Empirical bridge function for strongly coupled Yukawa systems

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A simple bridge function for strongly coupled Yukawa systems is developed based upon a form previously extracted for a one-component plasma [H. Iyetomi, S. Ogata, and S. Ichimaru, Phys. Rev. A **46**, 1051 (1992)]. Using the proposed bridge function in the modified hypernetted chain theory, excellent agreement is obtained with molecular dynamics simulations and the compressibility sum rule is satisfied to within a few percent. This result offers a simple and very accurate method to quickly compute correlation functions for Yukawa systems.

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I. INTRODUCTION

In the field of strongly coupled plasmas, one of the most well studied models is the classical one-component plasma (OCP) which corresponds to a system of identical interacting ions with charge Ze immersed in a uniform background of totally degenerate electrons [2]. In this idealized system, ions interact through the bare Coulomb potential since electrons do not screen the ion interaction.

A more realistic description of a strongly coupled plasma, which allows for electron screening, is the Yukawa model. In this description, ions interact through a screened potential

$$V(r)=\frac{Ze}{r}\exp\left(-\frac{r}{\lambda_s}\right), \tag{1}$$

where λ_s accounts for screening effects arising from the compensating background of electrons. For classical electrons, this corresponds to the Debye length while for partially degenerate electrons this length is modified [3] by quantum effects. In the emerging field of strongly coupled dusty plasmas [4,5], the effective interaction between micrometer-sized grains is well approximated to lowest order by a Yukawa model [5] with screening length determined by the weakly coupled background plasma (both ions and electrons).

Among the existing analytic theories of dense plasmas, the hypernetted chain (HNC) approximation [6] is known to be quite good [2] for describing interparticle correlations. In the fluid regime, the internal energy of an OCP calculated using the HNC approximation reproduces exact Monte-Carlo (MC) data [7] within errors of the order of 1%. However, other quantities computed within the HNC approximation, such as the excess specific heat, differ considerably from the MC data [2]. In addition, the HNC approximation suffers from an internal inconsistency, the violation of the compressibility sum rule [2]. In order to improve the accuracy, it is necessary to include a treatment for the bridge functions, the class of diagrams neglected within the HNC approximation.

The first attempt [8] to include the bridge function was based on the assertion that the functional form is independent of the detailed nature of the interaction. Using this universality ansatz, the known bridge function for a hard-sphere system was applied to both OCP and Yukawa interactions. The single free parameter in the hard-sphere bridge function, the packing fraction, was determined by requiring thermodynamic consistency. Results obtained using this scheme are in very good agreement with MC simulations [8].

Based on similar ideas from this initial work, many other integral structure theories have been proposed including the reference-hypernetted-chain equation [9], the mixed Percus-Yevick/hypernetted chain approach [10,11], and the perturbative hypernetted-chain equation [12,13]. Most of these approaches involve the use of a free parameter to enforce thermodynamic consistency and the results are in very good agreement with MC simulations. However, the free parameter search to obtain thermodynamic consistency can be time consuming. In addition, there is evidence that the universality ansatz breaks down for an OCP [14,15].

More recently, the bridge function for an OCP was extracted from a series of Monte Carlo simulations and fitted to an analytic form [1]. The extracted bridge function was constrained to satisfy the exact short-range Widom expansion [16] and the long-range boundary conditions arising from the compressibility sum rule. Since all parameters in the bridge function are predetermined, the numerical complexity is the same as the original HNC approach, thus providing a very quick and accurate method to compute correlations.

In this work, we extend the bridge function extracted for the OCP [1] to the Yukawa potential for which the OCP is a limiting case [$\lambda_s \to \infty$ in Eq. (1)]. The underlying basis for this extension is related to the universality ansatz; we assume that the functional form of the Yukawa bridge function is relatively insensitive to the amount of screening and simply rescale the extracted OCP bridge function. The proposed Yukawa bridge function is in excellent agreement with molecular dynamics (MD) simulation and furthermore satisfies the compressibility sum rule to within a few percent.

Although the resulting bridge function is empirical, all parameters are predetermined, allowing direct use in existing HNC algorithms. This provides a very quick method to accurately compute correlation functions, which in turn form the basic ingredient in many other calculations.

II. THEORY

For both the Yukawa and OCP models, a convenient length scale is the ion-sphere radius

$$a \equiv \left(\frac{3}{4\pi n} \right)^{1/3},$$

where n is the ion density. The most widely used dimensionless coupling parameter describing these systems is

$$\Gamma \equiv \frac{(Ze)^2}{a k_B T},$$

corresponding roughly to the ratio of mean potential to mean kinetic energy in an OCP. In dimensionless form, the Yukawa interaction of Eq. (1) is

$$\beta u(\hat{r}) = \frac{\Gamma}{\hat{r}} \exp(-\kappa \hat{r}),$$

where $\beta = (k_B T)^{-1}$, $u(\hat{r}) = ZeV(\hat{r})$, $\hat{r} = r/a$ and $\kappa \equiv a/\lambda_s$ is a dimensionless parameter characterizing the screening. A Yukawa system is completely specified by the two dimensionless parameters Γ and κ while the OCP model is recovered in the limit $\kappa \to 0$.

The integral structure theory may be expressed concisely in terms of the Ornstein-Zernike equation [17,18]

$$h(r) = c(r) + n \int c(r') h(|\mathbf{r} - \mathbf{r}'|) d\mathbf{r}', \tag{2}$$

and the formally exact closure relation [17,18]

$$g(r) = \exp[-\beta u(r) + h(r) - c(r) + B(r)], \tag{3}$$

where $g(r)$ is the radial distribution function, $h(r) = g(r) - 1$ is the pair correlation function, $c(r)$ is the direct correlation function and $B(r)$ is the bridge function. To complete the theory, an expression for $B(r)$ is needed. In the hypernetted chain approximation, the bridge functions are neglected, $B(r) = 0$.

As mentioned previously, the HNC approximation suffers from an internal inconsistency. Given a solution from HNC theory, one may compute the isothermal compressibility from either the compressibility equation

$$\beta \left(\frac{\partial P}{\partial n} \right)_T = 1 - n \int [c(r) + \beta u(r)] d\mathbf{r}, \tag{4}$$

or by differentiating the pressure equation

$$\beta \frac{P}{n} = 1 - \frac{\beta n}{6} \int [g(r) - 1] r \frac{du(r)}{dr} d\mathbf{r}. \tag{5}$$

For the approximate $g(r)$ and $c(r)$ resulting from the HNC theory, these two approaches yield significantly different results. Attempts to improve HNC have typically involved adjusting a free parameter to ensure the compressibility obtained using Eq. (4) is equal to the result obtained by differentiating Eq. (5).

We employ the same basic idea of universality for the Yukawa interaction, but instead of the hard-sphere bridge function we use the OCP bridge function extracted from Monte Carlo simulations [1]. Clearly, in the limit $\kappa \to 0$ the Yukawa bridge function must reduce to the OCP bridge function. In the opposite limit of large κ, the effective coupling strength is dramatically reduced and the bridge function should rapidly become negligible. Thus, for the Yukawa bridge function we propose a screening dependent rescaling of the OCP bridge function.

Through trial and error comparisons with the set of MD simulations described in Sec. III, we have identified a simple functional form for the Yukawa bridge function

$$B(r) = B_{OCP}(\Gamma, r) \exp\left(-\frac{\kappa^2}{4} \right), \tag{6}$$

which accurately reproduces the correlation functions and thermodynamic properties from MD simulation and satisfies the compressibility sum rule to within a few percent over the range of parameters considered. For the one-component plasma bridge function $B_{OCP}(\Gamma, r)$, we use Eq. (22) of Ref. [1].

III. RESULTS

We make use of simple iterative techniques [19,20] to solve Eqs. (2) and (3) including the bridge function of Eq. (6). Although more advanced Newton-Raphson techniques have been developed [21] to solve these equations, we found the simple iterative approach to be adequate for our purposes. In the rest of the paper, we will refer to these solutions as modified HNC.

The radial distribution function $g(r)$ was accurately calculated using MD simulation. The equations of motion for N particles interacting through a Yukawa pair potential [see Eq. (1)] were solved using the velocity Verlet finite difference method with periodic boundary conditions. All N^2 forces were computed in the simulation cell with the minimum image convention, which allowed us to simulate modest to large κ values. Systematic errors associated with particle numbers were investigated by simulating from 500 to 2500 particles, with 1000 particles typically needed for large Γ and small κ (towards the OCP limit). For example, we found the excess internal energy was typically 0.2% larger for 1000 particles versus 500 particles. Statistical errors associated with insufficient sampling were minimized by simulating long intervals for which the computed properties did not change significantly. To compare with Eq. (6), we performed simulations for $\Gamma = 25,50,75,100$ and $\kappa = 1,2,3,4$.

In Fig. 1, we compare the radial distribution functions resulting from MD, plain HNC (no bridge), modified HNC with Eq. (6) and modified HNC with the OCP bridge function [1]. The HNC result falls short of the peaks while the HNC solution with the OCP bridge overshoots the peaks. The screening dependent rescaling of the OCP bridge function (6) is in excellent agreement with the MD results. Further comparisons between MD and modified HNC are given in Fig. 2. In every case, the modified HNC result is nearly indistinguishable from the corresponding MD simulation. Although not shown here, the results for $\kappa = 4$ are also quite similar.

In order to verify the accuracy of the proposed bridge function, we have compared the excess internal energy and equation of state against MD simulation. In particular, we have verified the modified HNC results reproduce the entire

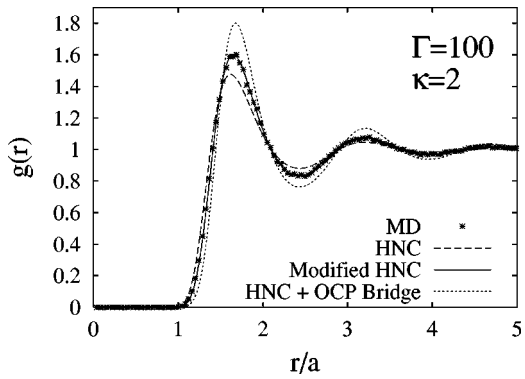

FIG. 1. Comparison of radial distribution functions for $\Gamma=100$ and $\kappa=2$. Results are from MD simulation (stars), HNC (dashed), modified HNC using Eq. (6) for bridge function (solid) and modified HNC with OCP bridge function of Ref. [1] (dotted).

range of excess energies in Table III of Ref. [22] nearly within the published uncertainties. In addition, we have computed the pressure resulting from modified HNC with two different approaches. The pressure may be computed directly from Eq. (5) or by performing an integration of the internal energy over the coupling parameter [22,23] to obtain the Helmholtz free energy F. The pressure is then computed by taking the partial derivative $P=-(\partial F/\partial V)_T$. In Table I, the pressure computed from modified HNC using both approaches is compared with results obtained from our MD simulations using Eq. (5). We also present the pressure obtained by differentiating a published Helmholtz free energy resulting from a series of MD simulations [24]. However, the free energy obtained in these simulations [24] is only valid

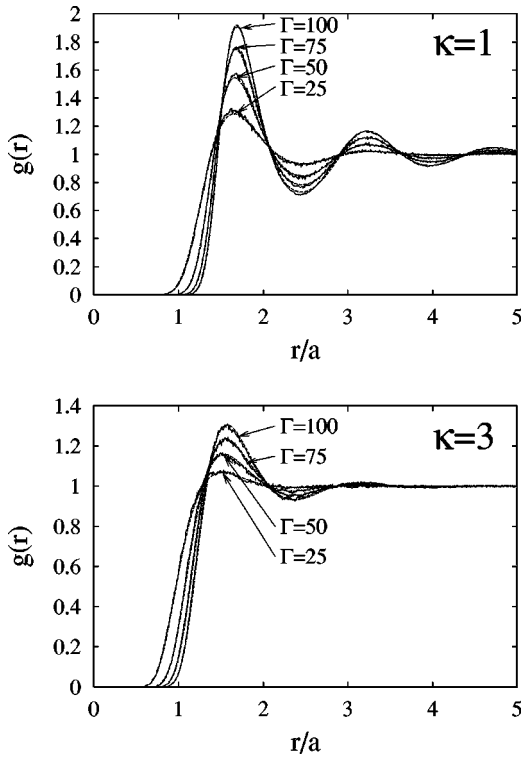

FIG. 2. Comparison of radial distribution functions resulting from modified HNC (dashed) and from molecular dynamics (solid) for a range of Γ and κ.

TABLE I. Pressure $P/(nk_BT)$ computed four ways: (1) modified HNC using the pressure equation [see Eq. (5)], (2) modified HNC via the Helmholtz free energy, (3) results from our MD simulations using the pressure equation and (4) results obtained by differentiating a published Helmholtz free energy [24] obtained using MD.

		$\kappa=1$	$\kappa=2$	$\kappa=3$	$\kappa=4$
	(1)	−5.019	−3.121	−1.582	−0.658
$\Gamma=25$	(2)	−5.004	−3.101	−1.579	−0.659
	(3)	−4.983	−3.105	−1.570	−0.655
	(4)	−5.028			
	(1)	−11.523	−7.797	−4.594	−2.591
$\Gamma=50$	(2)	−11.498	−7.769	−4.595	−2.597
	(3)	−11.456	−7.763	−4.576	−2.587
	(4)	−11.530			
	(1)	−18.088	−12.565	−7.691	−4.584
$\Gamma=75$	(2)	−18.057	−12.532	−7.698	−4.595
	(3)	−17.990	−12.509	−7.671	−4.590
	(4)	−18.094			
	(1)	−24.686	−17.378	−10.833	−6.609
$\Gamma=100$	(2)	−24.649	−17.340	−10.846	−6.624
	(3)	−24.539	−17.325	−10.815	−6.611
	(4)	−24.687			

for $\kappa<1.4$, thus we only show comparisons for $\kappa=1$. Agreement between the various approaches is excellent, confirming the accuracy of Eq. (6).

As a final stringent test of the proposed Yukawa bridge function, we examine the compressibility sum rule by computing the isothermal compressibility directly from Eq. (4) and comparing against the values obtained by differentiating the results from Eq. (5). The comparison is shown in Fig. 3 for a range of Γ and κ with typical differences on the order of a few percent. Significant differences arise only at small κ (near the OCP limit) and large Γ. Thus, it appears the functional fit to the OCP bridge function [1] gives a somewhat larger deviation from the compressibility sum rule at large Γ. This deviation is consistent with the results published in Fig. 12 of Ref. [1]. Since we have not included the Ewald sum,

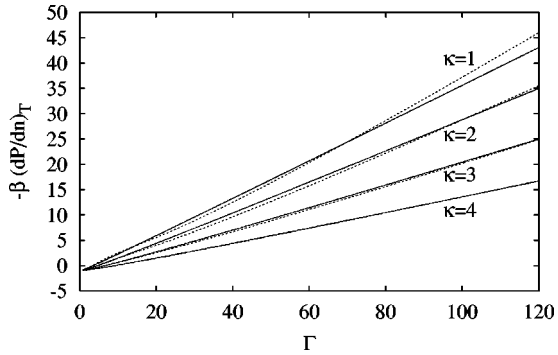

FIG. 3. Examination of compressibility sum rule as a function of Γ. The solid line is the compressibility $-\beta(\partial P/\partial n)_T$ computed by differentiating the pressure equation [see Eq. (5)] while the dashed line was computed directly from the compressibility equation [see Eq. (4)].

our MD code is not valid in the OCP limit $\kappa \to 0$. However, we have checked the modified HNC solutions for $g(r)$ against published Monte Carlo results for the OCP [25,26]. The results are nearly indistinguishable, except at large $\Gamma > 150$ where small differences arise. These differences are probably too small to effect quantities such as the pressure or excess energy, but may account for the small deviation in the compressibility at large Γ.

IV. CONCLUSIONS

We have proposed a bridge function for strongly coupled Yukawa systems based on a simple rescaling of the OCP bridge function extracted from Monte Carlo simulations [1]. The resulting correlation functions and thermodynamic properties are in excellent agreement with MD simulations and the compressibility sum rule is approximately satisfied over a broad range of parameters. Since all parameters are predetermined, including the proposed bridge function in an existing HNC algorithm is trivial. The resulting static correlation functions form a basic ingredient in nearly all theories describing strongly coupled regimes. Thus, we view the results of this work primarily as a useful tool in this regard.

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