PHYSICAL REVIEW E **83**, 015401(R) (2011)

Extent of validity of the hydrodynamic description of ions in dense plasmas

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(Received 7 September 2010; published 11 January 2011)

We show that the hydrodynamic description can be applied to modeling the ionic response in dense plasmas for a wide range of length scales that are experimentally accessible. Using numerical simulations for the Yukawa model, we find that the maximum wave number $k_{\max}$ at which the hydrodynamic description applies is independent of the coupling strength, given by $k_{\max}\lambda_s \simeq 0.43$, where λ_s is the ionic screening length. Our results show that the hydrodynamic description can be used for interpreting x-ray scattering data from fourth generation light sources and high power lasers. In addition, our investigation sheds new light on how the domain of validity of the hydrodynamic description depends on both the microscopic properties and the thermodynamic state of fluids in general.

DOI: 10.1103/PhysRevE.83.015401 PACS number(s): 52.27.Gr, 05.20.Jj

With the availability in the past decade of high power lasers and fourth generation x-ray sources, extreme states of matter found in inertial confinement fusion (ICF) and in the core of compact astrophysical objects, such as planets and stars, can be produced and diagnosed in the laboratory [1–5]. These experiments will require significant theoretical advances [6]. In particular, models are needed for the dynamical response of strongly correlated matter over a wide range of thermodynamic conditions—a goal that has thus far remained elusive. While a number of involved approaches have proven to be successful under some conditions [7–10], the hydrodynamic description retains a much simpler physical picture in terms of fundamental transport and thermodynamic properties of the plasma. In this Rapid Communication, we show that in fact this often overlooked description is applicable to conditions accessible to the experiments.

One ordinarily thinks of the hydrodynamic picture as applying only for wave numbers k such that $kl_f \ll 1$, with l_f the mean free path, and frequencies ω such that $\omega/\omega_c \ll 1$, with ω_c the mean collision frequency. These conditions, derived and already rather qualitative for a system governed by uncorrelated binary collisions (e.g., a dilute gas), become even more indeterminate when many-body correlations are present (as in the dense plasma case) because the concepts of mean free path and mean collision time cease to have a clear physical meaning. Indeed, we certainly expect the domain of validity of the hydrodynamic description to depend strongly on the thermodynamic state of the plasma. For instance, one expects that for the ions in a plasma, the description never applies on length scales smaller than the screening length λ_s of the effective ion-ion potential (i.e., $k\lambda_s \gtrsim 1$)—in other words, that the domain of validity will shrink as the screening length increases. In fact, in the extreme case of $\lambda_s = \infty$, the very existence of a hydrodynamic description is a known but unsolved problem [11].

Here, we address with numerical simulations the question of the extent of validity of the hydrodynamic description of ions in a plasma at or near equilibrium as the level of many-body correlations in the system is varied. We use the Yukawa interaction potential $v(r) = (Ze)^2 \exp(-r/\lambda_s)/(4\pi\epsilon_0 r)$, where Ze is the ionic charge, to represent the screened ion-ion interaction in a plasma [12]. The screening length λ_s [3,10,13] reduces to either the Debye-Huckel law or the Thomas-Fermi distance in the limiting cases of classical and degenerate electron fluid, respectively [1,14]. For $\lambda_s = \infty$ one recovers another standard model in plasma physics known as the one-component plasma (OCP) [11], which allows us to answer the question of the existence of the hydrodynamic limit referred to previously. Most importantly, the Yukawa model is very convenient here because it is known to be fully characterized by two dimensionless parameters only [12]—the reduced screening length $\lambda_s^* = \lambda_s/a$, where $a = (4\pi n/3)^{-1/3}$ is the Wigner-Seitz radius, and the coupling strength $\Gamma = q^2/(ak_bT)$, which itself characterizes completely the degree of many-body correlations present in the system for a given screening length [7] (here n and T are the ion number density and temperature, respectively). For a wide range of Γ and λ_s^* values, thus spanning states ranging from gaseous ideal plasmas to dense liquidlike plasmas [15], we determine the length and time scales at which the hydrodynamic description breaks down.

To accomplish this, we have computed with molecular dynamics (MD) simulations the dynamical structure factor, $S(k,\omega)$, that is the Fourier transform in space and time of the density autocorrelation function, for a wide range of Γ (0.1,1,5,10,50,120,175) and λ_s^* (0.5,1,1.4,2,3.3,10,∞) values. $S(k,\omega)$ contains complete information of the system dynamics at and near thermal equilibrium through the fluctuation-dissipation theorem, and can be obtained in inelastic light and neutron scattering experiments (e.g., Refs. [1,8,16]). Three main difficulties are involved with the MD calculation of $S(k,\omega)$. First, for large screening lengths (large λ_s^*), it is essential to include the Ewald summation; we compute this for all our λ_s^* values using the particle-particle-particle-mesh method [17]. Second, obtaining accurate MD data for $S(k,\omega)$ requires averaging the results of a large number of simulations to improve statistics. Third, in order to investigate the long wavelength dynamics that concern the hydrodynamic description, very large scale simulations (a large number of ions N) are needed: The minimum reduced wave vector $(ka)_{\min}$

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at which the system dynamics can be determined by using MD is $\propto N^{-1/3}$. These computational demands have made a thorough study such as ours impractical before now. In our computation of $S(k,\omega)$, we average the results of fully 25 simulations, each of duration $819.2\omega_p^{-1}$ (the ion plasma frequency $\omega_p = \sqrt{3q^2Ma^3}$ is the natural time scale for our system, where M is the ion mass), with up to 500 000 ions [18].

First, we consider the case of finite screening lengths ($\lambda_s^* < \infty$). In this case the MD data can be compared to the result obtained from the linearized hydrodynamic (Navier-Stokes) equations [8,19]

$$\frac{S^H(k,\omega)}{S(k)} = \frac{\gamma-1}{\gamma}\frac{2D_Tk^2}{\omega^2+(D_Tk^2)^2} + 1/\gamma\left(\frac{\sigma k^2}{(\omega+c_sk)^2+(\sigma k^2)^2}+\frac{\sigma k^2}{(\omega-c_sk)^2+(\sigma k^2)^2}\right), \quad (1)$$

where the static structure factor $S(k)$ in Eq. (1) is also determined from our MD simulations. Equation (1) consists of a central (Rayleigh) peak representing a diffusive thermal mode and two ion-acoustic (or more generally, Brillouin) peaks at $\omega = \pm c_sk$ corresponding to propagating sound waves in the plasma. As illustrated in the top panel of Fig. 1, at the smallest k value accessible to our MD simulations we find that the MD $S(k,\omega)$ can always (i.e., for all Γ and λ_s^*) be very accurately fitted to Eq. (1), thus giving numerical values for the thermal diffusivity D_T, sound attenuation coefficient σ, adiabatic sound speed c_s, and ratio of specific heats γ that appear in the hydrodynamic description. When obtained in this way, these parameters are found to be in very good agreement with previous equation-of-state and transport coefficient calculations for the Yukawa model [20]. In particular, we find that $\gamma \approx 1$—that is, the Rayleigh peak at $\omega = 0$ is negligible. In all cases, however, we find two ion-acoustic peaks, at $\omega = \pm c_sk$, representing damped ion-acoustic waves. Figure 2 shows the position of the ion-acoustic peak obtained from our MD simulations. We see that as the screening length becomes larger, it is necessary to look at increasingly long length scales (small ka) for the hydrodynamic description to be applicable. Clearly in all cases, at some k value, which we denote by k_{max}, the position $\omega(k)$ of the ion-acoustic peak as computed by MD diverges from the linear relation. Quantitatively, we define k_{max} as the minimum k value for which $\omega(k)/(c_sk) > 1.01$. Using this criterion, for all values of the coupling Γ, we find that $k_{max}\lambda_s \simeq 0.43$.

The k_{max} obtained from the peak position is found also to characterize well the departure of the height and width of the ion-acoustic peak from the predictions of the hydrodynamic description (Fig. 3). Therefore, k_{max} is the maximum wave vector at which the hydrodynamic description of Eq. (1) is applicable. As shown in Fig. 3, beyond k_{max} the height of the ion-acoustic peak decreases more slowly, and its width increases more slowly, than predicted by Eq. (1). Clearly, however, the hydrodynamic description is valid for a relatively large range of k values, well beyond $k = 0$. In real space, we find that the length scale $2\pi/k_{max}$ is, for all Γ values, greater

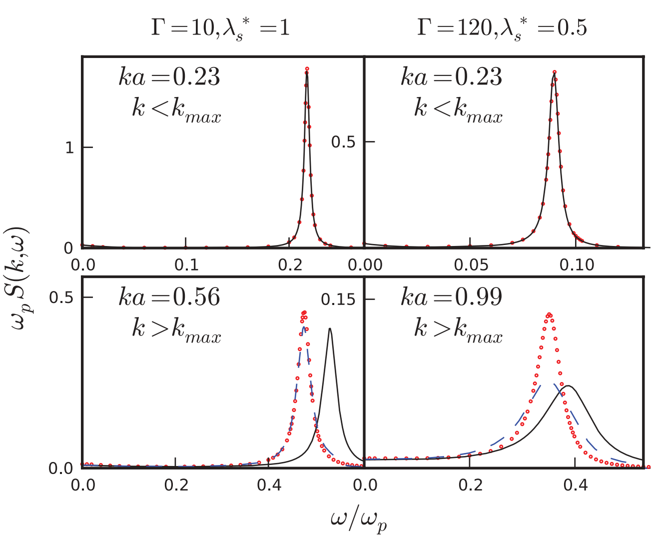

FIG. 1. (Color online) Sample of our MD results for $S(k,\omega)$ (dots) vs $S^H(k,\omega)$ in Eq. (1) (solid line) and when a "mean field" is added (dashed line—bottom panel only).

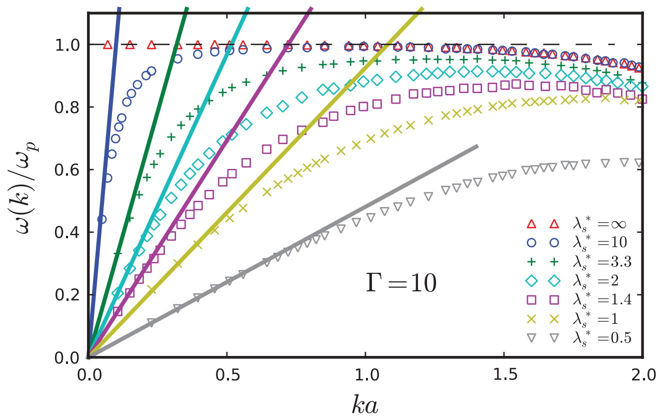

FIG. 2. (Color online) Ion-acoustic peak position $w(k)/\omega_p$ as obtained from MD (symbols), along with the corresponding linear relations $\omega = c_sk$ (solid lines).

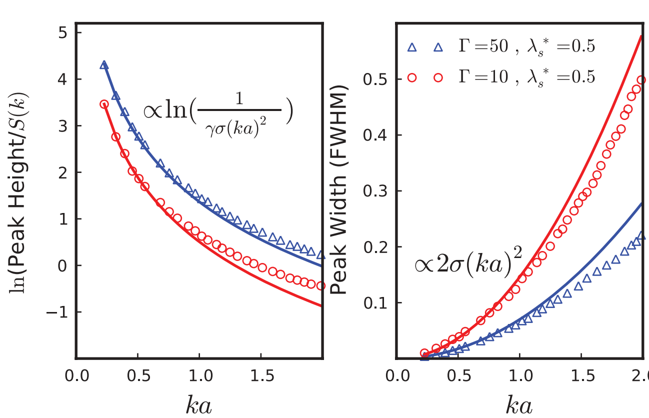

FIG. 3. (Color online) Height and width of the ion-acoustic peak as computed from MD (open symbols), and the predictions of Eq. (1) (solid lines).

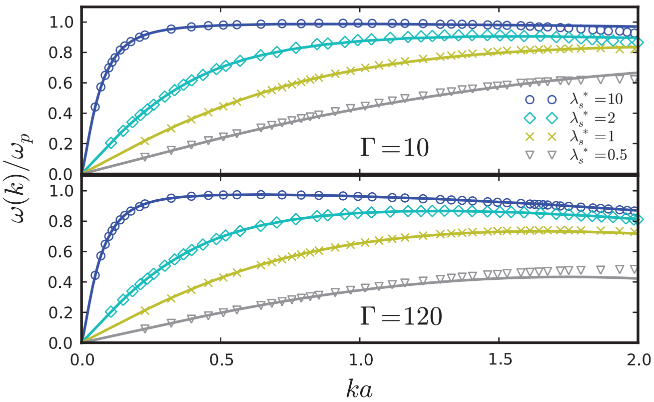

FIG. 4. (Color online) Ion-acoustic peak position as obtained from MD (symbols), and the prediction of Eq. (2) (solid lines).

than the short-range correlation length over which the pair correlation function $g(r)$ exhibits peaks and troughs [11]. It is remarkable that $k_{\max}$ does not depend on Γ; indeed, one would intuitively expect the domain of validity of Eq. (1) to increase as the system becomes more "collisional" (i.e., with increasing Γ). We also note that, provided $k < k_{\max}$, the hydrodynamic approximation of Eq. (1) for $S(k,\omega)$ is extremely accurate for all ω where $S(k,\omega)$ is not negligibly small; in this range, the ion-acoustic peaks exhaust the frequency sum rules (see the top panel of Fig. 1). The extensive domain of validity given by our criterion for $k_{\max}$ certainly has notable experimental applicability: For example, assuming a hydrogen plasma with $n = 1 \times 10^{23}\,\mathrm{cm}^{-3}$ and $T = 13\,\mathrm{eV}$ [6] (this gives $\Gamma \approx 1$ and we use the Debye length for λ_s), the hydrodynamic description can be expected to accurately model the ionic response in x-ray scattering experiments with a 4 keV probe up to a scattering angle of $\approx 15^\circ$ [16], which is large enough to be attainable in forthcoming experiments [21].

Much detailed work has been carried out to extend, from macroscopic to microscopic length scales, the domain in which ordinary hydrodynamics applies (e.g., Refs. [8,9,19]). Interestingly, we find that simply by adding to the usual stress tensor the mean field term, one can account very well for the position of the ion-acoustic peak. Microscopically, this additional term stems from the inclusion of a self-consistent "mean field" or "Vlasov" term—usually neglected because one considers length scales longer than the range of the potential—in the appropriate kinetic equation. By including the mean field term in the macroscopic equations, one obtains for the Yukawa model a modified expression for the position of the ion-acoustic peak [22]

$$\omega(k) = \left(K + \frac{\omega_p^2}{k^2 + \lambda_s^2}\right)^{\frac{1}{2}} k\,, \qquad (2)$$

where $K = c_s^2 - \omega_p^2/\lambda_s^2$. We note that for systems with $\gamma = 1$, which is a good approximation for the Γ and λ_s^* values considered here, the addition of the mean field does not change the hydrodynamic description of the height or width of the ion-acoustic peak (see Ref. [22] for details). As shown in Fig. 4, Eq. (2) gives a remarkably good description of the ion-acoustic peak position, even up to $ka \approx 2$ in most cases (although, as shown in Fig. 1, the height and width of the peak do not always compare well with the MD simulations). Indeed, this dramatic improvement is somewhat unexpected, since dynamics at these large wave vectors are not usually thought to be well described by macroscopic approaches.

For finite λ_s^*, the mean field only begins to play a role when $k\lambda_s > 0.43$ (i.e., when the range of the potential is large compared to the length scale of the density variations). Therefore, one may expect that in the OCP case of $\lambda_s^* = \infty$, when the interaction potential is Coulombic [23], the mean field is important at all length scales (in this case, our criterion $k_{\max}\lambda_s \simeq 0.43$ gives $k_{\max} = 0$). To be sure, the peculiarity of the Coulomb potential is very well known—in this case the longitudinal waves are not low-frequency sound waves, as for $\lambda_s^* < \infty$, but instead high-frequency plasma waves ($\omega \approx \omega_p$), even at $k = 0$. The resulting "plasmon" peak in $S(k,\omega)$, the position of which is illustrated in Fig. 2 (red upward pointing triangles), is certainly not described by the low-frequency hydrodynamic equations that lead to Eq. (1); one can indeed wonder why hydrodynamics should describe plasma oscillations at all. The difficulty here is underlined by a kinetic theoretical derivation of the hydrodynamic equations [11]: When proceeding with the Chapman-Enskog expansion of the appropriate kinetic equation, the mean field term is usually treated as a small perturbation, since, in the small-gradient region of interest to hydrodynamics, the kinetic equation is always dominated by the collision term. For the OCP, however, the mean field term cannot be considered as small, since its straightforward small-gradient expansion diverges with the characteristic Coulomb divergence (see Ref. [11] and references therein). Based on this analysis, Baus and Hansen [11] argued that only when the collisionality dominates the mean field, which they predicted would occur at sufficiently high coupling strength Γ, could a hydrodynamic description be expected for the OCP. In this case the hydrodynamic description is identical to Eq. (1) [24] but with $c_s k$ replaced with $\omega_p(1 + \frac{c_s^2 k^2}{2\omega_p^2})$ [25]. This macroscopic description is known not to work for small Γ [11]; exactly how large Γ has to be for it to be applicable was left as an open question until now. We show here that in fact the hydrodynamic description of the OCP is not valid at any Γ.

Baus and Hansen [11] based the arguments outlined earlier on an exact formula for $S(k,\omega)$ of the OCP, derived using generalized kinetic theory, which at small k is given by [24]

$$\frac{S^B(k,\omega)}{S(k)} = \frac{bk^2}{\left[\omega + \omega_p\left(1 + \frac{k^2}{2}a\right)\right]^2 + \left(\frac{k^2}{2}b\right)^2} + \frac{bk^2}{\left[\omega - \omega_p\left(1 + \frac{k^2}{2}a\right)\right]^2 + \left(\frac{k^2}{2}b\right)^2}, \qquad (3)$$

where a and b are generalized coefficients with k and ω dependence. They were able to show that only at large Γ would it be possible for these coefficients to equal their macroscopic counterparts [of Eq. (1)], c_s^2/ω_p^2 and 2σ, respectively [11]. We have estimated a and b by fitting $S(k,\omega)$ at the smallest k value accessible to our MD simulations to Eq. (3)—this gives a very good fit. However, as shown in Table I, the values obtained for

TABLE I. Comparison of the generalized coefficients obtained by fitting the MD $S(k,\omega)$ at our smallest k value to Eq. (3) with the analogous coefficients that appear in the hydrodynamic description. c_s is determined from the internal energy fit given in Ref. [26] while σ is obtained from Ref. [15].

Γ	a	c_s^2/ω_p^2	b	2σ
1	0.895	0.304	0.192	1.825
5	0.088	−0.034	0.109	0.333
10	−0.009	−0.080	0.078	0.235
50	−0.056	−0.112	0.032	0.212
120	−0.062	−0.127	0.021	0.349
175	−0.065	−0.129	0.009	0.550

a and b do not agree at all with their macroscopic counterparts, even at our highest coupling strength of $\Gamma = 175$, which is close to the freezing point of the system [11]. For example, the width of the plasmon peak b does not even follow the same trend predicted by the hydrodynamic scaling 2σ at our higher Γ values. From this we conclude that the combination of mean field and collisional effects means that the hydrodynamic description in the manner of Navier and Stokes is not valid for the OCP at any coupling strength Γ.

In summary, our results show that the conventional hydrodynamic description can be used to model ion dynamics in plasmas for a surprisingly large range of length scales: Our criterion of $k_{\max}\lambda_s \simeq 0.43$ gives a quantitative measure of this. What is more, below $k_{\max}$—which we find to be independent of the level of many-body correlations in the system (i.e., Γ)—the hydrodynamic equations give an accurate description of the entire ion-acoustic peak. For the OCP, $\lambda_s^* = \infty$, the persistence of both mean field and collisional effects causes the ordinary hydrodynamic approach to fail. As forthcoming x-ray scattering experiments on fourth generation light sources will be able to resolve the ion dynamics [21], we provide testable predictions that also significantly enhance our understanding of dense plasmas for conditions relevant to ICF and laboratory astrophysics.

This work was supported by the John Fell Fund at the University of Oxford and by EPSRC Grant No. EP/G007187/1. The work of J.D. was performed for the US Department of Energy by Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

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