved. Calculations based upon three different collision models are presented in Sec. III, and in Sec. IV we present our conclusions.

II. KINETIC EQUATION

For a hydrogen plasma the dynamic charge-charge structure factor is defined by

$$S_{QQ}(k,\omega)=\frac{e^2}{2}[S_{ii}(k,\omega)-2S_{ei}(k,\omega)+S_{ee}(k,\omega)] , \tag{2}$$

where the partial density correlation functions $S_{\alpha\beta}(\vec{k},\omega)$ with $\alpha,\beta=i,e$ are given by

$$S_{\alpha\beta}(k,\omega)=\int d\vec{p}\,d\vec{p}\,'\frac{1}{2\pi}\int dt\,e^{i\omega t}\frac{1}{N}\langle f_\alpha(k;\vec{p},t)f_\beta(-k;\vec{p}\,',t)\rangle\equiv\int d\vec{p}\,d\vec{p}\,'\int dt\,e^{i\omega t}S_{\alpha\beta}(k,t;\vec{p},\vec{p}\,') . \tag{3}$$

Here

$$f_\alpha(\vec{k};\vec{p},t)=\int d\vec{r}\,e^{-i\vec{k}\cdot\vec{r}}f_\alpha(\vec{r};\vec{p},t) \tag{4}$$

is the Fourier transform of the phase-space density

$$f_\alpha(\vec{r};\vec{p},t)=\sum_{j=1}^{N}\delta(\vec{r}-\vec{r}_j^{\,\alpha}(t))\delta(\vec{p}-\vec{p}_j^{\,\alpha}(t)) . \tag{5}$$

In Eq. (3), N is the number of ions in the system and angular brackets indicate an average over the equilibrium ensemble. It is not customary to calculate $S_{\alpha\beta}(\vec{k},\omega)$ directly, but rather to find it from

$$S_{\alpha\beta}(\vec{k},\omega)=2\,\mathrm{Re}\int d\vec{p}\,d\vec{p}\,'\tilde{S}_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,') , \tag{6}$$

where the Laplace transform function $\tilde{S}_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,')$ is

$$\tilde{S}_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,')=\int_0^\infty dt\,e^{izt}S_{\alpha\beta}(\vec{k},t;\vec{p},\vec{p}\,') . \tag{7}$$

The advantage is that the functions $\tilde{S}_{\alpha\beta}$ can be found from the solution to a coupled set of kinetic equations of the form[17]

$$\left[z-\frac{\vec{p}\cdot\vec{k}}{m_\alpha}\right]\tilde{S}_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,')+\frac{\vec{p}\cdot\vec{k}}{m_\alpha}M_\alpha(p)\sum_{\gamma=e,i}c_{\alpha\gamma}(k)\int d\vec{p}\,''\tilde{S}_{\gamma\beta}(\vec{k},z;\vec{p}\,'',\vec{p}\,')$$
$$-\sum_{\gamma=e,i}\int d\vec{p}\,''\Phi_{\alpha\gamma}(\vec{k},z;\vec{p},\vec{p}\,'')\tilde{S}_{\gamma\beta}(\vec{k},z;\vec{p}\,'',\vec{p}\,')=iS_{\alpha\beta}(\vec{k},t=0;\vec{p},\vec{p}\,') . \tag{8}$$

In Eq. (8), $M_\alpha(p)$ represents the Maxwell-Boltzmann distribution function (normalized to unity), and the $c_{\alpha\beta}$'s are the direct correlation functions defined by the Ornstein-Zernike relations

$$c_{\alpha\beta}(k)=h_{\alpha\beta}(k)-\sum_{\gamma=e,i}c_{\alpha\gamma}(k)h_{\gamma\beta}(k) , \tag{9}$$

where

$$h_{\alpha\beta}(k)=S_{\alpha\beta}(k)-\delta_{\alpha\beta} \tag{10}$$

and

$$S_{\alpha\beta}(k)=\int d\vec{p}\,d\vec{p}\,'S_{\alpha\beta}(k,t=0;\vec{p},\vec{p}\,') \tag{11}$$

are the static partial structure factors. [Note that in Eqs. (9) and (10) a factor of ion density has been absorbed into the usual definitions.] The effects of collisions are contained in the operators $\Phi_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,')$. Formally, exact expressions exist for these operators, but they will not be presented here. Instead, we will simply present results based upon various models for them.

Before proceeding we note for future convenience that, analogous to the single-species case,[13] Eq. (8) can be solved formally to obtain the Laplace-transformed functions

$$\tilde{S}_{\alpha\beta}(\vec{k},z)=\int d\vec{p}\,d\vec{p}\,'\tilde{S}_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,') \tag{12}$$

in terms of the functions

$$\tilde{J}_{\alpha\beta}(\vec{k},z)=\int d\vec{p}\,d\vec{p}\,'\tilde{J}_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,') , \tag{13}$$

where the $\tilde{J}_{\alpha\beta}$'s are solutions to the simplified kinetic equations

$$\left[z-\frac{\vec{p}\cdot\vec{k}}{m_\alpha}\right]\tilde{J}_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,')-\sum_{\gamma=e,i}\int d\vec{p}\,''\Phi_{\alpha\gamma}(\vec{k},z;\vec{p},\vec{p}\,'')\tilde{J}_{\gamma\beta}(\vec{k},z;\vec{p}\,'',\vec{p}\,')=M_\alpha(p)\delta(\vec{p}-\vec{p}\,')\delta_{\alpha\beta} . \tag{14}$$

Specifically, the results for a system of electrons and ions are

$$\tilde{S}_{ee}(\vec{k},z)=\frac{i}{E(\vec{k},z)}(E_i(\vec{k},z)[\tilde{J}_{ee}(\vec{k},z)S_{ee}(k)+\tilde{J}_{ei}(\vec{k},z)S_{ie}(k)]$$
$$+\{c_{ei}(k)-z[\tilde{J}_{ee}(\vec{k},z)c_{ei}(k)+\tilde{J}_{ei}(\vec{k},z)c_{ii}(k)]\}$$
$$\times[\tilde{J}_{ie}(\vec{k},z)S_{ee}(\vec{k})+\tilde{J}_{ii}(\vec{k},z)S_{ie}(k)]) \quad (15)$$

and

$$\tilde{S}_{ei}(\vec{k},z)=\frac{i}{E(\vec{k},z)}(E_e(\vec{k},z)[\tilde{J}_{ii}(\vec{k},z)S_{ie}(k)+\tilde{J}_{ie}(\vec{k},z)S_{ee}(k)]$$
$$+\{c_{ei}(k)-z[\tilde{J}_{ii}(\vec{k},z)c_{ie}(k)+\tilde{J}_{ie}(\vec{k},z)c_{ee}(k)]\}$$
$$\times[\tilde{J}_{ee}(\vec{k},z)S_{ee}(k)+\tilde{J}_{ei}(\vec{k},z)S_{ie}(k)]) , \quad (16)$$

where the functions $E_\alpha(\vec{k},z)$ and $E(\vec{k},z)$ are defined by

$$E_\alpha(\vec{k},z)=1-c_{\alpha\alpha}(k)+z[\tilde{J}_{\alpha\alpha}(\vec{k},z)c_{\alpha\alpha}(k)+\tilde{J}_{\alpha\beta}(\vec{k},z)c_{\beta\alpha}(k)], \quad \alpha\neq\beta \quad (17)$$

$$E(\vec{k},z)=E_e(\vec{k},z)E_i(\vec{k},z)-\{c_{ei}(k)-z[\tilde{J}_{ee}c_{ei}(k)+\tilde{J}_{ei}c_{ii}(k)]\}\{c_{ie}(k)-z[\tilde{J}_{ii}c_{ie}(k)+\tilde{J}_{ie}c_{ee}(k)]\} . \quad (18)$$

Various models for the collision operators will generate different approximations to the $\tilde{J}_{\alpha\beta}$'s. Using these in Eqs. (15) and (16), and their counterparts with the labels e and i interchanged will give estimates of the dynamic structure factors. These collision models will be studied in Sec. III.

III. COLLISION MODELS

In this section we will examine the charge-charge structure factors predicted by three different models for $\Phi_{\alpha\beta}$ and compare them to the MD results of Ref. 8. All three models will require as input the direct correlation functions $c_{\alpha\beta}(k)$ which will be obtained from the solution to the two-component HNC equation with the potential in Eq. (1). The first and simplest model we will investigate is the collisionless or generalized Vlasov model in which $\Phi_{\alpha\beta}=0$. The second model employs a simple Fokker-Planck–type collision operator developed by Lenard and Bernstein.[20] The final model is one suggested by Duderstadt and Akcasu[21] which incorporates the exact high-frequency behavior of $\Phi_{\alpha\beta}$ and models its time dependence by simple exponential decay.

A. Generalized Vlasov model

In this model we simply neglect $\Phi_{\alpha\beta}$ in Eq. (14) to obtain

$$\tilde{J}_{\alpha\beta}(\vec{k},z)=\delta_{\alpha\beta}[1+\chi_\alpha(\vec{k},z)]/z , \quad (19)$$

where

$$\chi_\alpha(\vec{k},z)=\int d\vec{p}\,\frac{(\vec{k}\cdot\vec{p}/m_\alpha)M_\alpha(p)}{z-\vec{k}\cdot\vec{p}/m_\alpha} \quad (20)$$

is the plasma response function. Substituting Eq. (19) into Eqs. (15) and (16) yields the usual random-phase approximation (RPA) results for $\tilde{S}_{\alpha\beta}(k,z)$ with one important difference. The results presented here contain the exact static correlation functions rather than their Debye-Hückel limits.

Taking these functions from HNC data, we calculated $S_{QQ}(k,\omega)$ for $\Gamma=0.5$ and $r_s=0.4$ at the same values of q $(=ka)$ used in the MD runs.[8] The results are shown in Fig. 1 where the standard RPA curves are presented for

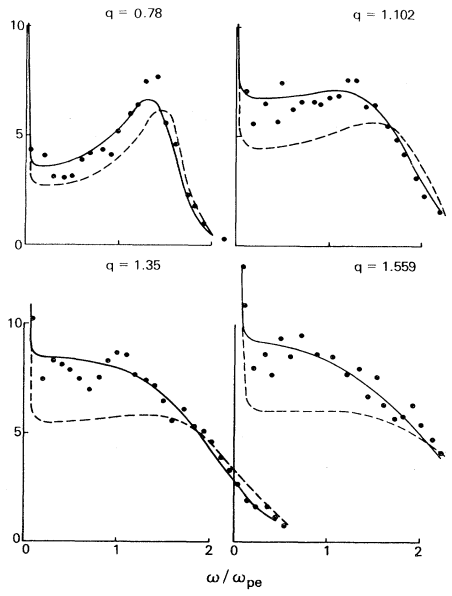

FIG. 1. $S_{QQ}(k,\omega)$ ($\times 100$) as a function of ω/ω_{pe} for four values of $q=ka$ at $\Gamma=0.5$ and $r_s=0.4$. ●, MD results; — — —, Vlasov spectrum; ——, generalized Vlasov with HNC statics.

comparison (the ordinate has been scaled by a factor of 100). It appears quite clear that even at the smaller values of the wave number q, where the collective modes will begin to exhibit evidence of dissipation not available in this collisionless model, that the generalized Vlasov results are in good agreement with the MD data.

Although this mean-field approximation may provide an adequate model of $S_{QQ}(k,\omega)$ for $\Gamma \leq 0.5$ (as long as $q \gtrsim 0.78$), it does not give a good representation of the charge-charge spectrum at $\Gamma=2$ unless q is restricted to large values. For appropriate comparison with MD results at this value of the coupling, we must introduce a reasonable approximation for $\Phi_{\alpha\beta}$ in Eq. (14) and solve for $\tilde{J}_{\alpha\beta}$.

B. Fokker-Planck model

A simple model for $\Phi_{\alpha\beta}$ that introduces an interparticle collision frequency ν and allows an analytic solution to Eq. (14) is[20]

$$\Phi^{\mathrm{FP}}_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,') = i\frac{m_\alpha}{\beta}\delta_{\alpha\beta}\nu_{\alpha\beta}\frac{\partial}{\partial\vec{p}}\cdot\left[\frac{\partial}{\partial\vec{p}}+\frac{\beta}{m_\alpha}\vec{p}\right]\delta(\vec{p}-\vec{p}\,') . \tag{21}$$

Substituting this approximate collision term into Eq. (14) and Fourier transforming in momentum allows one to find[13]

$$\tilde{J}_{\alpha\beta}(\vec{k},z)=\delta_{\alpha\beta}\tilde{K}_\alpha(k,z) , \tag{22}$$

where

$$\tilde{K}_\alpha(k,z)=-(i\beta m_\alpha\nu_{\alpha\alpha}/k^2)I_\alpha(Q^2,s_\alpha-1) \tag{23}$$

and

$$I_\alpha(Q^2,s_\alpha)=Q_\alpha^{-2(Q_\alpha^2+s_\alpha)}e^{Q_\alpha^2}\int_0^{Q_\alpha^2}dx\,e^{-x}x^{(Q_\alpha^2+s_\alpha)} . \tag{24}$$

In the above, $Q_\alpha^2=k^2/\beta m_\alpha\nu_{\alpha\alpha}^2$ and $s_\alpha=-iz/\nu_{\alpha\alpha}$.

Having introduced two collision frequencies ν_{ee} and ν_{ii} into our solution for $S_{QQ}(\vec{k},\omega)$ to allow for collisional damping, we must now select them with some care. It is well known that the ordinary Spitzer-type binary-collision times are inappropriate in moderately to strongly coupled plasmas. We can, however, utilize transport coefficients found directly from the molecular-dynamics simulations to obtain estimates of the required collision frequencies. In particular, using the self-diffusion coefficients given by Hansen and McDonald,[8] these frequencies are seen to be

$$\frac{\nu_{ee}^{\mathrm{MD}}}{\omega_{pe}}=\frac{1}{m_e\beta D_e}=\frac{1}{3\Gamma D_e^*}$$

and (25)

$$\frac{\nu_{ii}^{\mathrm{MD}}}{\omega_{pe}}=\left[\frac{m_e}{m_i}\right]^{1/2}\frac{1}{3\Gamma D_i^*} .$$

Collisions are found to be of negligible importance for $S_{QQ}(k,\omega)$ at $\Gamma=0.5$. They are, however, necessary when describing $S_{QQ}(k,\omega)$ at larger values of coupling. In Fig. 2 we compare the collisionless generalized Vlasov model calculations (using "correct" HNC-evaluated direct correlation functions) with the results employing $\nu_{\alpha\alpha}^{\mathrm{MD}}$ from Eq. (25) in the Fokker-Planck solution for the case $\Gamma=2$, $r_s=1$. From the figure it is clear that the model including collisions provides a much superior fit to the MD data than the collisionless model. For values of q smaller than 0.78, the discrepancy is still larger, indicating the failure of mean-field (RPA) descriptions of strongly coupled systems in the collective regime.

Even though the Fokker-Planck (FP) model considerably improves the shape of the spectrum, the electron peak intensity for the FP curve, which is a sensitive function of $\nu_{\alpha\alpha}$, falls below the MD data points at peak. In addition, the peak position is lower in frequency than is shown by the simulation. To correct this deficiency we must consider a different collision model.

C. Duderstadt-Akcasu-Linnebur (DAL) model

Neither of the first two models discussed above satisfies the fourth frequency-moment sum rule of $S_{QQ}(k,\omega)$. This sum rule will, however, be automatically satisfied by any model collision operator which incorporates the known high-frequency behavior of $\Phi_{\alpha\beta}$. One such model is that suggested by Duderstadt and Akcasu,[21] and later applied to weakly coupled two-component plasmas by Linnebur and Duderstadt,[17] in which the time dependence of $\Phi_{\alpha\beta}$ is modeled by two relaxation times. We define the DAL collision operator as

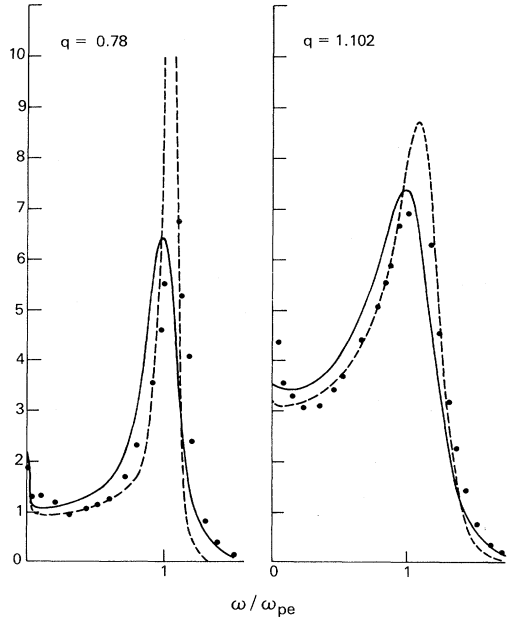

FIG. 2. $S_{QQ}(k,\omega)$ for two values of q at $\Gamma=2$, $r_s=1$. ●, MD results. — — —, generalized Vlasov with HNC statics; ——, FP model.

$$\Phi^{\mathrm{DAL}}_{\alpha\beta}(\vec{k},z;\vec{p},\vec{p}\,') = i\delta_{\alpha\beta}\frac{D_\alpha(0)}{z+ia^s_{\alpha\alpha}(k)}\frac{\partial}{\partial\vec{p}}\cdot\left[\frac{\partial}{\partial\vec{p}}+\frac{\beta}{m_\alpha}\vec{p}\right]\delta(\vec{p}-\vec{p}\,') + \frac{i}{z+ia^d_{\alpha\beta}(k)}M_\alpha(p)\vec{p}\cdot\overleftrightarrow{A}_{\alpha\beta}(\vec{k})\cdot\vec{p}\,' , \tag{26}$$

where

$$D_\alpha(0)=D_{\alpha\alpha}(0)+D_{\alpha\beta}(0),\quad \alpha\neq\beta \tag{27}$$

$$D_{\alpha\beta}(0)=\frac{1}{3\beta}\int d\vec{r}\,g_{\alpha\beta}(r)\nabla^2 v_{\alpha\beta}(r) , \tag{28}$$

and

$$\overleftrightarrow{A}_{\alpha\beta}(\vec{k})=\frac{\vec{k}\vec{k}}{m_\alpha m_\beta}c_{\alpha\beta}(k) - \frac{\beta}{m_\alpha m_\beta}\int d\vec{r}\,g_{\alpha\beta}(r)e^{i\vec{k}\cdot\vec{r}}\vec{\nabla}\vec{\nabla}v_{\alpha\beta}(r) . \tag{29}$$

The decay constants $a^s_{\alpha\beta}(k)$ and $a^d_{\alpha\beta}(k)$ are chosen to obtain the correct short and long time, as well as the known large and small wave-number limits of $S_{\alpha\beta}(\vec{k},\omega)$.

Using Eq. (26) in Eq. (14) and once again Fourier transforming in momentum leads to

$$\tilde{J}_{ee}(\vec{k},z)=\frac{\tilde{K}_e\left[1-\frac{im_i^2}{k^2}zy_{ii}\Delta_i\right]-\frac{im_e^2}{k^2}y_{ee}\Delta_e+\frac{m_e^2m_i^2}{k^4}z(y_{ei}^2-y_{ee}y_{ii})\Delta_e\Delta_i}{1-\frac{im_i^2}{k^2}zy_{ii}\Delta_i-\frac{im_e^2}{k^2}zy_{ee}\Delta_e+\frac{m_e^2m_i^2}{k^4}z^2(y_{ei}^2-y_{ee}y_{ii})\Delta_e\Delta_i} \tag{30}$$

and

$$\tilde{J}_{ei}(\vec{k},z)=\frac{im_em_i}{k^2}\frac{y_{ei}\Delta_e\Delta_i}{1-\frac{im_i^2}{k^2}zy_{ii}\Delta_i-\frac{im_e^2}{k^2}zy_{ee}\Delta_e+\frac{m_e^2m_i^2}{k^4}z^2(y_{ei}^2-y_{ee}y_{ii})\Delta_e\Delta_i} , \tag{31}$$

where $\tilde{K}_\alpha$ is defined as in Eq. (23), but with $\nu_{\alpha\alpha}$ replaced by $w_{\alpha\alpha}(k,z)$ which is given by

$$w_{\alpha\alpha}(k,z)=\frac{\beta}{m_\alpha}\frac{D_\alpha(0)}{z+ia^s_{\alpha\alpha}(k)} . \tag{32}$$

The remaining functions appearing in Eq. (31) are

$$y_{\alpha\beta}(\vec{k},z)\equiv\frac{1}{z+ia^d_{\alpha\beta}(k)}\hat{k}\cdot\overleftrightarrow{A}_{\alpha\beta}(\vec{k})\cdot\hat{k} \tag{33}$$

and

$$\Delta_\alpha\equiv zK_\alpha-1 . \tag{34}$$

The form of the damping functions is chosen to be

$$a^{s,d}_{\alpha\beta}(k)=a_{\alpha\beta}(0)[1+(k/k^{s,d}_{\alpha\beta})^2] , \tag{35}$$

where the unknown parameters $a_{\alpha\beta}(0)$ and $k^{s,d}_{\alpha\beta}$ are determined from known k and ω constraints on $S_{\alpha\beta}(k,\omega)$.[21,22] With these restrictions we are required to choose only two other collision frequencies to complete the description of the DAL model. Those coefficients are the electron-ion and ion-electron collision frequencies ν_{ei} and ν_{ie}, characterizing momentum transfer between particles.

We can find ν_{ei} from the coefficient of electrical conductivity provided by the MD data,

$$\frac{\nu_{ei}^{\mathrm{MD}}}{\omega_{pe}}=\frac{\omega_{pe}}{4\pi\sigma}=\frac{1}{4\pi\sigma^*} . \tag{36}$$

As an alternative to using the simulation derived conductivity to find ν_{ei}, we can employ a quantum-kinetic-theory treatment of plasma time-correlation functions[23] which leads directly to the calculation of the electrical conductivity.[24] This treatment can be thought of as a quantum generalization of the fully renormalized kinetic theory of Mazenko[15] in which the disconnected approximation (DA), is used to renormalize the potential terms in the collision operator. The application of this approximation to strongly coupled plasmas has been discussed in Ref. 23 and elsewhere.[25,26] More recently the theory has led to numerical evaluations of σ (or ν_{ei}, which we label ν_{ei}^{DA}) for the cases under consideration here.[27] We can estimate ν_{ee}^{DA} by taking

$$\nu_{ee}^{\mathrm{DA}}=\frac{\nu_{ee}^{\mathrm{MD}}}{\nu_{ei}^{\mathrm{MD}}}\nu_{ei}^{\mathrm{DA}} .$$

The collision frequencies are collected in Table I for the cases used in the simulation runs. The results employing the DAL model with MD and DA collision frequencies for a $\Gamma=2$, $r_s=1$ TCP are given in Fig. 3. At low k, it is apparent that the fits are superior to the FP model in peak position as well as the intensity of the resonance. At small

TABLE I. Collision frequencies (in units of ω_{pe}) derived from molecular-dynamics transport coefficients [MD, Eqs. (25) and (36)] and calculated from the disconnected approximation [DA, Ref. 27, Eq. (41)].

	$\Gamma=0.5,\ r_s=0.4$	$\Gamma=0.5,\ r_s=1$	$\Gamma=2,\ r_s=1$
ν_{ee}^{MD}	0.054	0.093	0.135
ν_{ee}^{DA}	0.111	0.225	0.201
ν_{ei}^{MD}	0.022	0.037	0.073
ν_{ei}^{DA}	0.045	0.090	0.109

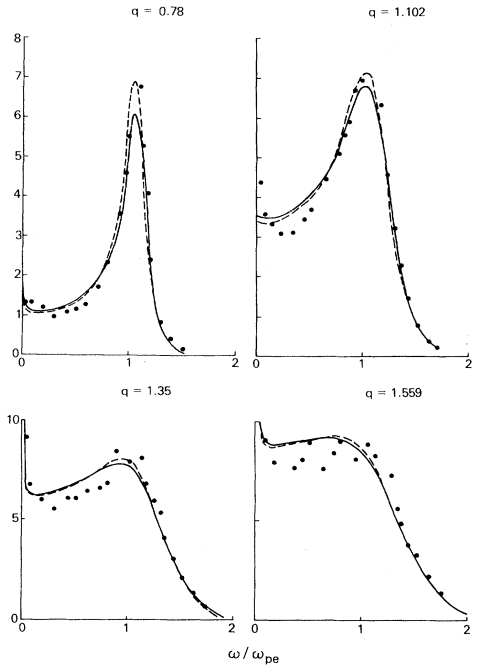

FIG. 3. $S_{QQ}(k,\omega)$ for four values of q at $\Gamma=2$, $r_s=1$. ●, MD results. Curves are DAL model results with $\nu=\nu^{DA}$ (dashes) and $\nu-\nu^{MD}$ (solid).

wavelengths the generalized Vlasov solution is nearly identical with those of the collision models, indicating the lack of importance of collisions in this regime.

In their paper, Hansen and McDonald[8] developed a memory function theory (MFT) based on the work of Abramo *et al.*[28] to describe the charge-fluctuation spectra obtained in the MD simulations. This theory builds a hierarchy of memory functions for linear combinations of momentum-integrated microscopic particle densities defined in terms of known sum rules. The hierarchy is truncated at the highest order in which the sum rules can be exactly calculated using two-particle radial distribution functions (the fourth-order sum rule). The highest-order memory functions are damped in time by an exponential or Gaussian approximation employing relaxation times defined, again, by the known sum rules.

The advantage of "MFT" lies in the fact that only two relaxation times are required and that these constants are determined within the framework of sum-rule calculations. The DAL model, on the other hand, requires the determination of four independent relaxation times by introducing four transport coefficients. However, since these time constants interpolate between hydrodynamic and Vlasov behavior, a knowledge of the needed transport coefficients (which can be accurately found from MD simulations or quantum kinetic theory) ensures correct small-k, small-ω limits of $S_{QQ}(k,\omega)$. The charge-fluctuation spectra predicted by the DAL model and MFT are very similar for all of the cases under consideration here (see Figs. 6 and 8 of Ref. 8). Results of $S_{\alpha\alpha}(k,\omega=0)$ for these models are collected in Table II.

As noted above, one may expect differences to occur at longer wavelengths where the DAL model has used transport coefficients to ensure correct hydrodynamic behavior. In Fig. 4 we present a comparison of MFT with the DAL model using values of the collision frequencies obtained from MD transport coefficients and the quantum-theoretical treatment with the disconnected approximation at $q=0.307$. The MFT results were taken from Figs. 9 and 10 of Ref. 8. The DAL model using ν^{MD} predicts a plasma peak of greater intensity and lower frequency than the MFT calculations. The DAL model using the larger values of ν^{DA} predicts a smaller intensity and a peak position closer to MFT. Differences between these theoretical approaches can be expected to increase as q is made smaller still. Unfortunately, there are no MD results at these wave numbers to indicate which is the preferable theoretical prediction.

IV. DISCUSSION

The collision approximations we have investigated for describing the TCP all utilize equilibrium correlation data

TABLE II. $S_{QQ}(k,\omega=0)$ for DAL, FP, and generalized Vlasov (GV) and Vlasov (V) collisionless models compared with MFT and MD simulation data. $\nu_{\alpha\beta}^{MD}$ was used in the DAL and FP calculations.

	$S_{QQ}(k,\omega=0)$											
	$\Gamma=0.5$, $r_s=0.4$						$\Gamma=0.5$, $r_s=1$					
q	MD	MFT	DAL	FP	GV	V	MD	MFT	DAL	FP	GV	V
0.78	0.26	0.32	0.31	0.31	0.31	0.39	0.33	0.40	0.35	0.36	0.35	0.39
1.10	0.86	0.79	0.78	0.78	0.77	0.80	0.85	0.83	0.79	0.79	0.78	0.80
1.35	1.20	1.26	1.21	1.23	1.21	1.17	1.28	1.22	1.18	1.18	1.16	1.17
1.56	1.45	1.60	1.59	1.60	1.58	1.38	1.80	1.51	1.48	1.48	1.45	1.38

	$S_{QQ}(k,\omega=0)$ $\Gamma=2$, $r_s=1$					
q	MD	MFT	DAL	FP	GV	V
0.78	0.02	0.025	0.022	0.022	0.021	0.064
1.10	0.07	0.045	0.036	0.036	0.033	0.16
1.35	0.21	0.15	0.13	0.12	0.12	0.29
1.56	0.40	0.32	0.29	0.29	0.29	0.39

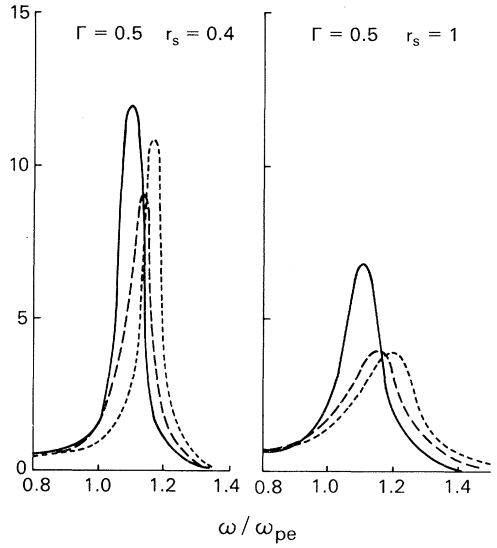

FIG. 4. Comparison of model results at $\Gamma=0.5$ for $q=0.307$. ----, MFT results of Hansen and McDonald; — — —, DAL model with $\nu=\nu^{DA}$; ——, DAL model with $\nu=\nu^{MD}$.

as input to the solutions. The data have been shown[8] to be accurate and easily obtained from the solution of the hypernetted-chain integral equations using the Deutsch potential as the effective interparticle interaction. We have used these data in all models considered with the exception of the usual Vlasov approximation.

As has already been shown,[8] the standard Vlasov equation, which contains neither collisional dynamics nor correct initial time-correlation information, does not reproduce any of the MD spectra accurately. The generalized Vlasov equation, in which the Fourier transform of the potential in the mean-field term is replaced by the exact direct correlation function, provides a reasonable fit to the data at $\Gamma=0.5$ for all r_s and q values simulated. This approximation is also adequate for large wave numbers at higher values of the coupling parameter.

At the higher value of Γ considered here, it is necessary to include collisions in order to damp the strongly spiking plasmon peak. The Fokker-Planck—type Lenard-Bernstein model approximates these effects by introducing two self-collision times into the solution of $S_{QQ}(k,\omega)$. Even though these constants are well known, the resulting spectra are only qualitatively similar to the MD data at smaller values of q. As we have noted, the FP term does not satisfy the fourth frequency moment sum rule. In addition, the collisional invariant of momentum is not satisfied by this model.[29]

The DAL model does incorporate exact sum rules up to fourth order and does satisfy conservation of momentum, leading to much improved results at low q in the case of large coupling.[30] The implementation of several relaxation times allows the collision dynamics to be interpolated from known hydrodynamic ($k\rightarrow 0,\omega\rightarrow 0$) forms of $S_{\alpha\beta}(k,\omega)$ to their Vlasov and free-particle forms. This approximate form of the collision term depends on the accuracy of the acquired hydrodynamic coefficients, but is seen here to give a good description of the MD charge-fluctuation spectra. This description is very similar to the MFT calculations except at low wave number where the interpolative DAL model should represent the spectra resonances as accurately as the transport coefficients provided. For all cases of Γ less than about 2 and q sufficiently large, the distinctions are negligible.

The primary limitation in this process in the accurate calculation of the radial distribution functions from the HNC procedure. This implies that the best solutions will arise from the most inclusive effective interionic potential. The Deutsch potential, Eq. (1), is not valid for Γ greater than about 2, but the HNC scheme should give reasonable distribution functions for a more general effective potential. From these functions relaxation times can be derived and used in the DAL collision term to provide accurate predictions of dynamic correlation functions in more strongly coupled two-component plasmas over a wide range of k and ω.

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