Viscosity estimates for strongly coupled Yukawa systems

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An analytic form for the shear viscosity of a Yukawa system, in terms of the known result for the one-component plasma, is given by establishing an analytic correspondence between the Yukawa and one-component plasma systems. The correspondence is found by ensuring that the Yukawa system and the reference one-component plasma have identical effective hard-sphere packing fractions, as determined by the Gibbs-Bogolyubov inequality. The resulting prediction for the freezing transition is compared with known simulation results. These results are useful for describing dynamical properties of Yukawa systems, and the method can be easily generalized to mixtures.

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I. INTRODUCTION

The strongly coupled, screened Coulomb system has attracted significant attention recently due to the relative ease of experimentally producing and diagnosing dilute systems. Strongly coupled Coulomb systems are Coulomb systems with an average potential energy that exceeds the average kinetic energy. Strong coupling is typically characterized by the Coulomb coupling parameter $\Gamma=\beta Q^2/a$, where Q is the charge, $a=(3/4\pi n)^{-1/3}$ is the ion-sphere radius in terms of the particle density n, and $\beta=1/T$ is the inverse temperature. Dusty (colloidal) plasmas have begun to elucidate many properties of such systems [1]. Dusty plasmas are normal plasmas that achieve strong coupling with micron-sized impurities that can acquire $\sim 10^5$ elementary charges. Recently, ultracold strongly coupled plasmas, as created by ionizing a dilute cold atomic gas, have been produced [2]. These plasmas show great promise for studying strongly coupled Coulomb systems over a wide parameter range.

Screened Coulomb systems are frequently modeled with the Yukawa (Y) interparticle interaction (in temperature units)

$$\beta u_Y(r)=\frac{\Gamma}{r}e^{-\kappa r}, \tag{1}$$

where Γ measures the strength of the interaction and κ measures the strength of the screening. (All lengths are in units of a.) This model, which results from a linear treatment of the screening, has been used to describe liquid metals [3], liquid metallic hydrogen and helium [4], screening of thermonuclear reaction rates in astrophysical settings [5], and plasmas and colloidal suspensions [6]. The Yukawa system is typically used as a model for the heaviest ion component under the assumption of linear, adiabatic screening by the background particles. The Yukawa system is chosen because of its generality: the dimensionless coupling and screening parameters are chosen to match the particular plasma conditions. For dusty plasmas, the coupling refers to the dust grains and the screening to the hot background electron-ion plasma. For ultracold plasmas, the coupling refers to the cold ions and the screening to the partially degenerate electron gas. Similar arguments hold for other situations.

Despite the ubiquity of Yukawa-like systems, less is known relative to the one-component plasma (OCP), for which the interparticle interaction is of the pure Coulomb ($\kappa=0$) form Γ/r. It is possible to take advantage of this situation by using the known properties of the OCP as a reference for the properties of screened systems. Such a correspondence has been carried out for dense matter by Galam and Hansen [7] using both thermodynamic perturbation theory and a variational method based on the Gibbs-Bogolyubov inequality (GBI). In their work, the screening was specifically described by the zero-temperature Lindhard dielectric function with local field corrections. Sensitivity to the form of the screening function was subsequently investigated by Iyetomi, Utsumi, and Ichimaru [8]. The hard-sphere (HS) system can also be used as the reference, although it is known that the OCP system gives a better (lower upper bound) estimate of the free energy [7,9]. An advantage of using the HS system, however, is that analytic results can be obtained [9–11]. Here a combination of both reference systems is used. First, the HS reference system is used as a reference for the Yukawa system. Then, an OCP reference system is found by ensuring that the OCP reference has the same HS packing fraction as the Yukawa system. This method has the advantages that the model potential is quite general, the results are analytic and require only solutions of transcendental equations, the OCP limit is an exact limit, and the generalization to mixtures is straightforward. The main disadvantage is that it is not easy to rigorously assign an accuracy to the procedure, although accuracy can be established *a posteriori* with simulation data. The final result is then used to calculate the freezing transition of the Yukawa fluid and the shear viscosity.

II. HARD-SPHERE REFERENCE

Consider a Yukawa system with fixed volume Ω, number of particles $N=n\Omega$, and temperature $T=1/\beta$. The Yukawa interparticle interaction energy is taken to be of the form (1), where Γ is assumed to be the same for all particles. The total excess energy $U_Y=\Sigma_{i<j}^N u_Y(r_{ij})+U_{bg}$ of the Yukawa system includes all pairwise contributions, as well as interactions involving a neutralizing background U_{bg}. Now, consider a reference HS system with hard-sphere diameter σ, packing

fraction $\eta=\pi N\sigma^3/(6\Omega)$, and interparticle interaction energy

$$\beta u_{HS}(r)=\begin{cases}\infty, & r<2\eta^{1/3}\\ 0, & r>2\eta^{1/3},\end{cases} \tag{2}$$

with the same macroscopic parameters $\{N,\Omega,T\}$. For a given configuration, the excess energy of the HS assembly is then $U_{HS}=\Sigma_{i<j}^{N}u_{HS}(r_{ij})$.

In terms of the excess energies, the excess Helmholtz free energies for the two systems are

$$\beta F_Y^{(ex)}(\Gamma,\kappa)=-\ln\left[\int\frac{d^{3N}r}{\Omega^N}e^{-\beta U_Y}\right], \tag{3}$$

$$\beta F_{HS}^{(ex)}(\eta)=-\ln\left[\int\frac{d^{3N}r}{\Omega^N}e^{-\beta U_{HS}}\right]. \tag{4}$$

From the GBI [12], we know these free energies satisfy

$$F_Y^{(ex)}(\Gamma,\kappa)\le F_{HS}^{(ex)}(\eta)+\langle U_Y(\Gamma,\kappa)-U_{HS}(\eta)\rangle_{HS}+F_0, \tag{5}$$

where $\langle\cdots\rangle_{HS}$ refers to an ensemble average over the HS distribution function. The quantity F_0 contains all structure-independent terms, which do not play a role here. After simplification this becomes

$$F_Y^{(ex)}(\Gamma,\kappa)/(NT)\le\frac{\eta(4-3\eta)}{(1-\eta)^2}+\frac{3\Gamma}{2}\int_0^\infty dr\, re^{-\kappa r}\times[g_{HS}(\eta,r)-1]+F_0, \tag{6}$$

where the approximate Carnahan-Starling [13] HS excess free energy has been used. The integral is over the hard-sphere radial distribution function $g_{HS}(\eta,r)$ and can be done analytically in the Percus-Yevick approximation [14] to yield

$$\int_0^\infty dr\, re^{-\kappa r}[g_{HS}(r)-1]=4\eta^{2/3}[G(2\eta^{1/3}\kappa)-(2\eta^{1/3}\kappa)^{-2}], \tag{7}$$

where

$$G(x)=\frac{xH(x)}{12\eta[H(x)-I(x)e^x]} \tag{8}$$

with

$$H(x)=12\eta[x(1+\eta/2)+2\eta+1],$$

$$I(x)=(1-\eta)^2x^3+6\eta(1-\eta)x^2+18\eta^2x-12\eta(1+2\eta). \tag{9}$$

The right-hand side of Eq. (6) can now be minimized with respect to η for fixed $\{\Gamma,\kappa\}$ to yield the optimal HS packing fraction $\eta=\eta(\Gamma,\kappa)$. Note that this procedure contains the OCP as the special case $\kappa=0$.

Solutions of the variational procedure were found for $\kappa=0,1,2,3$ and $\Gamma=1-180$; these solutions are shown in Fig. 1. Qualitatively we see that the weaker screening cases correspond to larger packing fractions. Calculations were also performed for $\kappa=0.25,0.5,1.5,2.5,3.5$ and the full set of solutions for $\Gamma>1$ was fit by the form

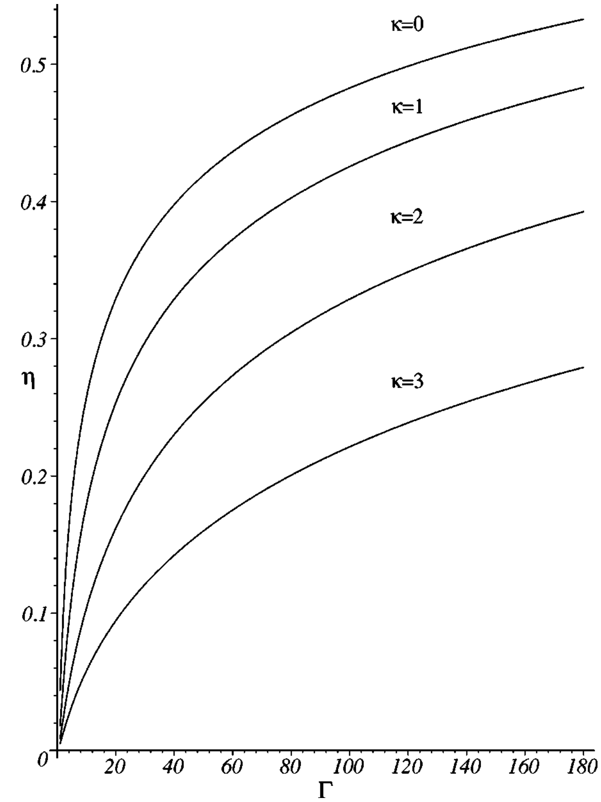

FIG. 1. Hard-sphere packing fraction η versus Coulomb coupling parameter Γ for a range of screening parameters κ.

$$\eta=a(\kappa)+\frac{b(\kappa)\ln(\Gamma)}{1+c(\kappa)\ln(\Gamma)}, \tag{10}$$

where

$$a(\kappa)=0.0255-0.0683\kappa+0.0267\kappa^2-0.003\kappa^3,$$

$$b(\kappa)=0.107\exp(-0.143\kappa-0.105\kappa^2),$$

$$c(\kappa)=-0.116+0.134\exp(-0.19\kappa-0.184\kappa^2). \tag{11}$$

It is also useful to compare Eq. (10) to previous results, most of which are for the OCP ($\kappa=0$) limit. In that limit we find from Eq. (10) that the OCP-HS correspondence is given by

$$\Gamma_{ocp}=\exp\left[\frac{\eta-0.0255}{0.107-0.018(\eta-0.0255)}\right], \tag{12}$$

whereas the OCP analytic result of Stroud and Ashcroft (SA) [10] is

$$\Gamma_{ocp}^{SA}=2\eta^{1/3}\frac{(2-\eta)(1+2\eta)^2}{(2+\eta)(1-\eta)^5}. \tag{13}$$

We found that over the range $\eta=0.1-0.6$ ($\Gamma_{ocp}\approx 2-300$), the quantity $|\Gamma_{ocp}^{SA}-\Gamma_{ocp}|/\Gamma_{ocp}^{SA}\times 100\%$ is less than 10%. The SA result for the OCP excess free energy in the strong coupling limit is known to agree with Monte Carlo results fairly well, and therefore we expect Eq. (12) to also give similar agreement. Of course, Eq. (10) generalizes the OCP case to the Yukawa case.

III. OCP-YUKAWA CORRESPONDENCE

Given known analytic forms for HS transport coefficients, Eq. (10) can be used to estimate the same properties for the Yukawa system. However, it is known that the OCP provides a better reference for the Yukawa system [7,9] and such a correspondence is guaranteed to give the exact $\kappa=0$ limit, whereas an HS reference does not give such a guarantee. An intuitive analytic mapping between the OCP and Yukawa systems is given by

$$\Gamma_{ocp}=\Gamma e^{-\kappa}, \tag{14}$$

which follows by simply replacing the average Coulomb energy by its screened value. It is possible to use Eq. (10) to develop a different mapping between the OCP and Yukawa systems that has somewhat better justification. The basic idea is to find the Yukawa and OCP systems that have identical packing fractions. Given a Yukawa system characterized by $\{\Gamma,\kappa\}$, we first find the corresponding hard-sphere packing fraction η that characterizes the hard-sphere system that best mimics (as defined by the Gibbs-Bogolyubov inequality) the Yukawa system. Now, given this hard-sphere system, we can then find which OCP system (as characterized by Γ_{ocp}) *also* corresponds to this hard-sphere system; that is, we solve

$$a(0)+\frac{b(0)\ln(\Gamma_{ocp})}{1+c(0)\ln(\Gamma_{ocp})}=a(\kappa)+\frac{b(\kappa)\ln(\Gamma)}{1+c(\kappa)\ln(\Gamma)} \tag{15}$$

for Γ_{ocp}, given $\{\Gamma,\kappa\}$. The results of this calculation are shown in Fig. 2. Qualitatively we see that strongly screened Yukawa systems are best modeled by relatively weakly coupled OCP systems, as expected. A fit to that data yields

$$\Gamma_{ocp}=A(\kappa)+B(\kappa)\Gamma+C(\kappa)\Gamma^2, \tag{16}$$

where

$$A(\kappa)=\frac{0.46\kappa^4}{1+0.44\kappa^4},$$

$$B(\kappa)=1.01e^{-0.92\kappa},$$

$$C(\kappa)=-3.7\times10^{-5}+9.0\times10^{-4}\kappa-2.9\times10^{-4}\kappa^2. \tag{17}$$

The functional forms for the κ-dependent coefficients were chosen to give a good fit, with the form for $B(\kappa)$ chosen specifically to compare with Eq. (14). It is interesting that the coefficient $B(\kappa)$ is quite similar to the intuitive guess of Eq. (14). However, the other coefficients in Eq. (16) give important corrections, as can be seen in Fig. 2, where the numerical results (lines), the simple estimate (14) (boxes), and the fit (16) (crosses) are compared. We see that the predictions based on this work give higher equivalent Γ_{ocp} values for a given $\{\Gamma,\kappa\}$ than Eq. (14); that is, Eq. (14) overestimates the effects of screening relative to Eq. (16). It should be mentioned that the fit (16) is most accurate for moderate to strong coupling ($\Gamma>5$). Since we know the intercept at small Γ of Eq. (16) is actually zero, we can take $A(\kappa)\approx0$. Given the smallness of $C(\kappa)$ in that same limit, we see that Eq. (14) may represent a reasonable approximate result for $\Gamma\approx1$.

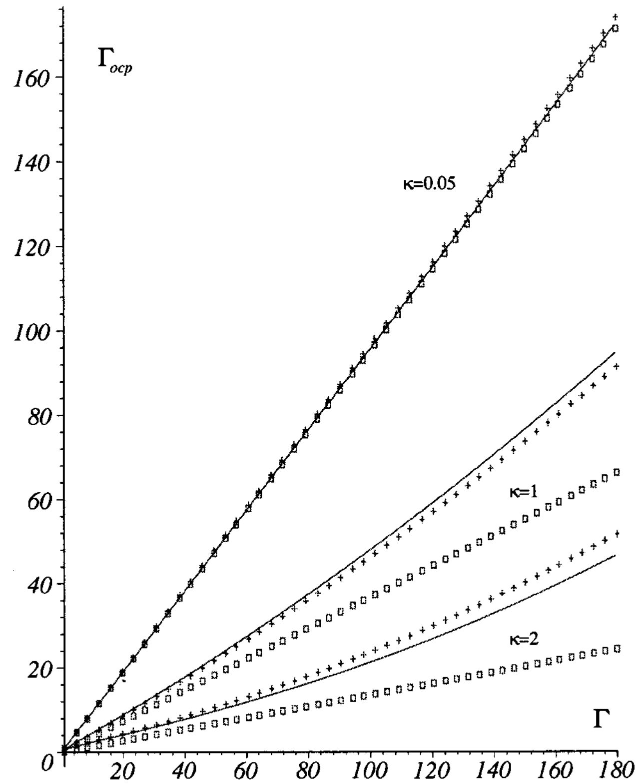

FIG. 2. The OCP coupling parameter versus the Yukawa coupling parameter for various κ values. The approximations given by Eqs. (14) and (16) are shown for comparison. The fit (16), shown as crosses, reproduces the results fairly well. The simple model of Eq. (14), shown as boxes, gives a lower equivalent OCP coupling value.

IV. PHASE BOUNDARY AND SHEAR VISCOSITY

Although the above results can be justified by the use of the variational principle, the optimal result of the GBI does not reveal how close the reference free energy is to the actual free energy or the accuracy of the correspondence implied by Eq. (15). To quantify the accuracy, the result (16) and the simple estimate of Eq. (14) are used to predict the liquid-solid phase boundary of the Yukawa fluid and to compare with the simulation data of Hamaguchi, *et al.* [15]. The phase boundary is found by solving for the critical coupling strength Γ_c for various κ with Eq. (15),

$$\Gamma_c=\exp\left[\frac{0.5295-a(\kappa)}{b(\kappa)-c(\kappa)[0.5295-a(\kappa)]}\right] \tag{18}$$

and with Eq. (14),

$$\Gamma_c=171.8e^{\kappa}, \tag{19}$$

where the OCP Γ_c is taken to be $\Gamma_c=171.8$ to be consistent with the simulation results. This procedure is motivated by noting that an HS packing fraction at freezing yields nearly the correct freezing point of the OCP [3] with Eq. (12) or Eq.

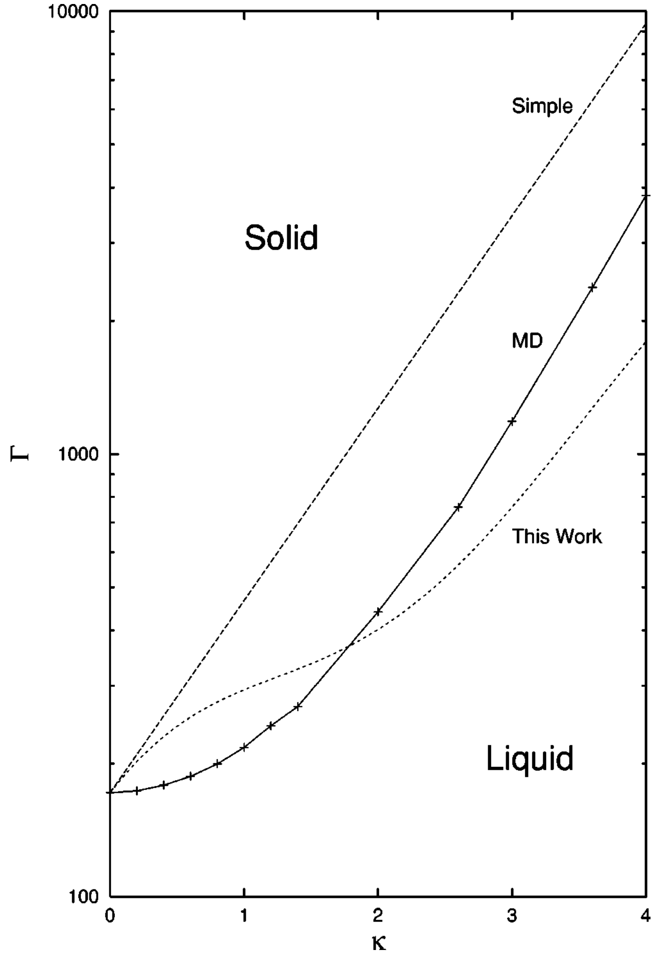

FIG. 3. Phase diagram of the Yukawa system in the $\{\Gamma,\kappa\}$ plane. The liquid-solid phase boundary is shown as predicted by the simple estimate $\Gamma=171.8\exp(\kappa)$ (top line), the solution of Eq. (18), and the simulation results of Hamaguchi *et al.* (line with circles). The results of this work are seen to give the phase boundary fairly well considering the simplicity of the theory.

(13). We assume here that a similar relation holds between the OCP and Yukawa systems. The result is shown in Fig. 3 where we see that the simple result of Eq. (14) predicts a larger coupling strength for freezing than the simulations indicate. The result (16) gives a considerable improvement in predicting the phase boundary, which suggests that Eq. (16) can describe semiquantitatively the properties of the Yukawa system.

As an example of the application of the above results, we consider the shear viscosity of a strongly coupled Yukawa system. The shear viscosity plays an important role in describing dynamical properties, such as collective modes. The viscosity enters both as a damping mechanism and contributes to the rigidity (high-frequency shear modulus) of the system. It therefore enters as a parameter in such theories, which have been recently applied to dusty plasmas [16,17]. Because of the lack of information on the Yukawa viscosity, Kaw and Sen [17] were forced to use the OCP viscosity. The shear viscosity will be denoted here by η^* to distinguish it from the packing fraction η; all viscosities are in dimensionless units in terms of the viscosity $\eta_0=nM\omega_p r_s^2$. We use the available analytic fit to the OCP viscosity given by Wallenborn and Baus [18] to ensure that the OCP limit is an exact

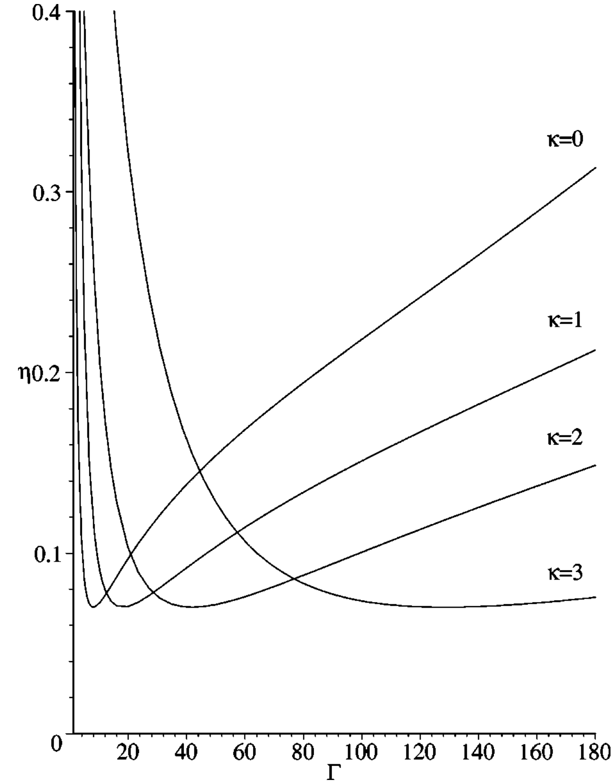

FIG. 4. The viscosity versus Γ for various values of κ. The $\kappa=0$ case is the Wallenborn-Baus OCP result and the remaining curves are the corresponding Yukawa estimates based on Eq. (15).

limit. Their result, which agrees well with simulation results [19], can be expressed as

$$\eta^*=\lambda I_1+\frac{(1+\lambda I_2)^2}{\lambda I_3}, \tag{20}$$

where

$$\lambda=\frac{4\pi}{3}(3\Gamma_{ocp})^{3/2},$$

$$I_1=(180\Gamma_{ocp}\pi^{3/2})^{-1},$$

$$I_2=\frac{0.49-2.23\Gamma_{ocp}^{-1/3}}{60\pi^2},$$

$$I_3=0.241\frac{\Gamma_{ocp}^{1/9}}{\pi^{3/2}}. \tag{21}$$

Together with Eq. (16), these equations represent a procedure for computing the Yukawa viscosity, as shown in Fig. 4. The results have the expected behavior in that the viscosity behaves like a weakly coupled system for strong screenings. Note that the viscosity minimum has moved to about $\Gamma\approx140$ for $\kappa=3$, where it occurs at $\Gamma\approx8$ for the OCP case. For large couplings of $\Gamma\approx180$, we see that using an OCP estimate for the viscosity overestimates the viscosity by nearly a factor of 4.

V. CONCLUSION

An analytic correspondence between the OCP and Yukawa systems has been given. The correspondence was achieved by using the HS system as a reference for each system and ensuring an identical HS packing fraction for both systems. The accuracy of this procedure has been shown by comparing a prediction of the freezing transition with simulation data. The result is shown to be superior to the intuitive guess $\Gamma_{ocp}=\Gamma\exp(-\kappa)$. The final result was used to compute the shear viscosity using the OCP analytic fit of Wallenborn and Baus. It was seen that screening moves the viscosity minimum to large coupling strengths and thereby reduces the viscosity at strong couplings relative to the OCP estimate. This reduction can have important consequences on the damping of collective modes and the onset of shear waves that are dependent on the rigidity of the system.

The method presented here is easily extended to other properties for which expressions are known for the OCP. General approximate relations, such as the Einstein relation between the diffusion coefficient and viscosity, can also be used to give estimates for some properties. Because of the simplicity of the theory, the same method can be easily applied to mixtures for which the HS expressions are already known [11].

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