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Excess pressure and electric fields in nonideal plasma hydrodynamics

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Nonideal plasmas have nontrivial space and time correlations, which simultaneously impact both the excess thermodynamic quantities as well as the collision processes. However, hydrodynamics models for designing and interpreting nonideal plasma experiments, such as inertial-confinement fusion experiments, typically neglect electrodynamics, although some models include electric fields indirectly through a generalized Fick's law. However, because most transport models are not computed self-consistently with the equation of state, there is double counting of the forces in the excess thermodynamic quantities and the collision terms. Here we employ the statistical mechanical hydrodynamic theory of Irving and Kirkwood [J. Chem. Phys. **18**, 817 (1950)] to examine inhomogeneous, nonideal plasmas that contain electric fields. We show that it is not possible to simultaneously separate terms that correspond to electric fields and excess pressure; rather, these quantities arise from the same interparticle Coulomb forces. Moreover, new terms associated with nonlocality appear in the presence of strong inhomogeneities.

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I. INTRODUCTION

Strong, self-generated electric fields [1,2] and barodiffusion [3,4] have been reported to play important roles during capsule implosions in inertial-confinement-fusion (ICF) experiments. Measurements of these phenomena [5–7] have renewed interest in models of multispecies phenomena in hot, dense plasmas [8–10]. Our ability to accurately model such heterogeneous, dense plasmas relies on a well-devised mathematical model that correctly reflects essential physical processes. For high energy-density matter, we rely heavily on hydrodynamic models, which may not properly or self-consistently describe the excess pressure (beyond the ideal-gas pressure), electric fields, and other nonlocal correlation effects. A rigorous hydrodynamic model would allow us to more accurately model a wide variety of phenomena, including shock waves and interfacial diffusive mixing, with a level of confidence similar to that provided by high-fidelity microscopic descriptions [11–14].

Euler hydrodynamic models [15] (those with vanishing Knudsen number), which rely on high-quality equations of state (EOSs)[16], are often used in the design and interpretation of highenergy-density experiments [2,17]. The Euler approximation is now known [18–20] to give imprecise explanations of recent experimental results, especially at higher temperatures, where the Knudsen number is finite. The discrepancies between experimental results and theoretical predictions observed in ICF are believed to emerge in large part from the absence of electric-field terms in the Euler hydrodynamic equations, barodiffusion [3,4], and thermodiffusion [21]. These effects are not included in standard dense-plasma fluid codes, which are based on a single-fluid description; however, generalization to a multifluid description with electric and magnetic fields is possible in principle.

At the microscopic level, the excess pressure, electric field, and collisions arise from the same potential energy term in the Liouville equation [22]. Therefore, care is needed to correctly separate the different contributions that arise from the interaction (potential-energy) terms to avoid double counting. Because it is not possible to obtain the correct excess pressure from a kinetic equation, it is necessary to find the hydrodynamic moments directly from the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy [23,24], which requires novel closures. Such a problem is generic, occurring widely in related fields, and free-energy methods have been used to create closures that avoid double counting. For example, building on work by Cahn [25] and time-dependent Ginzburg-Landau models [26], it is possible to formulate the dynamics of a many-body system near equilibrium using the free-energy functional $\mathcal{F}[n(\mathbf{r})]$, where $n(\mathbf{r})$ is the one-body density. Such approaches, called dynamical density functional theory (DDFT) [23,24,27–29], 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 as a closure for the momentum equation was first proposed by Ying [30], in the context of quantum hydrodynamics [31]. The principal idea of DDFT is to relate the two-body distribution function in the BBGKY hierarchy [22] distribution function to properties of the free energy $\mathcal{F}[n]$. However, it is not clear how to extend this approach to heterogeneous plasmas for which there are important excess-pressure and electric-field contributions; here we address the delicate problem of the form of the multifluid hydrodynamic equations (Euler), when correlation effects and electric fields are essential features of the system under consideration, by using the set of hydrodynamic equations derived by Irving-Kirkwood-Bearman [32].

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In Sec. II, which serves primarily as a review, we examine nonideal plasmas from the opposing points of view of equilibrium statistical mechanics and the Vlasov equation to establish the nature of the problem we wish to solve in the following sections. In Sec. III we derive the hydrodynamic equations from a fundamental, classical-mechanical description of the many-body problem, using the Liouville equation for multispecies plasmas. For simplicity, we consider only semiclassical, electrostatic plasmas; the generalization to electrodynamics and/or quantum plasmas [33] is straightforward and does not impact our main results in any way. We show that the local force, which contains information about thermal and interaction effects, can be decomposed into a pressure term with nonlocal gradient corrections and a residual term arising from plasma heterogeneity. Finally, we examine the modifications to the EOSs needed to ensure self-consistency when an electric-field force term is incorporated into the momentum equation.

II. CORRELATIONS IN NONIDEAL PLASMAS

Before we embark on the derivation of hydrodynamics for interacting charged-particle systems with electric fields in the next section, we review some basic and well-known classical mechanics results that we will refer to in the following sections. Consider a classical, multispecies plasma modeled through the Hamiltonian

$$H = K + U, \tag{1}$$

$$K = \sum_{i=1} \frac{p_i^2}{2m_i}, \tag{2}$$

$$U = \sum_{i<j} \frac{Z_i Z_j e^2}{|\mathbf{r}_i - \mathbf{r}_j|}, \tag{3}$$

where the sums are over all particles. Here K is the total kinetic energy, and U is the total potential energy. For simplicity, we have neglected other terms (e.g., external fields) that have no direct impact on the main results. The particles can be grouped into species, and we will rewrite the Coulomb energies between species α and β as $U_{\alpha\beta}(r)$ below.

Using the Hamiltonian (1), we can establish the equilibrium thermodynamic properties of the plasma. A well-known result from statistical mechanics [34] is that the total pressure for a uniform mixture at (common) temperature T (here in energy units such that $k_B = 1$) is given by

$$P = \sum_\alpha n_\alpha T - \frac{1}{6}\sum_{\alpha,\beta} n_\alpha n_\beta \int d^3r\, r g_{\alpha\beta}(r) \frac{dU_{\alpha\beta}}{dr}, \tag{4}$$

where n_α are species number densities, $g_{\alpha\beta}(r)$ are the partial radial distribution functions (RDFs), and $U_{\alpha\beta}(r)$ are the pair interactions between species α and β that arise from the potential energy in (3). The first term is the ideal-gas contribution, which is a sum over species of partial ideal pressures. The second term is referred to as the "excess pressure," which can be important in dense plasmas; obtaining accurate values of this term is the main challenge in building realistic EOSs. Note that when an EOS is constructed (e.g., in the form of a table), *all* contributions from the potential energy (3) are included as accurately as possible [e.g., through the integration over the forces $dU_{\alpha\beta}/dr$ in molecular dynamics (MD) simulations, or sampling of the partition function in Monte Carlo simulations]; the gradient of (3), of course, reveals that the Coulomb forces are electric fields. Moreover, note that the total pressure cannot be decomposed into intraspecies partial pressures because interspecies cross-terms appear in the second summation; this fact has implications for constructing multifluid hydrodynamic models because, in practice, EOS tables are typically constructed for the *total* pressure of a composite material. The lack of a simple decomposition can be seen explicitly by rewriting (4) as

$$P = \sum_\alpha \left[n_\alpha T - \frac{n_\alpha^2}{6} \int d^3r\, r g_{\alpha\alpha}(r) \frac{dU_{\alpha\alpha}}{dr} \right] - \frac{1}{6} \sum_{\alpha\neq\beta} n_\alpha n_\beta \int d^3r\, r g_{\alpha\beta}(r) \frac{dU_{\alpha\beta}}{dr}. \tag{5}$$

The contributions from the final term explicitly reveal interspecies pressure terms that spoil the concept of a species partial pressure; moreover, while the quantity in parentheses might appear to be the total partial pressure of species α, even this separation is artificial because the factors $g_{\alpha\alpha}$ should be computed self-consistently with the cross-terms $g_{\alpha\beta}$.

For a charged particle system with potential energies of the form (3), each of the integrals in (4) is separately divergent because of the long-range nature of electric fields; recall that $g_{\alpha\beta}(r) \to 1$ for large r. For a charge-neutral plasma with $n_e = \sum_i z_i n_i$, where $z_e = -1$ is the electron charge and z_i is the charge of the ith ion species (in units of e), it is useful to introduce pair correlation functions $h_{\alpha\beta}(r) = g_{\alpha\beta} - 1$, which have the property that $h_{\alpha\beta}(r) \to 0$ for large r, and we can rewrite (4) as

$$P = \sum_\alpha n_\alpha T - \frac{1}{6}\sum_{\alpha,\beta} n_\alpha n_\beta \int d^3r\, r h_{\alpha\beta}(r) \frac{dU_{\alpha\beta}}{dr}. \tag{6}$$

Thus, the total pressure includes the electric fields between all species, with the consequence that we need to introduce $h_{\alpha\beta}(r)$ to isolate divergent terms that arise from the Coulomb interactions (3); we are left with a finite excess pressure of a nonideal plasma that includes long-range electric fields. Note that the pressure is a local quantity that depends on local, average densities n_α; as we will see in the next section, complications arise for heterogeneous plasmas in which $n_\alpha = n_\alpha(\mathbf{r})$.

As a specific example, consider a hydrogen-carbon mixture with species densities 10^{23} cm^{-3} for a range of temperatures $T = 1$–1000 eV. We obtain the ionization state $\langle Z \rangle$ for the mixtures from a Thomas-Fermi average-atom model [35], and the mean ionization states are shown in the top panel of Fig. 1. An estimate of the pressure for this system provides some insight into the various contributions to the pressure. Approximate forms for the $g_{\alpha\beta}(r)$ are needed; we begin with the direct correlation functions $c_{\alpha\beta}(r)$, which are related to the pair-correlation functions $h_{\alpha\beta}(r)$ through the mixture Ornstein-Zernicke equations [36]

$$h_{\alpha\beta}(r) = c_{\alpha\beta}(r) + \sum_k n_k \int d\mathbf{r}' c_{\alpha k}(|\mathbf{r} - \mathbf{r}'|) h_{k\beta}(|\mathbf{r}'|). \tag{7}$$

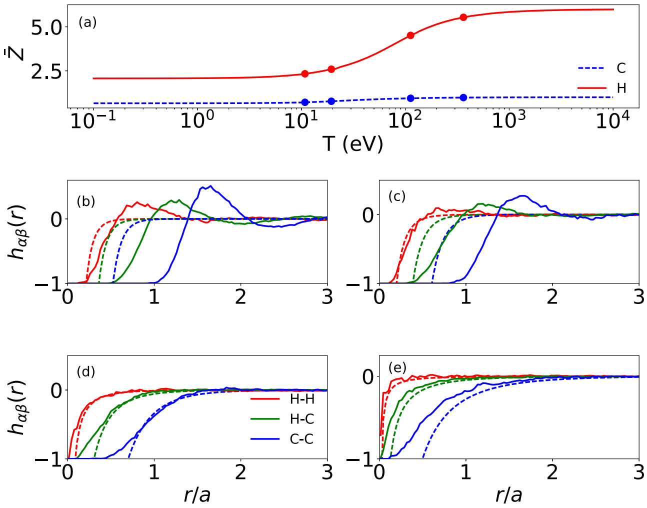

FIG. 1. Ionization and pair correlations for a binary-ionic mixture. (a) The top panel shows the mean ionization state (MIS) for a model system of plastic composed of equal densities of hydrogen and carbon (a CH plastic) with densities $n_H = n_C = 1 \times 10^{23}$ cm^{-3} and nuclear charges $Z = 1$ and $Z = 6$. (b)–(e) The various contributions of the total correlation functions $h_{\alpha\beta}(r)$ to the total pressure are shown for a model system of CH plastic, with $n_H = n_C = 1 \times 10^{23}$ cm^{-3}, heated to different temperatures: (b) 10 eV, (c) 21 eV, (d) 127 eV, and (e) 545 eV. The MD results are shown with solid lines, and the Debye-Hückel results (8) are shown with dashed lines. We see that the cross-correlation functions cannot be neglected because they are of the order of the mutual terms. Also, it is well known that the Debye-Hückel model does not capture the different peaks of the correlation functions, in contrast with MD.

At low densities, the direct correlation functions are known to be $Tc_{\alpha\beta}(r) \approx -Z_\alpha Z_\beta e^2/r$, which yield the Debye-Hückel (DH) pair-correlation functions for the mixture:

$$h_{\alpha\beta}(r) = -\frac{Z_\alpha Z_\beta e^2}{Tr}\exp(-r/\lambda_D), \tag{8}$$

where λ_D is the total Debye screening length defined through

$$\frac{1}{\lambda_D^2} = \sum_i \frac{1}{\lambda_{D_i}^2}. \tag{9}$$

Substituting (8) into (6) and integrating gives the total pressure

$$\frac{P}{nT} = 1 - \frac{\lambda_D}{2a}\Gamma^2 \sum_{\alpha,\beta} x_\alpha x_\beta Z_\alpha^2 Z_\beta^2, \tag{10}$$

where the coupling parameter is defined as $\Gamma = e^2/aT$, a is the interparticle radius given by $(3/4\pi n)^{1/3}$, $n = \sum_\alpha n_\alpha$ is the total density, and $x_\alpha = n_\alpha/n$ is the isotopic ratio. Equation (10) reveals the importance of the cross-term in coupling the species together.

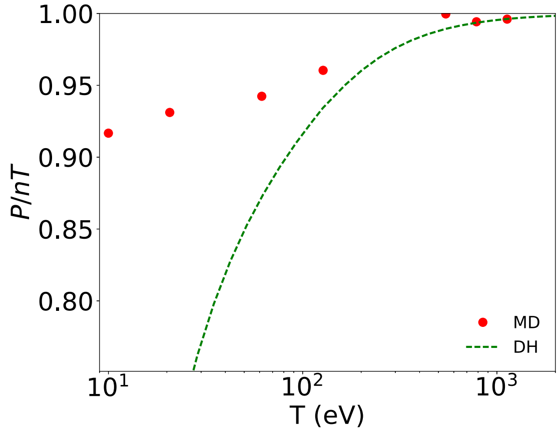

FIG. 2. The ionic pressure, in units of nT, as a function of temperature, from MD (dots) and the Debye-Hückel (dashed curve) prediction from (10). We see that the Debye-Hückel model is in good agreement with the MD results in the high-temperature limit but differs from the MD results in the low-temperature limit (i.e., in the strongly coupled regime).

While this analytical model provides valuable insights, the low-density approximation is not generally valid in nonideal plasmas, and another method is needed to obtain the correlation functions. We have performed MD simulations of a model system of hot plastic comprising carbon and hydrogen with equal number densities of 10^{23} cm^{-3} using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [37]. The binary ionic mixture consists of carbon and hydrogen ions embedded in a neutralizing electronic background. The particle interactions are modeled with Coulomb potentials, and long-range Coulomb forces are handled through an Ewald summation algorithm.

The MD simulations were set up as follows. We simulated a system of 4000 particles in a cube of volume L^3, with $L = 2.71$ nm. The equations of motion for N particles interacting through Coulomb potentials were solved using a velocity-Verlet integrator with periodic boundary conditions. We integrated the equations of motion in the canonical ensemble, with constant particle number, volume, and temperature maintained using a Nose-Hoover thermostat, over 10^6 time steps of 10^{-2} fs, to establish thermodynamic equilibrium at the desired temperature. Then the production runs were carried out in the microcanonical ensemble with 2×10^4 steps. Then the desired correlation functions $h_{\alpha\beta}$ were calculated with 330 bins in the range $0 < r < L/2$.

We obtain the pair-correlation functions $h_{\alpha\beta}(r)$ from the simulations and evaluate all of the contributions to the pressure. In Fig. 1 we plot the contributions of the pair-correlation functions $h_{\alpha\beta}(r)$ across a range of temperatures from $T = 10$ eV to $T = 1$ keV and compare them with the DH results obtained using Eq. (8). We see that the DH theory underestimates the RDF, as it misses all peaks in the structure for strongly coupled systems [low T here, as shown in Figs. 1(a) and 1(b)]. This is a well-known result, as the DH model is expected to hold only in the limit of small Γ; high-temperature and low-density results are shown in Figs. 1(d) and 1(e), where we observe qualitatively good agreement between the MD results and the DH model. More importantly, the interspecies term $P_{\alpha\beta}$ obtained by taking the moment force of the direct correlation functions $h_{\alpha\beta}$ cannot be neglected when evaluating the total pressure, as it is of the order of the intraspecies partial pressure terms. Finally, in Fig. 2 we observe again how important it is to account for the correlations in strongly coupled systems, where the DH model fails. This failure shows the need to go beyond the polytropic

EOSs for the ions used in multifluid codes [38] and consider more realistic EOSs.

Having established the equilibrium thermodynamic properties of a model plasma mixture, with a focus on the excess pressure, we now turn to a dynamic description of a plasma based on the Vlasov equation to explore how the EOS arises in that context and to compare it with the EOS description above. In a plasma mixture, the coupled Vlasov equations are [39]

$$\frac{\partial}{\partial t} f^{\alpha} + \mathbf{v} \cdot \nabla f^{\alpha} - \frac{q_\alpha \nabla \phi}{m_\alpha} \cdot \nabla_v f^{\alpha} = 0, \tag{11}$$

$$-\frac{1}{4\pi} \nabla^2 \phi = \sum_\alpha z_\alpha e \int d^3 v\, f^{\alpha}. \tag{12}$$

It is often stated that the Vlasov equation describes an ideal gas of charged particles interacting through a self-consistent electric field. This view is justified by the observation that the momentum equation, obtained by taking the $\mathbf{v}$ moment of the Vlasov equation, contains the term $\nabla \cdot \langle \mathbf{v}\mathbf{v} \rangle$, which arises from the advection term. Evaluated near thermal equilibrium, when that is valid, the diagonal portion of this tensor yields the ideal pressure through $\frac{1}{2} m_\alpha \langle (\mathbf{v} - \mathbf{u}_\alpha)^2 \rangle = \frac{3}{2} n_\alpha T$ [40]. Thus, we can write the full momentum equation as

$$\frac{\partial}{\partial t}(\rho_\alpha \mathbf{u}_\alpha) + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha \mathbf{u}_\alpha) + \nabla \cdot \mathbf{P}_0 = z_\alpha n_\alpha q_\alpha \mathbf{E}, \tag{13}$$

where $\rho_\alpha(\mathbf{r}) = m_\alpha \int d^3 v\, f_\alpha$ is the mass density of species α, $\mathbf{P}_0$ denotes the ideal-gas pressure tensor that arises solely from kinetic contributions, and $\mathbf{E}$ is the electric field. This form thus supports the narrative of an ideal gas interacting through a self-consistent electric field. In contrast with the statistical-mechanical description above, we note that two terms arise from the kinetic energy, one describing bulk motion and one describing internal kinetic energy (the second and third terms, respectively); neither of these terms involves forces. All contributions from forces appear in the electric-field term on the right-hand side.

Now, suppose that we have a nonideal plasma and that we have a precomputed EOS for our specific material, perhaps stored as a table. It is tempting to simply replace the ideal pressure with the total pressure by adding the excess pressure to the ideal pressure to obtain

$$\frac{\partial}{\partial t}(\rho_\alpha \mathbf{u}_\alpha) + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha \mathbf{u}_\alpha) + \nabla \cdot \mathbf{P} - z_\alpha q_\alpha n_\alpha \mathbf{E} \overset{?}{=} 0, \tag{14}$$

where $\mathbf{P}$ is the total pressure computed using a procedure similar to (4), although in practice, a quantum-mechanical version would be used. However, such a replacement is not possible, for two reasons. First, the total pressure cannot be decomposed into species-dependent portions, because of the interspecies contributions to the pressure; there are no well-defined partial "$\mathbf{P}_\alpha$" for each species, as shown above. Second, we have seen that the excess pressure arises from the interactions between species through electric fields, which already appear in the Vlasov force term as $\mathbf{E}$; this naive replacement would double count the forces. An alternative strategy is to retain $\mathbf{P}_0$ as the kinetic portion of the pressure and write the electric field in terms of the electrostatic potential, such that

$$P^{\mathrm{ex}} \overset{?}{=} \frac{z_\alpha}{m_\alpha} \phi(\mathbf{r}) \tag{15}$$

$$= \frac{z_\alpha e}{m_\alpha} \int_\Omega d^3 r\, \frac{n(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|}, \tag{16}$$

where $n(\mathbf{r}) = \sum_\alpha z_\alpha n_\alpha$ is the total density. However, two problems also arise with this viewpoint. First, it is not clear how correlations contained in $h_{\alpha\beta}(r)$ can be included in this approach. Second, this form does not lend itself to the usual EOS approach of precomputing (e.g., using tables) the pressure because the integration includes the inhomogeneous density $n(\mathbf{r}, t)$ over the *entire* volume Ω, which we do not know in advance; thus, electric fields contain a nonlocality not described in a standard EOS treatment, which, as we saw above, assumes that a plasma is infinite and homogeneous [41].

To summarize this review section, we note that standard EOS approaches assume homogeneity, disallow the concept of partial pressures for nonideal plasmas and naturally account for nonideality. In contrast, a standard Vlasov treatment includes an ideal-pressure term and an electric field that includes nonlocal contributions from the density, and the Vlasov approach neglects correlations beyond the mean field. We attempt to address these difficulties below by obtaining the mixture hydrodynamic equations from an exact formulation that includes all contributions self-consistently. Such an approach allows force terms to be isolated in a way that avoids double counting by isolating separate contributions, each of which arises from the same interaction terms.

III. IRVING-KIRKWOOD-BEARMAN HYDRODYNAMIC EQUATIONS

We employ an approach that does not assume a uniform system, as we did above in the statistical mechanical treatment; nor do we use the Vlasov approximation, as we did in the kinetic treatment. We begin with the same Hamiltonian in (1) and develop exact kinetic and hydrodynamic models, while allowing for a multifluid treatment.

Consider a mixture with ν different types of particles, with N_α being the number of types α, $\alpha = 1, \ldots, \nu$, and $N = \sum N_\alpha$ being the total number of particles contained in a volume V. The time evolution of the one-particle distribution function $f^{\alpha}(\mathbf{r}, \mathbf{v}, t)$ in phase space ($\mathbf{r}$ $\mathbf{v}$) obeys the lowest-order equation of the BBGKY hierarchy [22]:

$$\frac{\partial f^{\alpha}}{\partial t} + \mathbf{v} \cdot \nabla f^{\alpha} = \frac{1}{m_\alpha} \sum_{\beta=1}^{\nu} \int \nabla_{\mathbf{r}} U_{\alpha\beta} \cdot \frac{\partial f_2^{\alpha\beta}}{\partial \mathbf{v}}\, d\mathbf{r}'\, d\mathbf{v}', \tag{17}$$

where $U_{\alpha\beta}$ is the pair potential, and $f_2^{\alpha\beta}$ is the distribution of a pair of particles of types α and β. This equation and its coupling to the remainder of the BBGKY hierarchy are exact in the sense that, for a statistical description of a multispecies, classical, electrostatic Hamiltonian in (1), no approximations have been made. Of course, (17) is still too complex to deal with directly, but we can use it to obtain moments that are correspondingly exact. From those moments, we will attempt to systematically isolate the ideal pressure, excess pressure, and electric field. This work is restricted to classical plasmas. For modeling heterogeneous, nonequilibrium, quantum systems, many approaches based on quantum hydrodynamics—a computationally attractive approach with a rich history in statistical mechanics—have been developed [33,42,43].

The number density $n_\alpha(\mathbf{r},t)$ of particles of species α is given in terms of its single-particle distribution function $f^\alpha(\mathbf{r},\mathbf{v},t)$ in phase space as

$$n_\alpha(\mathbf{r},t) = \int d\mathbf{v} f^\alpha(\mathbf{r},\mathbf{v},t). \tag{18}$$

The local average velocity $\mathbf{u}_\alpha$ of species α is given by

$$\mathbf{u}_\alpha(\mathbf{r},t) = \frac{1}{n_\alpha(\mathbf{r},t)} \int d\mathbf{v}\mathbf{v} f_\alpha(\mathbf{r},\mathbf{v},t)\, d\mathbf{v}. \tag{19}$$

The local kinetic pressure (tensorial) exerted by species α is given by

$$\mathbf{p}_\alpha^{\mathrm{k}} = m_\alpha \int (\mathbf{v}_\alpha - \mathbf{u}_\alpha)(\mathbf{v}_\alpha - \mathbf{u}_\alpha) f^\alpha\, d\mathbf{v}. \tag{20}$$

Finally, we define the local kinetic energy as

$$e_\alpha(\mathbf{r},t) = \frac{1}{2} m_\alpha \int (\mathbf{v}_\alpha - \mathbf{u}_\alpha)^2 f^\alpha\, d\mathbf{v}. \tag{21}$$

The two-particle distribution function $f_2^{\alpha\beta}(\mathbf{r},\mathbf{v},\mathbf{r}',\mathbf{v}',t)$, which is proportional to the probability of species α being at ($\mathbf{r}$ in phase space, $\mathbf{v}$) with species β at ($\mathbf{r}'$, $\mathbf{v}'$) at time t, is related to the single-particle distribution function through

$$f^\alpha(\mathbf{r},\mathbf{v},t) = \sum_{\beta=1}^{N_\beta} \int d\mathbf{r}'\, d\mathbf{v}'\, f_2^{\alpha\beta}(\mathbf{r},\mathbf{v},\mathbf{r}',\mathbf{v}',t). \tag{22}$$

The relations (18) and (22) define our normalization for the multiparticle distribution functions. We also define a two-particle density $n_{\alpha\beta}$ of species α and β as

$$n_{\alpha\beta}(\mathbf{r},\mathbf{r}',t) = \int d\mathbf{v}\, d\mathbf{v}' f_2^{\alpha\beta}(\mathbf{r},\mathbf{v},\mathbf{r}',\mathbf{v}',t). \tag{23}$$

This quantity plays a key role in describing heterogeneous systems; in general, it is not a function of $\mathbf{r}-\mathbf{r}'$.

The velocity moments of (17) give the macroscopic equations for the plasma system. The full conservation laws for the density, momentum, and energy were derived by Irving and Kirkwood [44] for a one-component system and later extended to mixtures by Bearman and Irving [32]. The continuity, momentum, and energy equations for each component α of the plasma are obtained by multiplying (17) by $\varphi = \{1, m_\alpha \mathbf{v}, m_\alpha v^2/2\}$ and integrating over velocity. These operations yield

$$\frac{\partial n_\alpha}{\partial t} + \nabla\cdot(n_\alpha \mathbf{u}_\alpha) = 0, \tag{24}$$

$$\frac{\partial}{\partial t}(m_\alpha n_\alpha \mathbf{u}_\alpha) + \nabla\cdot(m_\alpha n_\alpha \mathbf{u}_\alpha \mathbf{u}_\alpha) = \boldsymbol{\sigma}_\alpha, \tag{25}$$

$$\frac{\partial}{\partial t}(n_\alpha \mathcal{E}_\alpha) + \nabla\cdot\left(n_\alpha \mathcal{E}_\alpha \mathbf{u}_\alpha + \boldsymbol{q}_\alpha^k\right) = \nabla\cdot(\mathbf{u}_\alpha\cdot\boldsymbol{\sigma}_\alpha), \tag{26}$$

where $\mathcal{E}_\alpha = e_\alpha + \frac{1}{2} m_\alpha \mathbf{u}_\alpha^2$ is the total (internal and bulk) kinetic energy, $\boldsymbol{q}_\alpha^k$ is the local kinetic heat flux, and $\boldsymbol{\sigma}_\alpha$ is the local force per unit volume arising from the interaction given by

$$\boldsymbol{\sigma}_\alpha = -\nabla\cdot\mathbf{p}_\alpha^{\mathrm{k}} - \sum_{\beta=1}^{\nu} \int \nabla_{\mathbf{r}} U_{\alpha\beta}\, n_{\alpha\beta}(\mathbf{r},\mathbf{r}',t)\, d\mathbf{r}'. \tag{27}$$

The set of hydrodynamic equations (24)–(26), known as the Irving-Kirkwood-Bearman equations, are still formally exact in the sense discussed above. They allow us to describe correlations in an arbitrarily complex geometry. The Irving-Kirkwood-Bearman equations need a closure for practical use; the local kinetic pressure, local heat flux, and intramolecular contribution to the local force are still unknown. The local kinetic pressure and heat flux cannot be computed without evolving their evolution equations or obtaining knowledge of the one-particle distribution function f^α, and the intramolecular term crucially includes all of the contributions from particle interactions: contributions that are referred to as electric fields, collisions, and local and nonlocal excess pressure. For collisional systems, the near-equilibrium expansion of f^α is often used, as in the familiar Chapman-Enskog expansion [22]. For the interaction contributions, we additionally need the two-particle distribution function $f_2^{\alpha\beta}$.

We seek to recast the interactions part of the total local force $\boldsymbol{\sigma}_\alpha$ exerted by species α into the form of an electric-field ($\mathbf{E}$) force term plus the divergence of the excess-pressure tensor $\boldsymbol{P}_{\mathrm{ex}}$. This separation is the subject of the remainder of this section.

A. Isolation of the electric field

A separation of the standard quantities, i.e., electric field and excess pressure, from the local force (27) is not straightforward. However, it is possible to decompose (27) in a way that isolates the electric field, and we examine this decomposition first. Let us write the two-body density in terms of one-body densities and a correlation term $\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{r}',t)$ as

$$n_{\alpha\beta}(\mathbf{r},\mathbf{r}',t) = n_\alpha(\mathbf{r},t) n_\beta(\mathbf{r}',t) + \mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{r}',t). \tag{28}$$

Substituting (28) into (27), we obtain

$$\begin{aligned}\boldsymbol{\sigma}_\alpha = {} & -\nabla\cdot\mathbf{p}_\alpha^{\mathrm{k}} - n_\alpha \sum_{\beta=1}^{\nu} \int \nabla_{\mathbf{r}} U_{\alpha\beta}\, n_\beta(\mathbf{r}',t)\, d\mathbf{r}' \\ & - \sum_{\beta=1}^{\nu} \int \nabla_{\mathbf{r}} U_{\alpha\beta}\, \mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{r}',t)\, d\mathbf{r}',\end{aligned} \tag{29}$$

where the second term can be written as

$$\mathbf{F}^C(\mathbf{r},t) = -\sum_{\beta=1}^{\nu} \int \nabla_{\mathbf{r}} U_{\alpha\beta}\, n_\beta(\mathbf{r}',t)\, d\mathbf{r}', \tag{30}$$

which we identify as the total Coulomb force $\mathbf{F}^C(\mathbf{r},t)$ on species α due to all of the species (including α); this is the "electric field." That this force is indeed the electric field can be shown explicitly by finding the divergence of $\mathbf{F}^C(\mathbf{r},t)$:

$$\frac{1}{Z_\alpha e}\nabla\cdot\mathbf{F}^C(\mathbf{r},t) = 4\pi e \sum_\beta Z_\beta n_\beta(\mathbf{r},t) \tag{31}$$

$$= 4\pi \rho_{tot}(\mathbf{r},t), \tag{32}$$

which we recognize as Gauss's Law. This result uses the usual Green function relation $\nabla^2 \frac{1}{|\mathbf{r}-\mathbf{r}'|} = -4\pi\delta(\mathbf{r}-\mathbf{r}')$, where the Coulomb potential arose from our original Hamiltonian in (1). However, it is interesting to note that the original Coulomb potential also gives rise to the additional term $\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{r}',t)$, which is often neglected in hydrodynamics models. It is tempting to associate $\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{r}',t)$ with the excess pressure, which would allow us to identify the ideal-pressure tensor, electric field, and excess pressure; together, the ideal and excess pressures could be precomputed and stored in EOS databases. Yet, as we have seen in Sec. II, the excess pressure is not computed relative to the electric field (i.e., the mean field), but, rather, directly from the Hamiltonian. However, in density functional theories, it is common practice to remove the mean-field portion to isolate the correlation term (or, the exchange-correlation term for quantum systems). In general, the correlation term, like the electric field, is nonlocal and cannot be tabulated for a fixed, specific density; integrating over all space (i.e., densities) is needed to find $\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{r}',t)$.

If we neglect the correlation terms $\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{r}',t) = 0$ and keep only the random-phase term in (28), the total local force exerted by species α is

$$\boldsymbol{\sigma}_\alpha = -\nabla\cdot\mathbf{p}^{\mathrm{k}}_\alpha + n_\alpha\mathbf{F}^C, \tag{33}$$

where again, $\mathbf{p}^{\mathrm{k}}_\alpha$ is the local kinetic-pressure tensor. The expression above is similar to what we obtained in Sec. II from a Vlasov description of a plasma, which correctly describes the physics of hot, dense, and weakly coupled plasmas. However, for strongly coupled plasmas where the Debye lewngth is such that $n\lambda_D^3 \ll 1$, the correlations beyond the mean-field approximation need to be taken into account. Replacing the ideal-gas pressure term in (33) with the total pressure from EOS tables, while keeping the electric-field term, would result in double counting the forces.

In summary, we have derived the local force on species α from the BBGKY hierarchy. This expression contains all of the force contributions and kinetic and interaction effects. We then separated out the mean-field electric-field term from the interaction term to recover the total force in a hydrodynamics-based Vlasov kinetic equation. With the mean-field electric field pulled into a separate term, the total local force becomes

$$\begin{aligned}\boldsymbol{\sigma}_\alpha(\mathbf{r},t) &= -\nabla\cdot\mathbf{p}^{\mathrm{k}}_\alpha + n_\alpha\mathbf{F}^C(\mathbf{r},t)\\ &\quad + \sum_{\beta=1}^{\nu}\int \nabla_{\mathbf{r}} U_{\alpha\beta}(|\mathbf{r}-\mathbf{r}'|)\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{r}',t)\,d\mathbf{r}',\end{aligned} \tag{34}$$

where again, we can identify the contribution of the ideal gas $\mathbf{p}^{\mathrm{k}}_\alpha$ and the total Coulomb force $\mathbf{F}^C$ on species α, and the last term, which contains $C_{\alpha\beta}$, incorporates all of the Coulomb contributions beyond the mean field. In the next section, we will examine how the excess pressure can be extracted from the last term of (34), and we will then consider its remainder.

B. Isolation of the excess pressure

Our goal now is to extract the excess-pressure tensor $\boldsymbol{P}_{\mathrm{ex}}$ from this remainder force term (34). Our strategy closely follows the derivation proposed by Irving-Kirkwood-Bearman [32]. Transforming the variables $(\mathbf{r}, \mathbf{r}')$ to $(\mathbf{r}, \mathbf{s})$, where $\mathbf{s} = \mathbf{r}-\mathbf{r}'$, (34) becomes

$$\boldsymbol{\sigma}_\alpha = -\nabla\cdot\mathbf{p}^{\mathrm{k}}_\alpha + n_\alpha\mathbf{F}^C + \sum_{\beta=1}^{\nu}\int \frac{\mathbf{s}}{s}\frac{dU_{\alpha\beta}}{ds}\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{r}+\mathbf{s})\,d\mathbf{s}. \tag{35}$$

It is convenient at this stage to change the notation: by setting the positions of particles of the species represented by the first subscript of $\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{s})$ as the first argument and the relative positions of the other particles as the second argument, we can rewrite the identity for heterogeneous systems $\mathcal{C}_{\alpha\beta}(\mathbf{r}_1,\mathbf{r}_2) = \mathcal{C}_{\beta\alpha}(\mathbf{r}_2,\mathbf{r}_1)$ as

$$\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{s}) = \mathcal{C}_{\beta\alpha}(\mathbf{r}+\mathbf{s},-\mathbf{s}). \tag{36}$$

If we now assume that $\mathcal{C}_{\beta\alpha}(\mathbf{r}+\mathbf{s},\mathbf{s})$ varies so slowly with its first argument that, with negligible error, we may retain only the first two terms in a Taylor series expansion about the point $\mathbf{s}$, then we can write

$$\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{s}) = \mathcal{C}_{\beta\alpha}(\mathbf{r},-\mathbf{s}) + \mathbf{s}\cdot\nabla_{\mathbf{r}}\mathcal{C}_{\beta\alpha}(\mathbf{r},-\mathbf{s}) + \cdots. \tag{37}$$

Inserting (37) into (35), we have

$$\begin{aligned}\boldsymbol{\sigma}_\alpha &= -\nabla\cdot\mathbf{p}^{\mathrm{k}}_\alpha + n_\alpha\mathbf{F}^C + \mathbf{B}_\alpha\\ &\quad + \frac{1}{2}\sum_{\beta=1}^{\nu}\int \frac{\mathbf{s}\mathbf{s}}{s}\frac{dU_{\alpha\beta}}{ds}\cdot\nabla_{\mathbf{r}}\mathcal{C}_{\beta\alpha}(\mathbf{r},\mathbf{s},t)d\mathbf{s} + \cdots,\end{aligned} \tag{38}$$

where $\mathbf{B}_\alpha$ is the local asymmetric force [44] arising from the heterogeneity of the system and is given by

$$\mathbf{B}_\alpha = \frac{1}{2}\sum_{\beta=1}^{\nu}\int \frac{\mathbf{s}}{s}\frac{dU_{\alpha\beta}}{ds}[\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{s}) - \mathcal{C}_{\beta\alpha}(\mathbf{r},\mathbf{s})]d\mathbf{s}, \tag{39}$$

which vanishes for homogeneous systems, where $\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{s}) = \mathcal{C}_{\beta\alpha}(\mathbf{r},\mathbf{s})$. The last term in (38) contains the local and nonlocal excess pressures; to isolate the different contributions, we proceed as follows. First, we recall the usual decomposition of $\mathcal{C}_{\alpha\beta}$ from statistical mechanics:

$$\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{s}) = n_\alpha(\mathbf{r})n_\beta(\mathbf{r}+\mathbf{s})h_{\alpha\beta}(\mathbf{r},\mathbf{s}). \tag{40}$$

The contributions of the interactions (potential energies) to the transport coefficients are neglected here. However, accounting for nonequilibrium fluctuations in the distribution functions would not change the form of the electric-field terms or the excess pressure, but rather would introduce transport terms (as in a Chapman-Enskog expansion). Forms of the hydrodynamic equations for heterogeneous systems with transport terms can be found in Refs. [45–47].

Next, expanding $n_\beta(\mathbf{s}+\mathbf{r})$ about $\mathbf{r}$ and retaining only the first term of the expansion, we can rewrite (40) as

$$\mathcal{C}_{\alpha\beta}(\mathbf{r},\mathbf{s},t) = n_\beta n_\alpha h_{\alpha\beta} + n_\alpha h_{\alpha\beta}\,\mathbf{s}\cdot\nabla_{\mathbf{r}} n_\beta + \cdots. \tag{41}$$

Substituting (41) into (38) and using (27), the local force becomes

$$\boldsymbol{\sigma}_\alpha = -\nabla\cdot\mathbf{p}^{\mathrm{k}}_\alpha + n_\alpha\mathbf{F}^C + \mathbf{B}_\alpha - \nabla\cdot\mathbf{P}^{\mathrm{ex}}_\alpha, \tag{42}$$

where the excess heterogeneous pressure tensor is given by

$$\mathbf{P}_\alpha^{\rm ex} = \frac{1}{2}\sum_{\beta=1}^{\nu} n_\alpha n_\beta \int \frac{\mathbf{ss}}{s}\frac{dU_{\alpha\beta}}{ds} h_{\beta\alpha}(\mathbf{r},\mathbf{s})\, d\mathbf{s} + \frac{1}{2}\sum_{\beta=1}^{\nu} n_\beta \nabla n_\alpha \int \frac{\mathbf{sss}}{s}\frac{dU_{\alpha\beta}}{ds} h_{\beta\alpha}(\mathbf{r},\mathbf{s})\, d\mathbf{s} + \cdots. \quad (43)$$

This result (43) includes a local kinetic-pressure force, electric term $\mathbf{F}^C$, local excess-pressure tensor (43), and asymmetric force term $\mathbf{B}_\alpha$ (39) on species α, which arises from the heterogeneity of the plasma [44] and vanishes for homogeneous plasmas, for which $h_{\alpha\beta}(\mathbf{r},\mathbf{s}) = h_{\beta\alpha}(\mathbf{r},\mathbf{s})$.

We have provided equations for the electric-force term, excess-pressure tensor, and asymmetric-force tensor from the total, local force. However, in order to apply our theory to nonuniform flows, we need information about the pair-correlation function $h_{\alpha\beta}(\mathbf{r},\mathbf{s})$. The exact form of $h_{\alpha\beta}(\mathbf{r},\mathbf{s})$ is unknown; nonetheless, it can be computed directly from first-principle calculations. The inhomogeneous pair-distribution function appearing in the above results is constructed using a generalization of the method proposed by Fischer-Methfessel [48]. This approximation expresses $h_{\alpha\beta}(\mathbf{r},\mathbf{s})$ formally in terms of the homogeneous pair-correlation function $h^0_{\alpha\beta}(|\mathbf{r}-\mathbf{s}|;\bar{n}_\alpha)$ as

$$h_{\alpha\beta}(\mathbf{r},\mathbf{s}) = h^0_{\alpha\beta}[|\mathbf{r}-\mathbf{s}|;\bar{n}_\alpha(\mathbf{R}_{\alpha\beta})], \quad (44)$$

evaluated at some effective density $\bar{n}_\alpha$ defined by

$$\bar{n}_\alpha(\mathbf{R}_{\alpha\beta}) = \frac{1}{v_\alpha}\int_{v_\alpha} n_\alpha(\mathbf{r}-\mathbf{R}_{\alpha\beta}), \quad (45)$$

where the density is averaged over a volume v_α of molecular size, and the mean location is given as $\mathbf{R}_{\alpha\beta} = (\mathbf{r}+\mathbf{s})/2$. Note that extensive studies have shown very good agreement between computer simulations and calculations made using the Fischer-Methfessel method [45,47–51]. Also, as Scriven *et al.* [47] pointed out, this method satisfies the the requirement for symmetry, that $h_{\alpha\beta}(\mathbf{r},\mathbf{s}) = h_{\beta\alpha}(\mathbf{s},\mathbf{r})$.

With the inhomogeneous pair-correlation function known, the total pressure for the mixture can be obtained by taking the diagonal sum of the total pressure tensor $P = -\frac{1}{3}\mathrm{Trace}(\mathbf{p}^{\rm k}_\alpha + \mathbf{P}^{\rm ex}_\alpha)$, given by

$$P = \sum_\alpha n_\alpha T - \frac{2\pi}{3}\sum_{\alpha,\beta} n_\alpha n_\beta \int s^3 \frac{dU_{\alpha\beta}}{ds} h^0_{\alpha\beta}(s) ds - \frac{2\pi}{3}\sum_{\alpha,\beta} n_\alpha \nabla_{\mathbf{r}} n_\beta \int s^4 \frac{dU_{\alpha\beta}}{ds} h^0_{\alpha\beta}(s)\, ds + \cdots. \quad (46)$$

Equation (46) is the main result of this work. It generalizes the standard isotropic and equilibrium EOSs for classical fluids to include nonlocal effects in terms of high-order gradient-density corrections. The first two terms of (46) constitute the isotropic pressure contained in EOS tables, while the third term is the correction for inhomogeneity. A common challenge for multifluid codes is to find an accurate description of the species EOSs, because EOS tables do not provides these quantities. Equation (46) provides a way to incorporate an accurate EOS with strongly coupled physics into multifluid codes to describe heterogeneous plasmas mixtures. The uniform pair-correlation function needed for these formulas can be directly computed with a hypernetted-chain solver or MD.

IV. CONCLUSIONS

We have derived Euler-based hydrodynamic equations for multicomponent and heterogeneous systems, in which self-generated electric fields can be substantial, with a moment-based method, using the first equation of the BBGKY hierarchy. We have also proposed an expression for the nonhomogeneous EOSs.

First, we presented a brief review of some basic classical mechanics results regarding the form of the EOSs for multispecies systems. In general, for homogeneous systems, the intramolecular part of the pressure of any material can be obtained by summing, over all species, the moment of the force times the uniform radial distribution functions. When considering nonideal and heterogeneous plasmas, it is very tempting to replace the ideal-gas pressure form with the EOSs from tables, while retaining the electric-field term. In general, this approach will result in double counting of force terms. To show how EOS tables can be used in the Euler hydrodynamic equation while retaining the electric field, we recalled the approach proposed by Irwing and Kirkwood [44].

From kinetic theory, we derived the total forces acting on species, which including local kinetic and interaction contributions. Introducing the heterogeneous pair-correlation function $h_{\alpha\beta}(\mathbf{r},\mathbf{r}')$ through the two-body density, defined as $n_{\alpha\beta}(\mathbf{r},\mathbf{r}') = n_\alpha(\mathbf{r})n_\beta(\mathbf{r}')[1+h_{\alpha\beta}(\mathbf{r},\mathbf{r}')]$, we separated out the mean-field electric-force term from the Coulomb interaction portion of the force. Unfortunately, the remainder of the interaction portion of the force is expressed in terms of the function $h_{\alpha\beta}(\mathbf{r},\mathbf{r}')$, which is complicated to compute. Although much progress has been made towards being able to evaluate this function [45,47,49,50], we have no detailed knowledge of its behavior for realistic inhomogeneous fluids. However, this difficulty can be resolved using the method of Fischer-Methfessel [45,48,50], in which the inhomogeneous pair-correlation function is replaced with its homogeneous counterpart, with the density evaluated at the mean location. This approximation has been extensively validated against MD simulations and is fairly accurate.

Using the Fischer-Methfessel approximation, the form of the EOS has been provided, and an expression that includes the first-order density-gradient correction is given. We showed that for a multicomponent system, an asymmetric force appears that can be attributed to the heterogeneity of the plasma. However, this force term vanishes for the one-fluid system. The local component of the pressure can be determined and stored into EOS tables, as it requires only knowledge of the homogeneous pair-correlation function. The exact form of this latter function is unknown; However, once the pair potential has been specified, it can be calculated using an integral-equation method such as a hypernetted-chain, MD, or Monte Carlo simulation method. This local pressure already occurs in hydrodynamics codes, through its EOS models or tables, which are usually for single fluids. Finally, we believe it should be straightforward to implement the nonlocal pressure and electric-field terms into existing multifluid codes.

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