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Static and dynamic properties of 2-dimensional strongly coupled Yukawa liquids

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Static and dynamical properties of strongly coupled Yukawa liquids are investigated. The particles are either (i) situated within an ideal 2-dimensional plane or (ii) are confined by an external parabolic potential to form a quasi-2-dimensional configuration. The static simulations (yielding pair correlation functions and correlation energies) and dynamical simulations (yielding spectra of density and current fluctuations) are carried out for a wide range of coupling (Γ) and screening (κ) parameters. The dispersion relations show good agreement with the predictions of the QLCA theory.

1 Introduction

Strongly coupled plasmas characterized by the Yukawa (screened Coulomb) interaction potential have been of current interest in relation to complex (dusty) plasmas. Earlier studies considered 3-dimensional systems [1, 2, 3, 4]; more recently attention has also turned towards 2-dimensional systems [5], due to their relevance to actual configurations formed in dusty plasmas [6].

In this paper we report our studies on two types of systems: (i) particles situated within an ideal 2-dimensional layer, and (ii) particles confined by an external parabolic potential to form a quasi-2-dimensional layer. We investigate these systems in the strongly coupled liquid phase. The particles interact through the Yukawa potential $\phi(r) = (q^2/r)\exp[-r/\lambda_{\rm D}]$ where q is the particle charge and $\lambda_{\rm D}$ is the Debye length. In addition to the screening parameter $\kappa = a/\lambda_{\rm D}$, the system is characterized by the coupling parameter $\Gamma = q^2/(ak_{\rm B}T)$, where T is the temperature, a is the Wigner-Seitz (WS) radius, $a = (n\pi)^{-1/2}$ and n is the surface density.

The simulations are based on the 3-dimensional Particle-Particle Particle-Mesh (PPPM) molecular dynamics technique, using periodic boundary conditions [7]. The calculations yield the static properties: pair correlation functions (PCF), correlation energy of the system and their dependence on the plasma coupling (Γ) and screening (κ) parameters, as well as the dynamical characteristics: spectra of the longitudinal and transverse current fluctuations, and dispersion relations for the collective excitations. The results of the simulations are compared to the predictions of the Quasi-Localized Charge Approximation (QLCA) theory [8].

2 2-dimensional Yukawa liquid

The effective coupling parameter for a Yukawa system is usually defined as $\Gamma^\star = \Gamma e^{-\kappa}$. We have found this definition inadequate since a fixed $\Gamma^\star$ may not uniquely determine the properties of the system (e.g. at $\Gamma^\star$=120 the

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system was found to be either in the liquid or in the solid phase, depending on the value of κ). A more appropriate definition of the effective coupling parameter Γ_0 can be given on the basis of the $g(r)$ pair correlation function so that Γ_0 represents a combination of (Γ, κ) pairs that leaves the amplitude of the first peak of the PCF invariant. In fact, as Fig. 1(a) shows, not only the amplitudes of the first peak, but the $g(r)$ functions in their entireties are nearly the same for a fixed Γ_0 but differing κ values. Moreover, at high values of Γ_0 the ratio Γ/Γ_0 depends only on κ, as shown in Fig. 1(b), i.e. $\Gamma_0(\Gamma, \kappa) = \Gamma f(\kappa)$, where $f(\kappa) = 1 - 0.388\kappa^2 + 0.138\kappa^3 - 0.0138\kappa^4$. It can be seen that the results accurately fit the above formula except for the lowest Γ_0 = 10 value. The correlation energy, calculated as $E_{\rm corr} = (q^2/a)\int d\overline{r} g(\overline{r}) e^{-\kappa\overline{r}}$ (where $\overline{r} = r/a$) is plotted in Fig. 1(c) as a function of κ, for different values of Γ_0. The results depend slightly on Γ_0 but vary strongly with κ, as expected, due to the exponential dependence of the interaction potential on the screening strength. The data can be approximated as $E_{\rm corr} = (q^2/a)[b(\kappa) + c(\kappa)\Gamma_0^{-2/3}]$, where $b(\kappa) = -1.103 + 0.505\kappa - 0.107\kappa^2 + 0.00686\kappa^3 + 0.0005\kappa^4$ and $c(\kappa) = 0.384 - 0.036\kappa - 0.052\kappa^2 + 0.0176\kappa^3 - 0.00165\kappa^4$.

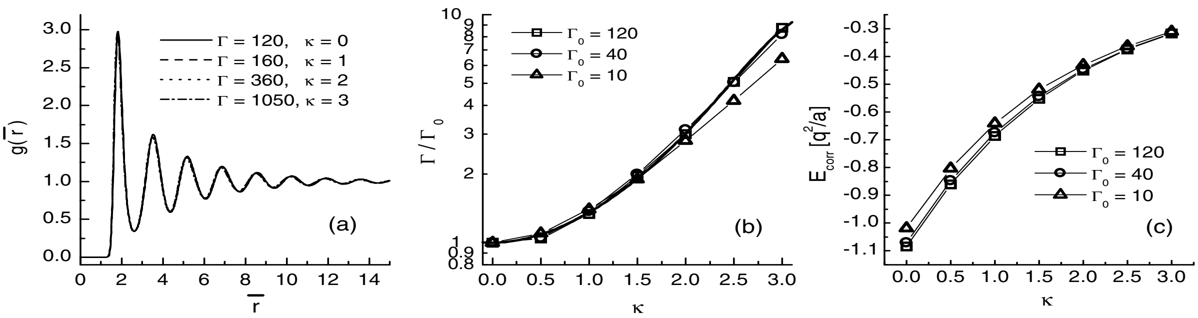

Fig. 1 (a) Pair correlation functions at an effective coupling Γ_0 = 120; (b) Γ/Γ_0 as a function of κ; the heavy line shows values calculated from the fitting formula; (c) correlation energy.

To obtain the spectra of longitudinal and transverse current fluctuations we use the standard simulation techniques [9]. The dispersion relations derived from these fluctuation spectra are displayed in Fig. 2(a) and (b), respectively, for the longitudinal and for the transverse mode. The results are shown for effective coupling Γ_0 = 120, at different values of κ. The quasi-acoustic $\omega/\omega_0 \propto \sqrt{\overline{k}}$ behavior of the longitudinal mode in the κ = 0 Coulomb limit changes to an acoustic $\omega/\omega_0 \propto \overline{k}$ behavior as the screening is introduced (ω_0 is the nominal 2D plasma frequency: $\omega_0 = (2\pi n q^2/ma)^{1/2}$ and $\overline{k} = ka$). The transverse mode also shows (although the data are less accurate due fact that this mode is quite weak) an approximately linear relationship between the frequency and the wave number, except that this mode has a cutoff at a finite frequency, similarly to the 3-dimensional case [1, 2]. The results of the simulations have been compared to the predictions of the QLCA theory that gives the frequencies of the longitudinal and transverse waves, respectively, as:

$$\frac{\omega_{\rm L}^2}{\omega_0^2} = \frac{\overline{k}^2}{2}\int d\overline{r}\Lambda(\overline{k}\overline{r}, \kappa\overline{r})g(\overline{r}) \quad , \quad \frac{\omega_{\rm T}^2}{\omega_0^2} = \frac{\overline{k}^2}{2}\int d\overline{r}\Theta(\overline{k}\overline{r}, \kappa\overline{r})g(\overline{r}) \tag{1}$$

$$\Lambda(x, y) = \frac{e^{-y}}{x^2}\left[(1 + y + y^2) - (4 + 4y + 2y^2)J_0(x) + (6 + 6y + 2y^2)\frac{J_1(x)}{x}\right], \tag{2}$$

$$\Theta(x, y) = 2\frac{e^{-y}}{x^2}(1 + y + y^2)[1 - J_0(x)] - \Lambda(x, y). \tag{3}$$

In (1) the $g(\overline{r})$ functions obtained from our MD simulations have been used as an input. There is a good quantitative agreement between the theoretical and simulation results. The only feature that the QLCA fails to reproduce is the cutoff of the transverse mode frequency at a finite wave number [1, 2].

3 Collective behavior of quasi-2-dimensional Yukawa liquid

When particles are confined by a parabolic potential, depending on the strength of the confining potential they arrange themselves in different numbers of layers [10]. Here we look at strong confinement when a single layer

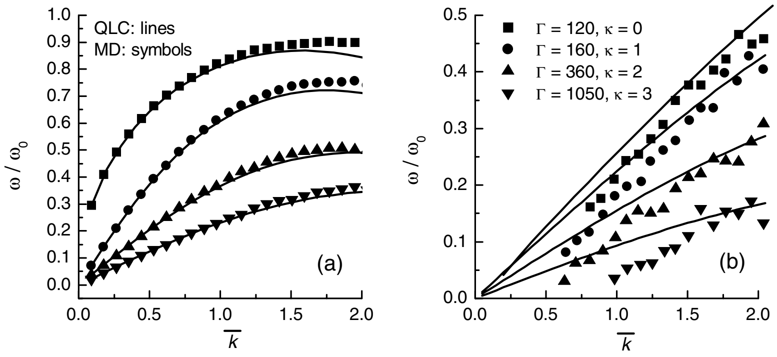

Fig. 2 Dispersion relations of the longitudinal (a) and transverse (b) modes at Γ_0 = 120; symbols: simulation results, solid lines: QLCA theory.

(with finite width) is formed. Compared to the ideal 2-dimensional configuration, there is an extra degree of freedom provided by the confinement of the particles by the external potential. This gives rise to an additional collective mode, the "perpendicular" mode, where the particles oscillate in the direction normal to the plane. Figure 3 shows the dispersion of the three modes, for $\Gamma = 100$, $\kappa = 0.26$, and for a confinement strength where the width of the layer is $\approx 0.3a$. The frequency of the perpendicular mode at $k = 0$ is determined by the confinement force. As the confinement force and the repulsive interparticle force act against each other, this mode exhibits a negative dispersion.

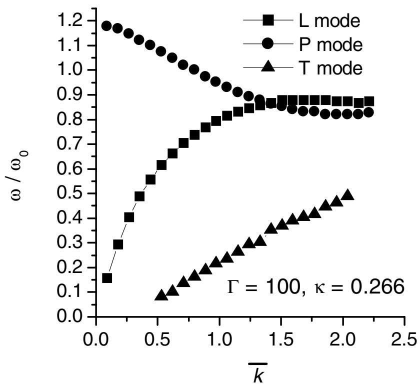

Fig. 3 Dispersion relations for the longitudinal (L), transverse (T) and perpendicular (P) modes in the quasi-2-dimensional system. The L and T modes behave similarly to the modes in the ideal 2-dimensional layer. Simulation parameters: $\Gamma = 100$, $\kappa = 0.26$, width of particle layer $\approx 0.3a$

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