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Generalized hydrodynamics model for strongly coupled plasmas

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A Generalized Hydrodynamics Model for Strongly Coupled Plasmas

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Beginning with the exact equations of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy, we obtain the density, momentum and stress tensor-moment equations. We close the moment equations with two closures, one that guarantees an equilibrium state given by density functional theory and another that includes collisions in the relaxation of the stress tensor. The introduction of a density functional-theory closure ensures self consistency in the equation-of-state properties of the plasma (ideal and excess pressure, electric fields, and correlations). The resulting generalized hydrodynamics thus includes all impacts of Coulomb coupling, viscous damping, and the high-frequency (viscoelastic) response. We compare our results with those of several known models, including generalized hydrodynamic theory and models obtained using the Singwi-Tosi-Land-Sjolander (STLS) approximation and the quasi-localized charge approximation (QLCA). We find that the viscoelastic response, including both the high-frequency elastic generalization and viscous wave damping, is important for correctly describing ion-acoustic waves. We illustrate this result by considering three very different systems: ultracold plasmas, dusty plasmas, and dense plasmas. The new model is validated by comparing its results with those of the current autocorrelation function obtained from molecular-dynamics simulations of Yukawa plasmas, and the agreement is excellent. Generalizations of this model to mixtures and quantum systems should be straightforward.

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I. INTRODUCTION

The advent of new high energy-density experimental facilities, such as the Linac Coherent Light Source (LCLS) [1] and the National Ignition Facility [2], have renewed interest in the physics of moderately to strongly coupled plasmas (SCPs). Furthermore, recent, smallerscale experiments with ultracold neutral plasmas (UC-NPs) [3, 4] and dusty plasmas (DPs) [5] continue to provide detailed information about these plasmas. Despite the breadth of our knowledge about these non-ideal plasmas [6-12], current applications are pushing our need for an understanding of plasma physics beyond that provided by the usual simplifications of homogeneous plasmas, linear transport coefficients, and linear collective processes. Modern experiments probe non-equilibrium, heterogeneous, and non-linear responses across large time and length scales; examples of such experiments include shock heating of inertial confinement fusion (ICF) capsules [7] and wave excitations in UCNPs [8]. Because molecular dynamics (MD) simulations cannot currently be performed over the time and length scales relevant for such experiments [6] and because kinetic equations do not include non-ideal plasma properties, it would be useful to develop a theoretical and computational model both applicable to the extreme conditions of current experiments and capable of reaching the relevant scales.

Models for large-scale dynamics are typically formulated in terms of the macroscopic equations of hydrodynamics [13]. While such equations can be derived directly from an underlying kinetic equation (e.g., the Boltzmann equation) [14], two issues arise. First, the kinetic equation should itself contain the physics of strong coupling, including *both* strong correlations and strong scattering, and most kinetic equations are lacking in this respect. Second, given a suitable kinetic equation, a moment hierarchy is generated that must be truncated through a suitable closure. For example, Murillo [15] obtained a hydrodynamic description that is derived from moments of a modified Vlasov equation that includes correlations through the equilibrium pair correlation function q(r), using a variant of the Singwi-Tosi-Land-Sjolander (STLS) [9] approximation, and this hydrodynamic description includes a simple closure at the level of the momentum equation. Upon further examination [16], SCPs require careful treatment of the high-frequency response, as well, including collisions, and improved closures [17] are therefore needed to obtain an adequate hydrodynamic description.

The high-frequency response of SCPs has also been examined by Golden and Kalman [10], who proposed the quasi-localized charge approximation (QLCA) to describe high-frequency waves. In this scheme, the particles are assumed to oscillate around localized positions. The QLCA is based on a time-scale separation in which particle positions are described by an equilibrium paircorrelation function g(r). Response functions were obtained, and results are in relatively good agreement with MD simulations. However, as is also true for the STLS approximation, the QLCA does not contain dissipative effects, and it is not applicable in the hydrodynamic limit.

The only existing hydrodynamic theory that accounts for both low-frequency collisional effects (e.g., viscous

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damping) and high-frequency response (e.g., elastic response) properties is the well-known generalized hydrodynamic (GH) theory [18]. GH is a phenomenological model that extends the usual Navier-Stokes equation to higher frequencies, and it is motivated by a model that combines the properties of both solid and liquid bodies by generalizing the transport coefficients in the Navier-Stokes equation, using a memory function. Such a GH model was first proposed by Frenkel [19] for viscoelastic liquids and was later used by Ichimaru [20] to study the dynamic properties of SCPs. Kaw and Sen [21] studied low-frequency modes in DPs using the GH equation for dust particles and assuming a Boltzmann distribution for electrons and ions. However, their GH model is valid only in the long-wavelength limit, and it was primarily developed for one-component plasmas (OCPs); ambiguities remain regarding the correct forms of GH equations [19, 21, 22].

However, the dynamics of SCPs may potentially be well-described using a kinetic formalism based on full Born-Bogolyubov-Green-Kirkwood-Yvon (BBGKY) hierarchy equations. In this paper, we derive a new hydrodynamic model that explicitly incorporates correlations, high-frequency (elastic) effects and viscous damping in a self-consistent and generalizable manner. This is done by inverting the usual order of closures: we first close the hydrodynamics equations and then close the underlying kinetic description. In the next section, we determine the hydrodynamic moment equations from the BBGKY hierarchy to describe the dynamics of non-ideal plasmas on a wide range of length and time scales. We discuss the two closures needed to obtain a generalization of the hydrodynamics model and highlight the approximations needed to do so. Connections to previous models of this type are discussed. Next, we use our new hydrodynamics model to obtain the properties of collective modes, including correlations and collisions, and we compare our results with those of previous models. We discuss our new MD results for the current autocorrelation function and compare these numerical results with the theoretical models. We then apply our results to three different plasma conditions to illustrate the implications of our new approach. Finally, we summarize and discuss the broad implications of our results to provide a perspective on the potential utility of this approach.

II. HYDRODYNAMIC MODEL

Deriving the macroscopic equations of hydrodynamics is a double closure problem in which, first, the BBGKY hierarchy is closed to obtain a kinetic equation (e.g., the Boltzmann equation) for the single-particle distribution function f_1 and, second, a hierarchy of moments is obtained and must also be closed [17]. In this section, we obtain the hydrodynamics equations for a strongly coupled system by inverting the order in which the closures are made; we first find the moments of the (unclosed) BBGKY hierarchy and then find closures for the resulting moment (hydrodynamics) equations that now contain self-consistent correlation information.

A. Moments of the BBGKY Hierarchy

We begin by considering a system of N particles of mass m, charge e, positions \mathbf{r}_i , velocities \mathbf{v}_i and Liouville distribution function $f_N(\mathbf{x}_1, ..., \mathbf{x}_N, t)$, where the $\mathbf{x}_i =$ $(\mathbf{r}_i, \mathbf{v}_i)$ are phase-space coordinates. The particles interact through an arbitrary pairwise potential $v(|\mathbf{r}_i - \mathbf{r}_j|)$ in the presence of an external potential $v_{ext}(\mathbf{r}_i, t)$. The evolution of the reduced distribution functions $f_{i=1,...,N-1}$, where

$$f_i(\mathbf{x}_1, \dots, \mathbf{x}_i, t) = \int d\mathbf{x}_{i+1}, \cdots, d\mathbf{x}_N f_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t), \quad (1)$$

is given by BBGKY hierarchy equations [23]. The first hierarchy equation is

$$\frac{\partial f_1}{\partial t} + \mathbf{v}_1 \cdot \nabla f_1 + \frac{\mathbf{F}_1^{ext}}{m} \cdot \frac{\partial f_1}{\partial \mathbf{v}_1} = -\frac{1}{m} \int \mathbf{K}_{12} \cdot \frac{\partial f_2}{\partial \mathbf{v}_1} \, d\mathbf{x}_2, \quad (2)$$

where $\mathbf{F}_{i}^{ext} = -\nabla_{i} v_{ext}(\mathbf{r}_{i}, t)$, $\mathbf{K}_{ij} = -\nabla_{i} v(|\mathbf{r}_{i} - \mathbf{r}_{j}|)$, and $f_{1}(\mathbf{x}_{1}, t)$ and $f_{2}(\mathbf{x}_{1}, \mathbf{x}_{2}, t)$ are the one- and two- body distribution functions, respectively. Typically, a kinetic equation is obtained at this point by finding a suitable functional relationship between f_{2} and f_{1} that closes the BBGKY hierarchy. We will now obtain the hydrodynamics equations from (2) directly.

We can obtain the moments of the distribution functions by multiplying (2) by some functions $\Phi(\mathbf{v}_1)$ and integrating over velocity. Choosing our set of functions to be $\Phi(\mathbf{v}) = \{1, \mathbf{v}_1, \mathbf{v}_1 \mathbf{v}_1\}$ and measuring moments relative to the mean velocity, we define

$$n(\mathbf{r}_1, t) = \int f_1(\mathbf{x}_1, t) \, d\mathbf{v}_1, \qquad (3)$$

$$u(\mathbf{r}_1,t) = \int \mathbf{v}_1 f_1(\mathbf{x}_1,t) \, d\mathbf{v}_1, \qquad (4)$$

$$\bar{\bar{\mathbf{P}}}(\mathbf{r}_1,t) = m \int (\mathbf{v}_1 - \mathbf{u}) (\mathbf{v}_1 - \mathbf{u}) f_1(\mathbf{x}_1,t) \, d\mathbf{v}_1, \quad (5)$$

$$\mathbf{Q}(\mathbf{r}_1,t) = m \int (\mathbf{v}_1 - \mathbf{u})^2 (\mathbf{v}_1 - \mathbf{u}) f_1(\mathbf{x}_1,t) \, d\mathbf{v}_1 \tag{6}$$

to obtain

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$$D_t n = -n\nabla \cdot \mathbf{u},\tag{7}$$

$$mnD_t \mathbf{u} = -\nabla \cdot \bar{\mathbf{P}} + n \mathbf{F}^{ext} - \mathcal{C}(\mathbf{r}_1, t), \qquad (8)$$

$$D_t P_{ij} = -P_{ij} \nabla_k u_k - P_{ik} \nabla_k u_j - P_{kj} \nabla_k u_i -\nabla_k Q_{ijk} - \mathcal{B}_{ij}(\mathbf{r}_1, t),$$
(9)

where

$$D_t = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla,$$

$$\mathcal{C}(\mathbf{r}_1, t) = \iint \mathbf{K}_{12} \mathbf{v}_1 \frac{\partial f_2}{\partial \mathbf{v}_1} d\mathbf{v}_1 d\mathbf{x}_2,$$

$$\mathcal{B}_{ij}(\mathbf{r}_1, t) = \iint \mathbf{K}_{12} (\mathbf{v}_1 - \mathbf{u})_i (\mathbf{v}_1 - \mathbf{u})_j \frac{\partial f_2}{\partial \mathbf{v}_1} d\mathbf{v}_1 d\mathbf{x}_2.$$

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The three final equations, which are still exact, are the continuity equation (7), the momentum equation (8), and the stress tensor equation (9). Note that the terms C and \mathcal{B}_{ij} contain all of the contributions from interparticle forces, and these two terms give rise to electric fields, collisions, and excess energy and pressure. As written above, these equations are not closed for two reasons: (1) we have not written an equation of motion for the heat flow, \mathbf{Q} , and (2) obtaining C and \mathcal{B}_{ij} requires knowledge of the two-particle distribution function f_2 . Nevertheless, this form illustrates how correlations formally enter into a hydrodynamic description. In the next subsection, we will employ dynamical density functional theory (DDFT) to achieve a partial closure.

B. Dynamical Density Functional Theory (DDFT)

Building on work by Cahn [24] and time-dependent Ginzburg-Landau models [25], it is possible to formulate the dynamics of a many-body system near equilibrium using the free energy functional $\mathcal{F}[n]$. Such DDFTs [26, 27] employ generalized forces (chemical potentials) in terms of the functional derivative $\delta \mathcal{F}[n]/\delta n(\mathbf{r})$. The use of density functional theory (DFT) as a closure for the momentum equation was first proposed by Ying [28], in the context of quantum hydrodynamics. Recently, Lutsko [29] has shown a more systematic way to derive a self-contained momentum equation using DDFT. The principal idea of DDFT is to relate the f_2 distribution function to properties of the free energy, $\mathcal{F}[n]$. We propose to introduce this approach as a closure for the SCP momentum equation.

First, let us briefly present some results of classical DFT [30] for equilibrium systems. The central result of DFT is that for a given density $n(\mathbf{r})$, there is a unique Helmholtz free energy functional $\mathcal{F}[n]$ with a form that does not depend on the external potential. Consequently, knowledge of $\mathcal{F}[n]$ completely determines the microscopic structure of the system. The (thermal) equilibrium density is given by the Euler-Lagrange equation

$$\frac{\delta \mathcal{F}[n]}{\delta n(\mathbf{r})} = \mu, \tag{10}$$

where μ is the chemical potential. The free-energy functional $\mathcal{F}[n]$ is typically decomposed into the four contributions of the non-interacting free energy $\mathcal{F}^{id}[n]$, the external potential energy $\mathcal{F}^{ext}[n]$, the Hartree energy $\mathcal{F}^{H}[n]$, and the correlation functional $\mathcal{F}^{cor}[n]$, as

$$\mathcal{F}[n] = \mathcal{F}^{id}[n] + \mathcal{F}^{ext}[n] + \mathcal{F}^{H}[n] + \mathcal{F}^{cor}[n], \qquad (11)$$

where the non-interacting free energy \mathcal{F}^{id} can be written explicitly (for classical plasmas) as

$$\mathcal{F}^{id}[n] = \beta^{-1} \int d\mathbf{r} \left[n \ln \left(\Lambda^3 n \right) - n \right], \qquad (12)$$

where $\beta = 1/k_B T$, k_B is Boltzmann's constant, T is the temperature, $\Lambda = h/2\pi\sqrt{mk_BT}$ is the thermal wavelength, and h is Planck's constant. The external potential contribution is given by

$$\mathcal{F}^{ext}[n] = \int n(\mathbf{r}) \, v_{ext}(\mathbf{r}) \, d\mathbf{r}.$$
 (13)

The Hartree term is

$$\mathcal{F}^{H}[n] = \frac{1}{2} \iint d\mathbf{r} d\mathbf{r}' \ n(\mathbf{r}) n(\mathbf{r}') v(|\mathbf{r} - \mathbf{r}'|), \qquad (14)$$

where $v(|\mathbf{r} - \mathbf{r}'|)$ is the pairwise potential. While the Hartree term is the mean-field portion of the interacting energy, it is the same term that gives rise to the self-consistent electric field in the context of plasma physics. Thus, this decomposition (11) ensures self-consistency among each of the contributions to the free energy; quantities such as the "electric field" and the various contributions to thermodynamic properties are not double-counted. The exact form of $\mathcal{F}^{cor}[n]$ is unknown [31, 32]; however, it can be expressed formally in terms of the direct correlation function $c(\mathbf{r}, \mathbf{r}')$, as follows:

$$c(\mathbf{r}, \mathbf{r}') = -\beta \frac{\delta^2 \mathcal{F}^{cor}[n]}{\delta n(\mathbf{r}) \delta n(\mathbf{r}')}.$$
 (15)

The direct correlation function is related to the static structure factor by the Ornstein-Zernike relation, which, in Fourier space, reads as

$$S(k) = \frac{1}{1 - n c(k)},$$
(16)

where k is the wavevector. Once the pair potential v(r) has been specified, c(r) can be calculated using integral equations, MD or Monte Carlo simulations, and the self-consistent \mathcal{F} is obtained.

Using (11)-(14) in (10) gives

$$\beta^{-1}\nabla \ln n(\mathbf{r}) + \nabla v_{ext} + \nabla U + \nabla \frac{\delta \mathcal{F}^{cor}[n]}{\delta n(\mathbf{r})} = \nabla \mu, \quad (17)$$

where

$$U(\mathbf{r}) = \int d\mathbf{r}' \, n(\mathbf{r}') v(|\mathbf{r} - \mathbf{r}'|) \tag{18}$$

is the mean-field potential. Note that for an inhomogeneous interacting fluid, the chemical potential is a constant, so $\nabla \mu = 0$ [30]. We are now in a position to use DFT to ensure that the equations of BBGKY yield the correct thermodynamic ground state.

In equilibrium, the velocity portions of the distribution functions are Maxwellian. In this limit, we multiply (2) by **v** and integrate it over velocity to obtain

$$\beta^{-1}\nabla n(\mathbf{r}_1) - n(\mathbf{r}_1)\mathbf{F}^{ext} = \int \mathbf{K}_{12} \, n_2(\mathbf{r}_1, \mathbf{r}_2) \, d\mathbf{r}_2, \quad (19)$$

where

$$n_2(\mathbf{r}_1, \mathbf{r}_2) = \iint d\mathbf{v}_1 d\mathbf{v}_2 f_2(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2).$$
(20)

Equation (19) is the equilibrium balance between the fluid pressure and the electrostatic pressure of the internal and external fields. This result is the first equation in the Yvon-Born-Green hierarchy. By ensuring consistency between (17) and (19), we can relate the unknown two-body distribution to the free-energy functional by writing

$$\nabla U(\mathbf{r}_1) - \nabla \frac{\delta \mathcal{F}^{cor}[n]}{\delta n(\mathbf{r}_1)} = \frac{\beta}{n(\mathbf{r}_1)} \int \mathbf{K}_{12} n_2(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_2.$$
(21)

This result corresponds to a specific sum rule for a fluid in DFT, and it relates the direct correlation function $c(\mathbf{r}_1, \mathbf{r}_2)$ to the two-particle density $n_2(\mathbf{r}_1, \mathbf{r}_2)$ [30]. DDFT assumes that for an arbitrary density of a fluid, it is always possible to find an external potential that forces the system into equilibrium. This configuration corresponds to an instantaneous value of the one-particle density $n(\mathbf{r}_1, t)$. Consequently, the two-particle density $n_2(\mathbf{r}_1, \mathbf{r}_2, t)$ can be replaced by its equilibrium value, $n_2(\mathbf{r}_1, \mathbf{r}_2)$, at any time. Substituting (17) into (19), the DDFT closure is readily found to be

$$\nabla U(\mathbf{r}_1) - \nabla \frac{\delta \mathcal{F}^{cor}[n]}{\delta n(\mathbf{r}_1, t)} = \frac{\beta}{n(\mathbf{r}_1, t)} \int \mathbf{K}_{12} n_2(\mathbf{r}_1, \mathbf{r}_2, t) d\mathbf{r}_2.$$
(22)

This closure was first obtained by Marconi and Tarzaconi [26] for classical fluids and was later extended to multibody interactions by Archer and Evans [27].

Note that the right-hand side of (22) is $C(\mathbf{r}_1, t)$; we can now eliminate $C(\mathbf{r}_1, t)$ in (8) to obtain the hydrodynamic equations

$$D_t n = -n\nabla \cdot \mathbf{u}, \tag{23}$$

$$mnD_t \mathbf{u} = -\nabla \cdot \bar{\mathbf{P}} + n\mathbf{F}^{ext} + n\nabla U - n\nabla \frac{\delta \mathcal{F}^{cor}}{\delta n}, (24)$$

$$D_t P_{ij} = -P_{ij} \nabla_k u_k - P_{ik} \nabla_k u_j - P_{kj} \nabla_k u_i \qquad (25)$$
$$-\nabla_k Q_{ijk} - \mathcal{B}_{ij}.$$

Our fluid equations are not yet closed. We now need to find approximations for the high-order moments: the stress tensor and the heat flow. To do so, we proceed as follows. In the hydrodynamic limit, where the mean free path of the particles, λ_{mfp} , is smaller than the macroscopic length of our system, $L = |\nabla n/n|^{-1}$, although the heat flow and the moments beyond are not zero, they can be neglected. Finally, the term \mathcal{B}_{ij} , which contains the two-particle distribution function, is estimated using a relaxation model; this procedure will be discussed in the next section.

C. Relaxation Closure of Higher Moments

Elastic effects were introduced in the classical fluid equations in the form of a memory function originally developed by Frenkel [19]. Our goal here is to include these effects in our model via the stress tensor equation.

To evaluate the stress tensor $\bar{\mathbf{P}}$, it is customary to decompose it as

$$\mathbf{P}_{ij} = P\delta_{ij} - \Pi_{ij},\tag{26}$$

where the diagonal terms of the stress tensor correspond to the pressure P, and the off-diagonal terms correspond to the dissipative effects Π_{ij} . Thus, using the Einstein summation convention, we insert (26) into (24) and (25) and separate the diagonal from the off-diagonal to find

$$mnD_{t}\mathbf{u} = -\nabla P + \nabla \cdot \Pi + n\mathbf{F}^{ext} + n\nabla U \qquad (27)$$
$$-n\nabla \frac{\delta \mathcal{F}^{cor}}{\delta n},$$
$$D_{t}P = -\frac{5}{3}P\nabla_{k}u_{k} - \frac{2}{3}\Pi_{ik}\nabla u_{i} - \mathcal{B}_{ii}, \qquad (28)$$
$$D_{t}\Pi_{ij} = -\Pi_{ij}\nabla_{k}u_{k} - \Pi_{ik}\nabla_{k}u_{j} - \Pi_{kj}\nabla_{k}u_{i},$$
$$+\frac{2}{3}\delta_{ij}\Pi_{lk}\nabla_{k}u_{l} + \mathcal{B}_{ij}$$

$$-P\left(\nabla_i u_j + \nabla_j u_i - \frac{2}{3}\delta_{ij}\nabla_k u_k\right). \quad (29)$$

An important approximation is to assume that the velocity gradients are small, so that the convective terms can be neglected: $\Pi_{ij} \nabla \mathbf{u} \sim 0$ and $P \nabla \mathbf{u} \sim 0$. If the velocity gradients are large, then one must take into account the convective terms; this situation will be discussed below. To retain elastic effects, we do not use a thermodynamic closure of the pressure tensor, but rather allow the two-particle distribution function \mathcal{B}_{ij} in (29) to fluctuate on a time scale τ using a phenomenological relaxation model. Combining these two approximations, we obtain for the pressure tensor

$$D_t P = \frac{P^0 - P}{\tau}, \tag{30}$$

$$D_t \Pi_{ij} = \frac{\Pi_{ij}^0 - \Pi_{ij}}{\tau}, \qquad (31)$$

where Π^0 and P^0 are the *equilibrium* values of the dissipative stress and the pressure, and here, Π and P are fluctuating quantities. Taking the convective derivative of (27) and using the spatial gradient of (31), we obtain

$$D_t \left[mnD_t \mathbf{u} + \nabla P - n\mathbf{F}^{ext} + n\nabla U + n\nabla \frac{\delta \mathcal{F}^{corr}}{\delta n} \right] = (32)$$
$$\frac{\nabla \cdot \Pi^0 - \nabla \cdot \Pi}{\tau}.$$

Finally, we replace the dissipative term $\nabla \cdot \Pi$ in the righthand side of (32) using (27) to yield a self-contained hydrodynamic model

$$D_t n + n\nabla \cdot \mathbf{u} = 0 \tag{33}$$

$$1 + \tau D_t \left(m n(\mathbf{r}, t) D_t \mathbf{u} + \nabla P - n(\mathbf{r}, t) \mathbf{F}^{tot} + n(\mathbf{r}, t) \nabla \frac{\delta \mathcal{F}^{cor}[n]}{\delta n(\mathbf{r}, t)} \right) = \nabla \cdot \Pi^0,$$
(34)

where $\mathbf{F}^{tot} = \mathbf{F}^{ext} - n(\mathbf{r}, t) \nabla U(\mathbf{r})$ is the external and the mean-field forces. Equations (33) and (34) are the main results of this work. We will refer to this new model as the viscoelastic-density functional (VEDF) model. It generalizes the hydrodynamic momentum equation to account for dissipative effects, elastic effects, and all impacts of Coulomb coupling through a self-consistent equation of state. In contrast with current hydrodynamic models, the VEDF satisfies a low-frequency sum rule through the density functional closure, and a high-frequency sum rule through the relaxation time τ . The usual Navier-Stokes equation for a viscous gas is recovered when τ is very small, and the correlation term \mathcal{F}^{corr} is negligible. We recover the hydrodynamic Bloch equations for fluids proposed by Ying [28] when we neglect viscoelastic effects.

When velocity gradients are large, the neglected terms in (29) become important. The relaxation time in the left-hand side of (34) can be seen as the first-order expansion of the elastic term around the velocity divergence,

$$\tau(\mathbf{u}) = \tau + \alpha \nabla \cdot \mathbf{u} + \dots, \tag{35}$$

where τ is the Maxwell relaxation time, and α is related to the microscopic effects of the fluid.

The VEDF model includes the relaxation time, viscosity and correlations in the form of external parameters. These quantities are determined as follows. For a fluid system, the rate of stress can be written as

$$\Pi_{ij} = \eta \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) + \xi \frac{\partial u_k}{\partial x_k} \delta_{ij}, \quad (36)$$

where η and ξ are the shear and bulk viscosities, respectively. The Maxwell relaxation time is given by

$$\omega_p \tau = \frac{3\,\bar{\eta}\Gamma}{1 - \gamma_i \mu + \frac{4}{15}E_c}.\tag{37}$$

Here, $\omega_p = (4\pi e^2 n_0/m)^{1/2}$ is the plasma frequency, $a_i = (3/4\pi n_0)^{1/3}$ is the Wigner-Seitz radius, $\Gamma = e^2/k_B T a_i$ is the coupling parameter, γ is the adiabatic index, μ is the compressibility, $E_c(\Gamma, \kappa)$ is the correlation energy in units of temperature $k_B T$, $\kappa = a_i/\lambda_{De}$ is the screening parameter, λ_{De} is the Debye length, and the normalized viscosity $\bar{\eta}$ is defined as

$$\bar{\eta} = \frac{\frac{4}{3}\eta + \xi}{m n_0 \,\omega_p \,a_i^2}.$$
(38)

The equations are still not closed because we must specify the viscosity and correlation energy. These quantities are determined through MD and integral equations, as will be described below.

An approximation for the free energy $\mathcal{F}[n]$ remains to be found. While we have an analytical expression for the density functional for the non-interacting fluid, the correlation energy $\mathcal{F}^{cor}[n]$ is unknown. Various models have been developed to estimate the free excess energy [31, 32]. We recall here the expression of the free excess energy obtained by Ramakrishnan and Yussouff [33]; this expression is obtained from the Taylor expansion of the direct correlation around a uniform density n_0 . The firstorder terms of this expansion can be written as

$$\mathcal{F}^{cor}[n] = \mathcal{F}^{cor}[n_0] - \frac{1}{2\beta} \iint \bar{n}(\mathbf{r}')\bar{n}(\mathbf{r})c(|\mathbf{r} - \mathbf{r}'|)d\mathbf{r}d\mathbf{r}', (39)$$

where $\bar{n}(\mathbf{r}) = n(\mathbf{r}) - n_0$. In this work, the direct correlation function is obtained using a hypernetted chain (HNC) approximation.

In the next section, we compare the new VEDF model to previously developed models.

III. REVIEW OF PREVIOUS THEORETICAL MODELS

A. Generalized Hydrodynamics (GH)

Classical fluid theory, as expressed by the Navier-Stokes equation, does not incorporate elastic effects. To remedy this deficiency, Frenkel [19] extended classical hydrodynamic theory to elastic fluids by replacing the viscosity coefficient with a nonlocal operator that accounts for the elastic properties of fluids.

The GH equations describing the dynamics of a fluid, obtained by Frenkel [19] and applied to dense plasmas by Kaw and Sen [21], can be written for the momentum equation as

$$\left(1+\tau\frac{\partial}{\partial t}\right)\left[m\,n\frac{\partial\mathbf{u}}{\partial t}-en\,\mathbf{E}+\nabla P\right]=\nabla\cdot\Pi^{0},\quad(40)$$

where **E** is the self-consistent electric field, P is the pressure, and Π^0 is the dissipative term.

Note the way that the derivatives $\frac{\partial}{\partial t}$ and D_t appear in (34) and (40). In previous studies [20, 21, 34, 35] that employed models like (40), different combinations of a partial time derivative $(\frac{\partial}{\partial t})$ and a convective derivative (D_t) have appeared. However, our derivation from the BBGKY hierarchy reveals that both of the derivatives in these equations should be D_t . However, in the case of

linear low-frequency modes, the convective derivative will have no effect on the dispersion relation because $\mathbf{u} \cdot \nabla \mathbf{u}$ is a second-order term and can consequently be neglected. For nonlinear waves in SCPs, additional terms may be important.

Another important difference between the VEDF model and the GH model is that the VEDF model describes viscoelastic effects, excess pressure and collisions, whereas GH considers collisions only through the viscoelastic term. It follows that to improve the GH approach, one must find a way to include a better equation of state to account correctly for correlations. Toward this end, Shukla [34] added a new force, which is supposed to represent the polarizing force between strongly coupled ions and electrons, to the generalized momentum equation. The generalized momentum equation proposed by Shukla can be written as

$$\left(1+\tau\frac{\partial}{\partial t}\right)\left[mn\frac{\partial \mathbf{u}}{\partial t}-(1-R)en\mathbf{E}+\nabla P\right]=\nabla\cdot\Pi^{0}.(41)$$

Here, R accounts for the polarization force emanating from the interactions between the thermal electrons and the strongly coupled ions and is given by $R = e^2/4k_BT_e\lambda_{De} \leq 1$, where T_e corresponds to the electron temperature. In comparison with (34), we are unable to justify a term of the form in (41).

B. Singwi-Tosi-Land-Sjolander (STLS) Closure

Murillo [15] developed a hydrodynamic model for SCPs based on the STLS [9] closure of BBGKY,

$$f_2(\mathbf{x}_1, \mathbf{x}_2) = f_1(\mathbf{x}_1, t) f_1(\mathbf{x}_2, t) g(\mathbf{r}_1 - \mathbf{r}_2), \qquad (42)$$

where $f_1(\mathbf{x}, t)$ is the one-body distribution function, and $g(\mathbf{r}_1 - \mathbf{r}_2)$ is the equilibrium pair correlation function. This approximation satisfies the relevant (for hydrodynamics) low-frequency sum rules but violates highfrequency sum rules. (This approach was later extended using a generalized Navier-Stokes approach [16].)

With the closure (42), the hydrodynamics equations for the density and the momentum become

$$\frac{\partial n}{\partial t} + \nabla \cdot \left(n\mathbf{u} \right) = 0, \qquad (43)$$

$$m\frac{\partial(n\mathbf{u})}{\partial t} + \nabla \cdot \left[n\langle \mathbf{v}\mathbf{v}\rangle\right] = n\left(\mathbf{F}^{corr} + \mathbf{F}^{ext}\right), \quad (44)$$

where

$$\mathbf{F}^{corr}(\mathbf{r}_{1},t) = \int \mathbf{K}_{12} n_{2}(\mathbf{r}_{1},\mathbf{r}_{2},t) g(\mathbf{r}_{1}-\mathbf{r}_{2}) d\mathbf{r}_{2},(45)$$
$$n_{2}(\mathbf{r}_{2},t) = \int f_{1}(\mathbf{x}_{2},t) d\mathbf{v}_{2}.$$
(46)

J
he term
$$\nabla \cdot [n \langle \mathbf{v} \mathbf{v} \rangle]$$
 which describes both the ideal

The term $\nabla \cdot \lfloor n \langle \mathbf{v} \mathbf{v} \rangle \rfloor$, which describes both the ideal pressure and the viscosity, was neglected in the original

work by Murillo [15]. Here, including this term, the momentum equation becomes

γ

$$nnD_t \mathbf{u} + \nabla \cdot \bar{\bar{P}} = n \big(\mathbf{F}^{corr} + \mathbf{F}^{ext} \big). \tag{47}$$

Assuming an equilibrium closure for the pressure tensor, we see that STLS hydrodynamics results in the usual Euler hydrodynamics equations in terms of the effective force

$$\mathbf{K}_{12}^{eff} \equiv \mathbf{K}_{12}(\mathbf{r}_1 - \mathbf{r}_2)g(\mathbf{r}_1 - \mathbf{r}_2).$$
(48)

Thus, as opposed to the VEDF model, STLS hydrodynamics does not account for viscosity or collisions, although it does include pair correlations associated with "excess" thermodynamic quantities. It is important to note that the STLS approach incorporates the physics of strong coupling directly through the two-body distribution function g(r), in contrast with the GH approaches of Kaw and Sen [21] and Shukla [34]. The VEDF model (34) consistently includes *both* contributions.

STLS hydrodynamics can be extended further by noting that higher-order moments would lead, in some circumstances, to non-spherical distributions and, therefore, to transport.

IV. COLLECTIVE MODES IN DENSE PLASMAS

In this section, we apply the VEDF formalism to study the properties of ion-acoustic waves (IAWs) in dense plasmas. First, we derive the dispersion relation of the wave, then we compare it with the results obtained with GH, QLCA and MD simulations. The features that these results have in common and that differentiate between the models are also discussed.

Let us consider, at time t = 0, a plasma composed of both electrons, with density n_{e0} and temperature T_e , and ions, with density n_0 , temperature T, and mass m. The ion temperature is assumed to be negligible compared with the electron temperature. Because the electron mass is small with respect to the ion mass, one can assume that the electrons are in Boltzmann equilibrium, with the self-consistent electrostatic potential ϕ .

At time t > 0, the ion dynamics are described by the VEDF equations (33) and (34). The electron-density distribution is determined by the Boltzmann distribution

$$n_e(\mathbf{r}, t) = n_{e0} \exp\left(\frac{e\phi}{k_B T_e}\right). \tag{49}$$

The electric potential ϕ is given by the Poisson equation

$$\nabla^2 \phi = 4\pi e \left(n_e - n \right). \tag{50}$$

To study the collective modes, we consider small densities and velocity perturbations as follows:

$$n_e(\mathbf{r},t) = n_{e0} + \frac{e\phi}{k_B T_e} n_{e0},$$
 (51)

$$n(\mathbf{r},t) = n_0 + \delta n, \tag{52}$$

$$\mathbf{u}(\mathbf{r},t) = \delta \mathbf{u}. \tag{53}$$

We insert these expressions into Eqs. (33), (34), and (50) and perform time and space Fourier transforms. The resulting dispersion relation takes the form

$$\frac{\omega^2}{\omega_p^2} = \frac{q^2}{3\,\Gamma\,S(q)} - \frac{i\,\bar{\eta}\,q^2}{1 - i\,\omega\,\tau}\frac{\omega}{\omega_p},\tag{54}$$

where $q = ka_i$ is the normalized wave vector. To find the static structure factor S(q), we have performed numerical simulations with a code constructed using the HNC approximation for Yukawa systems. The HNC approximation has been modified with a bridge function to describe SCPs. The numerical code is presented in more detail in [36]; it has been validated by comparisons with MD simulations.

The dispersion relation of IAWs in the GH model is given by

$$\frac{\omega^2}{\omega_p^2} = \frac{q^2}{\kappa^2 + q^2} + \frac{q^2}{3\Gamma} - i\frac{\bar{\eta}\,q^2}{1 - i\omega\tau}\frac{\omega}{\omega_p}.\tag{55}$$

Now, assuming finite off-diagonal contributions to the pressure tensor, the Navier-Stokes variant of STLS hydrodynamics yields the following dispersion relation for IAWs:

$$\frac{\omega^2}{\omega_p^2} = \frac{q^2}{q^2 + \kappa^2} \left[1 - G(q) \right] + \frac{q^2}{3\Gamma} - i\,\bar{\eta}\frac{\omega}{\omega_p}q^2, \qquad (56)$$

where the static local field correction G(q) serves as a generalized compressibility. The second and third terms on the right-hand side of (56) correspond to the thermal portion of the pressure and the viscous damping, respectively, which were previously neglected in [15].

However, the generalization of STLS hydrodynamics in (56) is not closed because of the appearance of the viscosity, which must be considered as a phenomenological, constitutive property. In fact, we also typically specify G(q); in this sense, (42) is not a true closure because it requires the specification of g(r). Originally, STLS imposed a self-consistency condition to obtain g(r), whereas Murillo employed the HNC approximation to avoid unphysical (negative) properties of g(r).

To be complete, let us now discuss the QLCA. It is a theory with a microscopic basis that provides a good description of waves for SCPs. In the QLCA [10], particles are assumed to occupy local mean positions and to diffuse slowly. Since these positions change over a much longer time scale than the characteristic diffusion time, they are replaced by equilibrium configurations using the equilibrium pair-correlation function. This model has been designed to satisfy a high-frequency sum rule and is restricted to SCPs ($\Gamma \gg 1$). QLCA yields the dispersion relation for the IAW

$$\frac{\omega^2}{\omega_p^2} = \frac{q^2}{q^2 + \kappa^2} + \frac{q^2}{\Gamma} \left[\frac{4}{45} E_c - \frac{2}{45} y \frac{\partial E_c}{\partial y} + \frac{4}{15} y^2 \frac{\partial^2 E_c}{\partial^2 y} \right],\tag{57}$$

where $y = \kappa^2$, and $E_c(\Gamma, \kappa)$ is the correlation energy. For $\kappa \leq 1$, we evaluate $E_c(\Gamma, \kappa)$ and its derivative using the expression given in [37]. For $\kappa = 2$, we use values reported in Table VIII of [38].

A detailed comparison of these different analytical expressions for the dispersion relations of the IAWs will be presented in the next section, along with results obtained from MD simulations. First, we will discuss the procedure we have followed to extract the dispersion relation of IAWs from MD-simulation results.

V. MOLECULAR DYNAMICS (MD) SIMULATIONS AND DISCUSSION

To validate the models examined in this study, we carried out MD simulations to extract the dispersion relation of IAWs. Details of the code that we used have been described previously [39]. In our simulations, the ions interact through the Yukawa potential,

$$v(r) = \frac{\Gamma \exp(-\kappa r_{ij})}{r_{ij}},\tag{58}$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|/a_i$ is the relative distance between two particles, and v(r) is in units of $k_B T$. We integrate the equations of motion of N = 5000 particles with the Yukawa potential, using a second-order symplectic integrator (velocity-Verlet) with cubic periodic boundary conditions over a period of $5000 \, \omega_p^{-1}$. Excellent energy conservation was obtained with an integration time step of $10^{-2} \, \omega_p^{-1}$.

Using the computed positions $\mathbf{r}_i(t)$ and velocities $\mathbf{v}_i(t)$, we construct the current $\mathbf{j}(\mathbf{q}, t)$ for a given normalized wave vector \mathbf{q} at time t as follows:

$$\mathbf{j}(\mathbf{q},t) = \sum_{i=1}^{N} \mathbf{v}_i(t) \exp[i \,\mathbf{q} \cdot \mathbf{r}_i(t)].$$
 (59)

We then compute the time-dependent longitudinal current autocorrelation function,

$$C_l(q,t) = \frac{1}{N} \left\langle \left[\mathbf{q} \cdot \mathbf{j}_l(\mathbf{q},t) \right] \left[\mathbf{q} \cdot \mathbf{j}_l(-\mathbf{q},0) \right] \right\rangle, \quad (60)$$

by averaging the longitudinal component $\mathbf{q} \cdot \mathbf{j}_l(\mathbf{q}, t)$ over all of the particles in our system. The spectrum of the longitudinal current autocorrelation is obtained by taking the Fourier transform of (60) to obtain

$$C_l(q,\omega) = \int_0^\infty dt \, C_l(q,t) \cos(\omega t). \tag{61}$$

For a given value of the wave number q, the dispersion relation of IAWs $\omega = \omega(q)$ corresponds to the peak of $C_l(q, \omega)$.

A selection of our results is shown in Figure 1, which displays the normalized longitudinal current autocorrelation function $C_l(q,t)$ (top panel) and its spectrum for $\Gamma = 2, \kappa = 0.1$ and for a range of the wave number q(bottom panel). This procedure was performed repeatedly to obtain the dispersion relation of IAWs for a wide





FIG. 1: (Color online) Normalized longitudinal current autocorrelation function as function of time $\omega_p t$ and its spectrum for $\kappa = 0.1$ and $\Gamma = 2$.

range of values of Γ and κ . In the subsections below, we explore the results of the VEDF model for specific types of plasmas: UCNPs, DPs and high energy-density plasmas (HEDPs).

A. Ultracold Neutral Plasmas (UCNPs)

It is possible to produce an UCNP via photo-ionization of laser-cooled atoms or molecules [40]. In such plasmas, the electron and ion temperatures are ~ 10 mK and ~ 10 μ K, respectively, with plasma densities in the range 10^{9-10} cm⁻³. These SCPs typically have coupling parameters in the range $\Gamma ~ 1-5$ and screening parameters in the range $\kappa ~ 0.5-3$, allowing us to probe plasma properties in a regime where the physics of strong coupling is moderate, but not perturbative. Thus, UC-NPs allow us to explore predictions of the VEDF model in the intermediate regime between traditional plasmas and very SCPs.

Using the Yukawa model for the ions in an UCNP, we have computed the dispersion relation for IAWs using several models and MD. Panels (a) and (b) of Figure 2 show the normalized dispersion relations obtained using the VEDF model, the usual GH model, the QLCA and MD simulations for typical UCNP conditions. The agreement between the VEDF model and the MD results is excellent. The GH model discussed above (in section III A) departs significantly from VEDF and MD results in the short-wavelength limit; this difference may be explained by the fact that the GH model was developed primarily for OCPs [20], and it does not include the correct Yukawa equation of state. We also observe that the QLCA approximation [10], which was designed for very SCPs ($\Gamma \gg 1$), is quite inaccurate in this intermediate coupling regime.

The dispersion relation of IAWs in UCNP has been measured in the long-wavelength regime by Killian and coworkers [8]. These investigators measured the density modulation of the waves and extracted the dispersion relation of the IAW using mean-field theory (Vlasov). Figure 3 (a) shows the dispersion relation of IAWs in the long-wavelength limit obtained using Vlasov theory, GH, QLCA and the VEDF model for $\Gamma = 5$ and $\kappa = 1$. It can be seen that the Vlasov dispersion relation is in quite good agreement with the other theoretical models for these plasma conditions at long wavelengths. This can be understood by noting that the long-wavelength sound speed is inversely related to the compressibility, which, in turn, is related to the long-wavelength limit of the static structure factor S(0). In Figure 3 (b), we compare the structure factors obtained using the HNC approximation and Vlasov theory, with the inset showing the results at very long wavelengths. One can clearly see that the Vlasov theory captures most of the compressibility for these plasma conditions, suggesting that c(r) plays a small role. Because the mean-field theory is a reasonable approximation in the hydrodynamic limit $q \rightarrow 0$ and because the MD results reveal larger discrepancies at shorter length scales, UCNP experiments could potentially be performed at very short wavelengths.

B. Dense, High Energy-Density Plasmas (HEDPs)

Dense plasmas are readily created in the laboratory with radiation, shocks, and beams [1, 2, 7]; in many cases, the resulting plasmas are strongly coupled [12]. Such plasmas are electron-ion mixtures describable in terms of generalized Coulomb coupling parameters $\Gamma_{ij} =$ $Z_i Z_i e^2 / a_{ij} K$, where K is the mean kinetic energy. For a near-equilibrium classical plasma, T is just the usual, common temperature of the species, whereas, for degenerate electrons, K is modified to include Pauli exclusion [12]; when the ions are moderately to strongly coupled and the electrons are partially degenerate, the plasma is referred to as "warm dense matter" (WDM). Dense plasmas differ from the UCNP discussed above in that a larger range of ion coupling is possible, the electrons may or may not be degenerate, and the ionization state is not necessarily well known or defined [41]. For example, in ICF experiments [2, 7], the target materials range from condensed matter through WDM to a nearly ideal plasma. Conversely, experiments at the LCLS create very strongly coupled matter on the cool side of WDM [1].

Properties of IAWs corresponding to conditions over the wide range of high energy-density conditions are displayed in Figures 2 (b)-(d). For strongly coupled plasmas with screening parameter $\kappa \leq 2$, the QLCA successfully compares with the VEDF model, as shown in Figures 2 (b) and (c). Figure 2 (d) shows the dispersion relations of the same models for $\Gamma = 100$ and $\kappa = 2$, and excellent agreement between the VEDF model and MD results can be seen. It should be noted that the GH curve is completely separated from the curves obtained from MD simulations and the VEDF model for SCPs, even



FIG. 2: (Color online) Dispersion relations of the longitudinal waves obtained using the VEDF model (green solid line) for a range of Γ and κ . The results of the VEDF model are compared with those of the QLCA model (red square line), the GH model (blue dashed line) and MD simulations (black dots). The frequency is normalized by an ion plasma frequency $\omega_p = (e^2 n_0 / \epsilon_0 m^2)^{1/2}$ and the wave vector $q = |k|a_i$ with the Wigner-Seitz radius $a_i = (3/4\pi n_0)^{1/3}$.



FIG. 3: (Color online) (a) Dispersion relations of longitudinal waves obtained using the usual Vlasov dispersion relation, GH, the VEDF model and the QLCA for $\Gamma = 5$ and $\kappa = 1$. (b) The static structure factor obtained using the HNC approximation and the mean-field theory (Vlasov) for the same parameters as in Figure 2. The insert shows detail around wavelengths where $q = ka \leq 0.5$, corresponding to the regimes accessible by experiments and measured by Killian and coworkers [8].



FIG. 4: (Color online) Dispersion relations of longitudinal waves obtained from VEDF, GH, QLCA and MD simulations for $\Gamma = 150$ and $\kappa = 0.1$. In this figure the MD data is taken from Ref. [43]. The agreement between the molecular dynamics data and the VEDF model is excellent.

in the hydrodynamic limit. Similarly, the phase velocity of the wave obtained with the QLCA is strongly reduced in the short-wavelength limit, leading to a large disagreement with the VEDF model and MD results. The QLCA tends to be very accurate when the effective coupling is very large [42]. To illustrate this, in Figure 4, we compare the MD results of Ohta and Hamaguchi [43] with the predictions of the VEDF, QLCA and GH models, for $\Gamma = 150$ and $\kappa = 0.1$. Here, the agreement between MD, the VEDF model and the QLCA results is rather good. In general, however, the VEDF model yields very accurate results over the entire range of dense plasma experiments within the Yukawa approximation.

C. Dusty Plasmas (DPs)

Dusty plasmas (DPs) are normal plasmas that have a background composed of electrons, ions and neutrals but also contain micron-scale particulates ("grains" or "dust") that are highly charged by fluxes from the background plasma species. While the dust particles are fairly dilute $(n \sim 10^4/\text{cc})$, they are cooled by dust-neutral collisions and can have charges in the $Q/e \sim 1,000-10,000$ range; because Γ scales with the square of that charge, DPs are very SCPs and readily crystallize. The properties of the background plasma are consistent with those of a very weakly coupled plasma, making the Yukawa model for three dimensional DPs quite reasonable. (In laboratory experiments in which the sheath is used to trap the grains, wake potentials can form [11]; nevertheless, the Yukawa approximation still serves as a generic model for such plasmas, especially monolayers.) Here, we do not consider dust lattice waves, but we note that Figures 2 (d) and 4 illustrate the dispersion relations of dust-acoustic waves for plasmas with parameters similar to those of DPs. The VEDF model describes such DPs very well.

VI. CONCLUSION

In this paper, we have derived a new hydrodynamic model (VEDF) for SCPs through a moment-based method within a kinetic theory framework. Rather than obtaining moments from a closure of the BBGKY hierarchy, such as the Boltzmann equation, and then closing the moment hierarchy, we obtain the hydrodynamic moments directly and exactly from the full BBGKY hierarchy. This yields (unclosed) equations for the plasma density, momentum and stress tensor; these moments contain all correlation information and allow us to introduce a different set of closures that retain correlations. Because it is important to avoid double-counting in field terms, correlation terms, and collision terms, we ensure that the equilibrium limit of the momentum equation is connected with the thermodynamic ground state specified by DFT through a DDFT approach. This approximation assumes that the equilibrium condition that expresses the two-body distribution with the free excess energy functional holds when the system is out of equilibrium. The second approximation is the relaxation model for the stress tensor.

We have also compared the results of the VEDF model with previous results in this area. Despite the various approximations that were needed, the approach lends itself to systematic generalizations and helps to resolve discrepancies among previous models [19, 21, 22]. In contrast with existing approaches, including GH, the STLS approximation, and the QLCA, the VEDF model presented here explicitly incorporates a self-consistent equation of state and dissipative and elastic effects. In addition, the VEDF formalism satisfies both low- and high-frequency sum rules. Furthermore, the hydrodynamic model based on the STLS ansatz proposed by Murillo [15] was generalized here to include dissipative effects. When the elastic effects are small, the VEDF model reduces to this hydrodynamic approach.

In the second part of this paper, we used the VEDF model to study collective modes in Yukawa fluids. Explicit expressions for the dispersion relations of the longitudinal wave were analytically derived from the VEDF model, GH, and the QLCA and evaluated numerically. The correlation density functional $\mathcal{F}^{cor}[n]$ in the VEDF model was estimated using the Ramakrishnan and Yussouff [33] Taylor expansion around a uniform density of the direct correlation function $c(\mathbf{r})$. Thus, the direct correlation function was provided by the HNC approximation [36]. We evaluated the relaxation time τ using the data for the correlation energy given in [37] and [20]. The values for the viscosity were taken from [38]. We used MD simulations to obtain the dispersion relation of the IAWs for different types of plasmas by calculating the current autocorrelation. The results obtained with the VEDF model were successfully confirmed by MD data.

The dispersion relation of IAWs was measured experimentally by Killian and coworkers for UCNPs in the hydrodynamic limit. Their results show good agreement with results obtained using mean-field theory. The reason for this agreement is that the contribution of the correlations to the compressibility is very small. Here, we have not found numerical results for our main result, (34), but rather have focused on linear waves in dense plasmas. In this regard, the effects of the nonlinear physics that it contains remain an open area of investigation.

We conclude by mentioning that it should be convenient to use the VEDF formalism to describe a large number of physical problems: shock waves in DPs [35], quantum properties in plasmas [28], vapor condensation and turbulence in clouds [44], and blood-particle deposition [45]. Extension of this model to magnetized plasmas, quantum systems [46], nonlinear problems and mixtures is left for future work.

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- [1] C. Bostedt *et al.*, J. Phys. B **46**, 164003 (2013).
- [2] O. Hurricane *et al.*, Nature **506**, 343 (2014).
- [3] T. C. Killian, Science **316**, 705 (2007).
- [4] M. Lyon, S. D. Bergeson, A. Diaw, and M. S. Murillo, Phys. Rev. E 91, 033101 (2015).
- [5] T. M. Flanagan and J. Goree, Phys. Plasmas 17, 12 (2010).
- [6] F. Graziani *et al.*, High Energy Density Phys. 8, 105-131 (2011).
- [7] A. J. MacKinnon *et al.*, Phys. Plasmas **21**, 5 (2014).
- [8] T. C. Killian, P. McQuillen, T. M. O'Neil, and J. Castro, Phys. Plasmas 19, 055701 (2012).
- [9] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).
- [10] M. Rosenberg and G. Kalman, Phys. Rev. E 5, 1862 (1998).
- [11] J. E. Hammerberg, D. S. Lemons, M. S. Murillo, and D, Winske, IEEE Trans. Plasma Science 29, 247 (2001).
- [12] M. S. Murillo, Phys. Plasmas **11**, 2964 (2004).
- [13] M. M. Marinak et al., Phys. Plasmas 8, 2275 (2001).
- [14] J. H. Irving and J. G. Kirkwood, J. Chem. Phys. 18, 817 (1950).
- [15] M. S. Murillo, Phys. Plasmas 5, 3116 (1998).
- [16] M. S. Murillo, Phys. Plasmas 7, 33 (2000).
- [17] C. D. Levermore, J. Stat. Phys. 83, 5 (1996).
- [18] J. P. Boon and S. Yip, *Molecular Hydrodynamics* (Dover, New York 1980).
- [19] J. Frenkel, Kinetic Theory of Liquids, (Clarendon, Oxford) (1946).
- [20] Ichimaru, H. Iyetomi, and S. Tanaka, Phys. Rep. 149, 91 (1987).
- [21] P. K. Kaw and A. Sen, Phys. Plasmas, 5 10 (1998).
- [22] M. A. Berkovsky, J. Plasma Phys. **50**, 359 (1993).
- [23] R. L. Liboff, Kinetic theory : classical, quantum, and relativistic descriptions (Springer, New York 2003).
- [24] J. W. Cahn and J. E. Hilliard, J. Chem. Phys. 28, 258 (1958).
- [25] P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. 49,

435 (1977).

- [26] U. M. B. Marconi and P. Tarazona, J. Chem. Phys. 110, 8032 (1999).
- [27] A. J. Archer and R. Evans, J. Chem. Phys. **121**, 4246 (2004).
- [28] S. Ying, Nuovo Cimento B, Series 11 23, 270 (1974).
- [29] J. F. Lutsko, Adv. Chem. Phys. **144**, 92 (2010).
- [30] R. Evans, Adv. Phys. 28, 143 (1979).
- [31] Y. Rosenfeld, Phys. Rev. Lett. 63, 980 (1989).
- [32] J. K. Percus, J. Stat. Phys. 15, 505 (1982).
- [33] T. V. Ramakrishnan and M. Youssouf, Phys. Rev. B 19, 2775 (1979).
- [34] P. K. Shukla, Phys. Lett. A **374**, 3656-3657 (2010).
- [35] A. A. Mamun and R. A. Cairns, Phys. Rev. E 79, 055401(R) (2009).
- [36] W. Daughton, M. S. Murillo, and L. Thode, Phys. Rev. E 61, 2129 (2000).
- [37] M. Rosenberg and G. Kalman, Phys. Rev. E 56, 7166 (1997).
- [38] S. Hamaguchi, R. T. Farouki, and D. H. E. Dubin, Phys. Rev. E 56, 4671 (1997).
- [39] M. S. Murillo, Phys. Rev. Lett. 87, 115003 (2001).
- [40] J. P. Morrison, C. J. Rennick, J. S. Keller and E. R. Grant, Phys. Rev. Lett. 101, 205005 (2008).
- [41] M. S. Murillo, J. W., S. B. Hansen, and M. W. C. Dharma-wardana, Phys. Rev. E 87, 063113 (2013).
- [42] T. Ott, M. Bonitz, L. G. Stanton, and M. S. Murillo, Phys. Plasmas 21, 113704 (2014).
- [43] H. Ohta and S. Hamaguchi, Phys. Rev. Lett. 84, 6026 (2000).
- [44] G. Falkovich, A. Fouxon, and M. Stepanov, Nature 419, 151 (2002).
- [45] P. Worth Longest and C. Kleinstreuer, J. Biomech. 36, 421 (2003).
- [46] Yu. V. Arkhipov, A. B. Ashikbayeva, A. Askaruly, A. E. Davletov, and I. M. Tkachenko, Phys. Rev. E 90, 053102 (2014).