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Numerical simulation of the dynamic structure factor of a two-component model plasma

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Abstract

Using molecular dynamics simulations we investigate the dynamic structure factor $S(k, \omega)$ of a two-component model plasma where the Coulomb interaction is regularized at short distances. New simulation results are presented and discussed, and they are used to verify different theoretical treatments: the standard random-phase approximation, a dynamic local field correction with input from HNC calculations and a new approach, which includes a dynamic collision frequency via the Mermin ansatz.

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1. Introduction

Many real plasmas, such as hydrogen or electron–hole systems, can be modelled by the two-component plasma (TCP) of two species of charged particles. It has, however, to be treated by quantum mechanics. A classical description is made possible by regularizing the Coulomb interaction at short distances which avoids the Coulomb collapse in the classical limit. Molecular dynamics (MD) simulations are a powerful tool to investigate such strongly coupled TCP-like systems and to verify results of analytical treatments. Here, we consider a two-component model plasma (TCMP) defined as a system of two species α (e.g. electrons e and ions i) with masses m_α and charges q_α and pair interactions $V_{\alpha\beta}$ ($r = |\boldsymbol{r}_\alpha - \boldsymbol{r}_\beta|$) which are finite at small distances, i.e. $\lim_{r\to 0} V_{\alpha\beta}(r) = C_{\alpha\beta} < \infty$, and merge into the Coulomb interaction at distances which are large compared to the mean inter-particle spacing a, i.e. $V_{\alpha\beta}\ (r \gg a) \sim q_\alpha q_\beta/(4\pi\epsilon_0 r)$. These TCP-like systems have a well-defined classical limit. In this paper, we consider interactions of the specific form

$$V_{\alpha\beta}(r) = \frac{q_\alpha q_\beta}{4\pi\epsilon_0 r}\left[1 - \exp\left(-\frac{r}{\lambda_{\alpha\beta}}\right)\right] \tag{1}$$

which is motivated by the quasi-classical effective interactions derived by, e.g. Kelbg [1] and

Deutsch [2] from quantum-statistical expressions. But here we take it as a definition of our model and the $\lambda_{\alpha\beta}$ as given, external parameters.

In the following, we assume a hydrogen-like TCMP with $q_i = -q_e = e$ and charge neutrality, $n_i = n_e = n$. In equilibrium, at density n and temperature T, and in the classical limit ($\hbar \to 0$), the system is completely characterized by the scaled parameters $\lambda_{\alpha\beta}/a$ of the interactions (1) and the coupling parameter $\Gamma = e^2/(4\pi\epsilon_0 a k_B T)$, where $a = (3/4\pi n)^{1/3}$. Small $\Gamma \ll 1$ indicate ideal, collisionless plasmas and $\Gamma \gtrsim 1$ strongly coupled systems.

The properties of two-component model plasmas using effective interactions have already been investigated by MD simulations during the last three decades, starting with the pioneering work of Norman [3] and Hansen [4–6] and followed by various other studies such as the more recent ones reported in [7–13]. Many of them, e.g. [4, 5, 7, 9, 11], also dealt with the dynamic structure factor. Our present MD studies complement and extend these previous investigations mainly in two respects: (1) a more systematic analysis of the sensitivity of a dynamic observable such as the dynamic structure factor on a variation of the effective potential, i.e. the $\lambda_{\alpha\beta}$, at fixed plasma conditions (n, T), (2) an extension to larger simulation cubes and thus smaller k-values. This allows a better evaluation of analytical treatments for the dynamic density response of nonideal plasmas, as the influence of the nonideality on the damping of plasma oscillations is in general much larger at lower k-values.

2. Dynamic response of a two-component model plasma

Important quantities to study the dynamic properties of a plasma are the charge-density response function $\chi_{qq}(\boldsymbol{k}, \omega)$ and the charge-density auto-correlation function or dynamic structure factor $S(\boldsymbol{k}, \omega)$, respectively. While $\chi_{qq}(\boldsymbol{k}, \omega)$ is defined through the variation of the charge density $\delta\rho(\boldsymbol{k}, \omega) = \chi_{qq}(\boldsymbol{k}, \omega)\phi(\boldsymbol{k}, \omega)$ when applying an external potential $\phi(\boldsymbol{k}, \omega)$, the structure factor $S(\boldsymbol{k}, \omega)$ represents the spectrum of the charge-density fluctuations in the equilibrium system. Within the linear response theory, both quantities are related via the fluctuation–dissipation theorem, and we have

$$S(k, \omega) = \frac{1}{N}\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\langle \rho_k(t)\rho_k(0)\rangle = -\frac{2k_B T}{\omega}\frac{\Omega}{N}\,\mathrm{Im}\,\chi_{qq}(k, \omega) \tag{2}$$

for a classical system, see e.g. [14]. Here ρ_k is the microscopic fluctuating charge density $\rho_k = \sum_\alpha q_\alpha \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_\alpha)$, N is the number of particles, $\langle\cdots\rangle$ denotes a statistical average, and Ω is the volume of the system. Because we assume a homogeneous and isotropic system, all quantities depend only on $|\boldsymbol{k}|$.

2.1. Random-phase approximation (RPA)

For ideal plasmas ($\Gamma \ll 1$), the charge-density response can be calculated in lowest-order perturbation theory within the standard random-phase approximation (RPA) (see e.g. [15]). For the TCMP with interactions (1), i.e. $V_{\alpha\beta}(k) = q_\alpha q_\beta \big/ \big[\epsilon_0 k^2\big(\lambda_{\alpha\beta}^2 k^2 + 1\big)\big]$, this yields the density-response function [16, 17]

$$\chi_{qq}^{\mathrm{RPA}}(k, \omega) = e^2\frac{\chi_{ii}^0\big(1 - V_{ee}\chi_{ee}^0\big) + \chi_{ee}^0\big(1 - V_{ii}\chi_{ii}^0\big) - 2\chi_{ii}^0\chi_{ee}^0 V_{ei}}{\big(1 - V_{ii}\chi_{ii}^0\big)\big(1 - V_{ee}\chi_{ee}^0\big) - V_{ei}V_{ie}\chi_{ee}^0\chi_{ii}^0} \tag{3}$$

with the free density–density-response functions $\chi_{\alpha\alpha}^0$ of the non-interacting system(s) ($V_{\alpha\beta} = 0$). In a classical treatment, $\chi_{\alpha\alpha}^0$ is given by the Vlasov function [18]

$$\chi_{\alpha\alpha}^0(k, \omega) \overset{\hbar\to 0}{=} \frac{n_\alpha}{k_B T}\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{\sqrt{2\pi}}\frac{x\exp(-x^2/2)}{\zeta_\alpha - x + \mathrm{i}\eta} \qquad \zeta_\alpha = \frac{\omega}{k}\left(\frac{m_\alpha}{k_B T}\right)^{1/2} \tag{4}$$

and $\eta \to 0^+$. In the special case $\lambda_{\alpha\beta} = 0$, equation (3) drastically simplifies to the standard expression for a TCP, $\chi_{qq}^{\mathrm{RPA}} = e^2\big(\chi_{ii}^0 + \chi_{ee}^0\big)\big/\big(1 - V_{ii}\chi_{ii}^0 - V_{ee}\chi_{ee}^0\big)$.

2.2. Dynamic local field correction (DLFC)

For strongly coupled systems, short-range correlations have to be included. It is convenient to implement them by introducing the dynamic local field corrections $G_{\alpha\beta}(k,\omega)$, see, e.g., [19], that is, by replacing the bare interactions $V_{\alpha\beta}(k)$ in the RPA expression for χ_{qq}, equation (3), with $U_{\alpha\beta}(k,\omega) = V_{\alpha\beta}(k)[1 - G_{\alpha\beta}(k,\omega)]$.

Various approaches to determine the $G_{\alpha\beta}(k,\omega)$ have been developed. In this paper, we apply the approach proposed by Ichimaru *et al* [20]. It is based on the low and high ω-limits of the $U_{\alpha\beta}$ (or likewise the $G_{\alpha\beta}$), and the interpolation

$$U_{\alpha\beta}(k,\omega) = \frac{\omega U_{\alpha\beta}^{\infty}(k) + \mathrm{i}\omega_{\alpha\beta}U_{\alpha\beta}^{0}(k)}{\omega + \mathrm{i}\omega_{\alpha\beta}} \tag{5}$$

with $\omega_{\alpha\beta}^2 = \big(\omega_{p\alpha}^2 + \omega_{p\beta}^2\big)\big/2$ and the plasma frequencies $\omega_{p\alpha}^2 = q_\alpha^2 n_\alpha\big/\epsilon_0 m_\alpha$. The $U_{\alpha\beta}^0$ and $U_{\alpha\beta}^\infty$ are fixed by the static properties of the system contained in the pair-distribution functions $g_{\alpha\beta}(r)$ or the partial static-structure factors $S_{\alpha\beta}(k)$, where $[2S_{\alpha\beta}(k) - \delta_{\alpha\beta}] = n_\alpha \int \mathrm{d}^3 r\, g_{\alpha\beta}(r)\exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})$. They are given through

$$U_{\alpha\beta}^0(k) = \frac{S_{\alpha\beta}(k)}{2\big(S_{ii}(k)S_{ee}(k) - S_{ie}^2(k)\big)} - \delta_{\alpha\alpha} \tag{6}$$

$$U_{\alpha\beta}^\infty(k) = \int \frac{\mathrm{d}^3 r}{k^4} \sum_\gamma \left[(\boldsymbol{k}\cdot\boldsymbol{\nabla})(\boldsymbol{k}\cdot\boldsymbol{\nabla})\frac{V_{\alpha\gamma}(r)}{k_B T}\right] g_{\alpha\gamma}(r)(n_\gamma\delta_{\alpha\beta} - n_\alpha\delta_{\gamma\beta}\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}). \tag{7}$$

To evaluate equations (6) and (7), we have calculated the $g_{\alpha\beta}(r)$ from the fully coupled hypernetted-chain (HNC) equations for the TCMP with interactions $V_{\alpha\beta}$ (1).

2.3. Dynamic collision frequency (DCF)

Alternatively, the short-range correlations can be accounted for by including ion–electron collisions. This has been done recently [17] by replacing the free-density response $\chi_{\alpha\alpha}^0$ in the RPA expression, equation (3), with the Mermin response function $\chi_{\alpha\alpha}^{\nu,0}$,

$$\chi_{\alpha\alpha}^{\nu,0}(k,\omega) = (\nu(\omega) - \mathrm{i}\omega)\left[\frac{\chi_{\alpha\alpha}^0(k,\omega + \mathrm{i}\nu(\omega))\chi_{\alpha\alpha}^0(k,0)}{\nu(\omega)\chi_{\alpha\alpha}^0(k,\omega + \mathrm{i}\nu(\omega)) - \mathrm{i}\omega\chi_{\alpha\alpha}^0(k,0)}\right] \tag{8}$$

and introducing a complex, frequency-dependent collision frequency $\nu(\omega)$. The use of such a dynamic collision frequency generalizes the original Mermin ansatz with a frequency-independent relaxation time [21] and results in a considerably improved density-response function $\chi_{qq}^{\mathrm{DCF}}(k,\omega)$ as shown and discussed in [17]. The dynamic collision frequency $\nu(\omega)$ itself is derived from a perturbation treatment of a generalized linear response theory [22–24]. In this framework, it is calculated in a first-order Born approximation from the force–force correlation function based on the ion–electron interaction V_{ie}, equation (1). See [17, 24, 25] for details.

2.4. Numerical treatment

To study the full many-body dynamics, we performed MD simulations [26], i.e. the classical equations of motion for a hydrogen-like TCMP of $N = N_p + N_e = 1414$ particles of masses

$m_\alpha = m_p, m_e$ ($m_p/m_e = 1836$) and charges $q_\alpha = \pm e$ have been numerically integrated using a velocity verlet algorithm. The elementary simulation cube of length L is periodically continued in all three spatial directions. This introduces a discrete set of allowed wave vectors $\boldsymbol{k} = 2\pi \boldsymbol{m}/L$ with a smallest wave number $k = 2\pi/L$, where $2\pi a/L = 0.438$ in our case. The actual simulations run over a typical time of $\tau = 310\omega_{pe}^{-1}$ at constant total energy in an equilibrium state, which is prepared by a preceding simulation at constant temperature. Their accuracy and stability are monitored using the total energy, which is conserved with an accuracy of typically better than $10^{-4} \ldots 10^{-3}$ at a global time step $\triangle t = 0.0105\omega_{pe}^{-1}$. Special attention is paid to close encounters of particles and the arising large forces, in particular for the ion–electron interaction. Here close colliding particles are propagated as subsystems with a reduced time step [27, 28].

From the positions $\{\boldsymbol{r}_\alpha(t)\}$ ($\alpha = 1, \ldots, N$) of the particles, the microscopic charge density ρ_k is sampled as $\rho_k(t) = \sum_\alpha q_\alpha \exp(-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}_\alpha(t))$ for values $ka = 0.438$, 0.619, 0.758, 0.875 and 1.75. The desired correlation function is evaluated as time average over the simulation time τ and an ensemble average $\langle \cdots \rangle$ over typically ten individual runs with microscopically different initial configurations. The error is deduced from the fluctuations within this ensemble. Inclusive of a final numerical Fourier transform, the dynamic structure factor (2) is thus given through

$$S(k,\omega) = \frac{1}{2\pi} \int_{-\tau}^{\tau} \mathrm{d}t \, \mathrm{Re} \left[\frac{1}{N} \frac{1}{\tau} \int_0^\tau \mathrm{d}t' \langle \rho_k(t'+t) \rho_k(t') \rangle \right] \cos(\omega t). \tag{9}$$

3. Analysis of the results

We determined the dynamic structure factor $S(k, w)$ for the hydrogen-like TCMP with interactions (1) for coupling parameters $\Gamma = 0.5$, 1, 2 and 4 and potential parameters $\lambda/a \equiv \lambda_{ie}/a = 0.1$, 0.2, 0.4 and 0.8. The interactions V_{ee} and V_{ii} have been fixed by using $\lambda_{ee} = 2^{1/2}\lambda_{ie}$ and $\lambda_{ii} = (2m_e/m_p)^{1/2}\lambda_{ie}$. The main objective of our studies is to verify theoretical treatments of nonideal classical TCMPs by comparing them with the simulation results. But the TCMP can also be viewed as an appropriate model of a real TCP when quantum diffraction effects are fairly well approximated by the effective potentials (1). This is expected to be the case for temperatures $k_B T \gtrsim 1$ Ry, λ about the thermal wavelength of the electrons and sufficiently nondegenerate systems, i.e. $\lambda/a \lesssim 1$, see [5] for a more detailed discussion. For the present set of parameters, the TCMP might thus be a reasonable approximation for a dense-hydrogen plasma in the parameter region $T/\mathrm{K} \sim 10^5 \ldots 10^6$ and $n/\mathrm{cm}^{-3} \sim 10^{23} \ldots 10^{25}$, about the same parameter region as given in [5]. The quasi-classical treatment of a TCP under these conditions is, however, justified only for static and statistical considerations. If such simple local effective potentials can also be used for a quasi-classical description of the dynamic properties of a real TCP is still an open question.

Results from the MD simulations and the three outlined theoretical approaches are shown in figures 1 and 2 for some examples of combinations of Γ and λ at specific k-values. The general observations we made are as follows: as expected, the MD results (filled circles with errorbars) show for increasing coupling Γ an increasing damping of the plasmon mode, i.e. a broadening of the corresponding peak in $S(k, \omega)$ around $\omega \approx \omega_p$. This can be seen best from the growing deviations between MD and RPA (dashed curves). But in addition, the damping of the plasmon mode also increases with decreasing λ (see figures 1 and 2(a), (b)). Both dependencies have to be attributed to the rising influence of strong short-range ion–electron correlations on the collective mode, including the formation of classically bound states. Accordingly, the RPA agrees with the simulation results only at low coupling Γ and

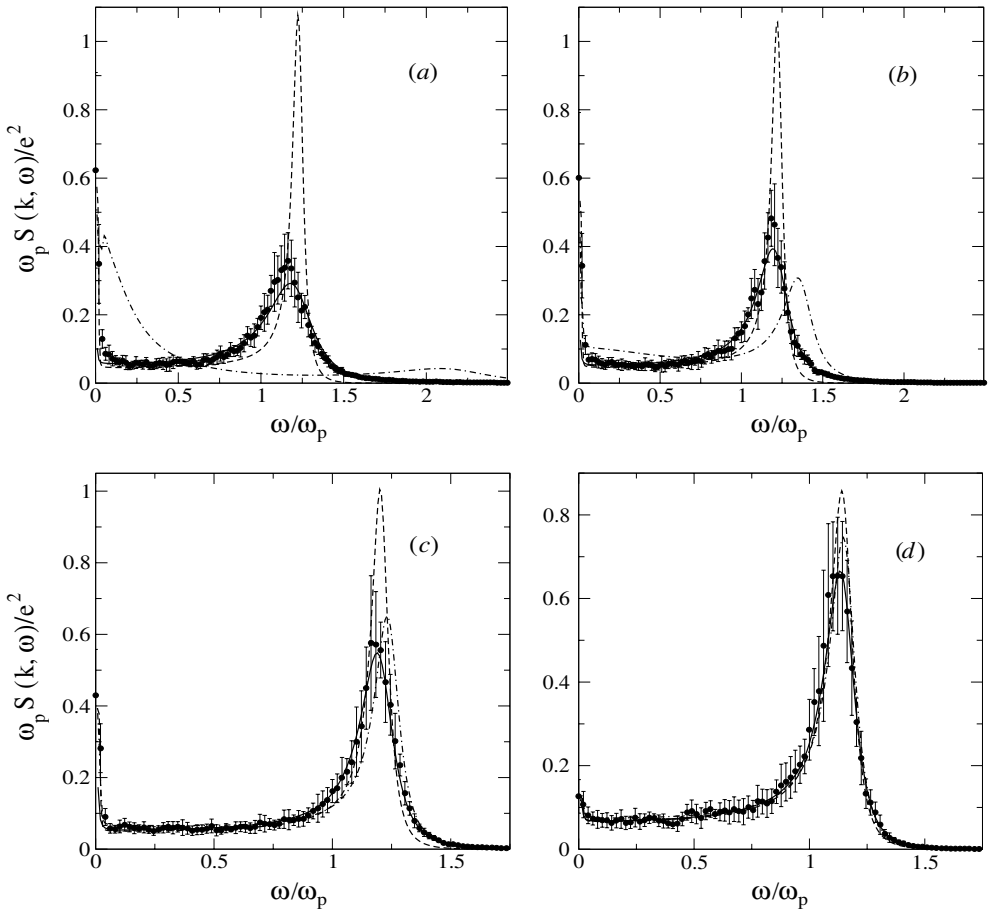

Figure 1. Dynamic structure factor $S(k, \omega)$ for a proton–electron model plasma as a function of ω in units of the electron-plasma frequency $\omega_p \equiv \omega_{pe}$ from the MD simulations (● with errorbars) and the different analytical treatments: RPA (- - - -), DLFC (— · —) and DCF [29] (——). The parameters are $\Gamma = 0.5$, $ka = 0.438$ and: (*a*) $\lambda/a = 0.1$, (*b*) $\lambda/a = 0.2$, (*c*) $\lambda/a = 0.4$ and (*d*) $\lambda/a = 0.8$.

large λ (see, e.g., figure 1(*d*), where $\Gamma = 0.5$ and $\lambda = 0.8a$). It grossly underestimates the damping in all other cases, but, very surprisingly, predicts the position of the plasmon rather well for most of the studied parameters. We also compare our recent simulation results with those of Hansen and McDonald [5] who used the same effective potentials (1), however for somewhat different values of λ and ka. Two examples are given in figure 3 for the lowest k-value, $ka = 0.78$, accessible in these early MD simulations with $N = N_p + N_e = 250$, and $\Gamma = 0.5$, $\lambda/a = 0.45$ (open squares on the left) and $\Gamma = 2.0$, $\lambda/a = 0.56$ (open squares on the right). At $\Gamma = 0.5$, there are only small deviations from our results mainly coming from the sightly different parameters ($ka = 0.76$ and $\lambda/a = 0.40$ in our simulations). The good agreement with the RPA result in this case compared to the considerable deviation at $ka = 0.438$ (but otherwise unchanged parameters, see figure 1(*c*)) clearly demonstrates the importance of an extension towards smaller k-values in order to improve the evaluation of theoretical approaches. The comparison shown in the right part of figure 3, on the other hand, again points out the rather large sensitivity on a variation of the effective interaction, i.e. on λ, where λ runs

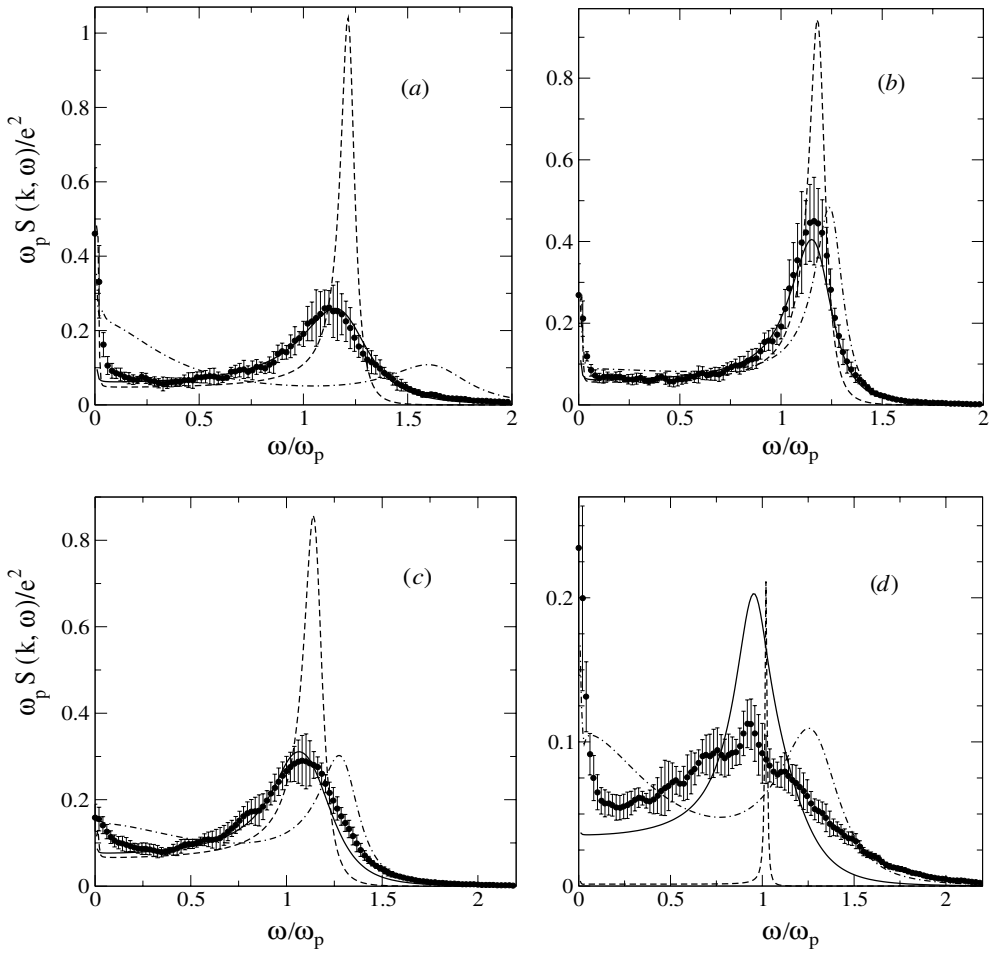

Figure 2. Dynamic structure factor $S(k, \omega)$ for a proton–electron model plasma as in figure 1 for: (*a*) $\Gamma = 1$, $ka = 0.619$, $\lambda/a = 0.2$, (*b*) $\Gamma = 1$, $ka = 0.619$, $\lambda/a = 0.4$, (*c*) $\Gamma = 2$, $ka = 0.875$, $\lambda/a = 0.4$, (*d*) $\Gamma = 4$, $ka = 0.875$, $\lambda/a = 0.4$. In case (*d*), the RPA result (- - - -) is divided by 20.

from 0.8 over 0.56 to 0.4. Once more, the RPA predicts the position of the collective mode rather well, but grossly underestimates the damping. The DLFC (dash-dotted curves in figures 1 and 2), which claims to account for short-range correlations, in fact shows a strong broadening of the plasmon peak. But at small λ, it significantly overestimates the damping and furthermore develops a spurious diffusive mode at low frequencies (see, e.g., figures 1(*a*) and 2(*a*)). And, moreover, the DLFC approach provides a marked displacement of the position of the plasmon in all cases where correlations are relevant, i.e. where MD and RPA deviate significantly (see, e.g., figures 1(*a*), (*b*) and 2). In view of this poor agreement of the DLFC with the simulation results, we carefully checked the pair correlation functions $g_{\alpha\beta}(r)$ used in equations (6) and (7) as well as the moments of the structure factor $\langle\omega^m\rangle = \int \mathrm{d}\omega\, \omega^m S(k, \omega)$ for $m = 0, 2, 4$. The $g_{\alpha\beta}(r)$ obtained from the HNC calculations agree, however, very well with those from the MD, and with respect to the moments, the DLFC and MD results diverge typically less than a few per cent. Note that the theoretical $g_{\alpha\beta}(r)$ and moments of $S(k, \omega)$ have been calculated using exactly the same effective potentials (1) as in the MD simulations and for the

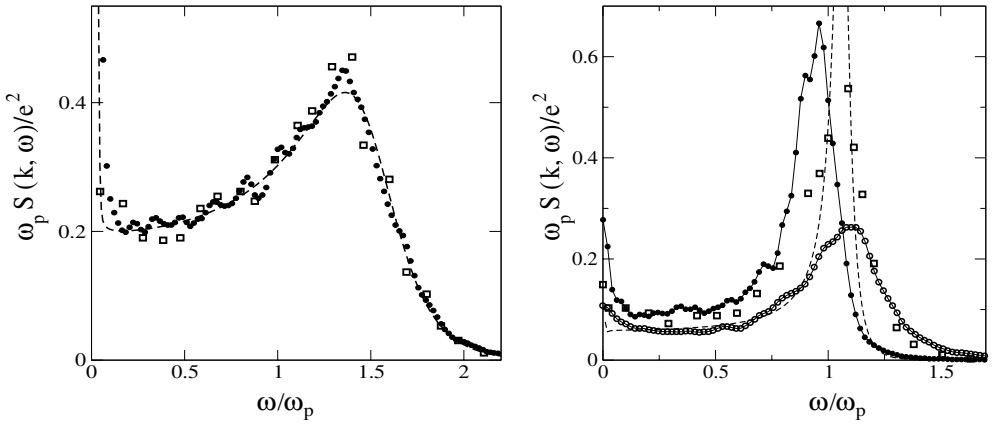

Figure 3. Dynamic structure factor $S(k, \omega)$ for a proton–electron model plasma as in figure 1. Left: $\Gamma = 0.5$; MD results from [5], $ka = 0.78$, $\lambda/a = 0.45$ (□); MD present work, $ka = 0.76$, $\lambda/a = 0.40$ (●); RPA: $ka = 0.76$, $\lambda/a = 0.40$ (- - - -). Right: $\Gamma = 2.0$; MD results from [5], $ka = 0.78$, $\lambda/a = 0.56$ (□); MD present work, $ka = 0.76$, $\lambda/a = 0.80$ (●), $ka = 0.76$, $\lambda/a = 0.40$ (○); RPA: $ka = 0.78$, $\lambda/a = 0.56$ (- - - -).

RPA predictions. Also a variation of the interpolation procedure equation (5), while redistributing the position of the peaks and its total strength, does not ameliorate the results. The DCF (solid curves, data kindly provided by Millat [29]), based on a dynamic collision frequency, on the other hand excellently reproduces the numerical results within the errors for coupling parameters $\Gamma \lesssim 2$. At even higher coupling, it still predicts fairly well the peak position and gives a reasonable estimate of the damping (figure 2(d)).

4. Summary and conclusion

From the whole parameter range which we have studied so far, we find that the DLFC procedure in its presented form seems to improve the description only in those cases where correlations merely affect slightly the dynamic properties. The DCF, on the other hand, gives a very satisfactory description of the dynamic density response of a strongly coupled TC(M)P. This suggests the conjecture that inherent dynamic approaches, such as the DCF, are much better suited for describing the dynamic properties of nonideal plasmas than methods which aim at constructing dynamic correlations from static properties. But to verify this surmise, a further evaluation of existing theoretical treatments is needed, comprising other approaches also based on the moments and sum-rules for $S(k, \omega)$, e.g. the treatment of Adamjan *et al* [30]. Such work is in progress.

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