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Dynamic Shear Viscosity in a 2D Yukawa System

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We present non-equilibrium molecular dynamics simulation studies on the dynamic (complex) shear viscosity of a 2D many-particle system interacting via a Yukawa (Debye-Hückel) type inter-particle potential. Our investigations reveal the complex interplay of dissipative and elastic processes, as well as the effect of single particle resonances and enhanced collective excitations, and the influence of the external forces on the structural correlations in the system.

Viscosity, the measure of the plastic response of matter (primarily liquids and soft matter) to applied forces, is a central quantity in rheology. The shear viscosity η relates the "transverse" momentum flux j_y to the velocity gradient $\partial v_x/\partial y$ (also termed the shear rate $\dot{\gamma}$), as $j_y = -\eta(\partial v_x/\partial y)$.

Continuum hydrodynamics successfully uses the concept of viscosity, usually as input parameter as an intrinsic property of the material under investigation, in the Navier-Stokes equation. One has to note, however, that the Newtonian concept of viscosity is applicable only (i) at small shear rates, (ii) long length scales, and (iii) at low frequencies. In many physical systems, these conditions are clearly violated [1].

The generalization of the concept of the flux equation to periodic excitations can be expressed as $j_y \mathrm{e}^{i(\omega t-\phi)} = -\eta(\omega)\dot{\gamma}\mathrm{e}^{i\omega t}$, where ω is the frequency of the harmonic excitation and $\phi = \phi(\omega)$ is the phase (time) shift (delay) observed between the excitation and the response. The frequency dependent viscosity coefficient in this case is a complex number and can be expressed as $\eta(\omega) = \eta_0(\omega)\mathrm{e}^{-i\phi(\omega)} = \eta'(\omega) - i\eta''(\omega)$.

Since the pioneering work of Lin I in 2001 [2], who has applied a shearing laser beam to a single layer dusty plasma system to measure shear viscosity, the rheological properties of both 2D and 3D dusty plasmas are of ongoing interest [3–7].

Complementing the experimental efforts, the shear viscosity has been derived in a number of simulation studies, both for three-dimensional (3D) and two-dimensional (2D) settings [8–13]. In [14, 15], besides calculations of the "equilibrium" ($\bar{\gamma} \to 0$) static viscosity, predictions for the shear-thinning effect (typical for complex molecular liquids) were given at high shear rates. The frequency dependence of the complex shear viscosity, which combines the dissipative and the elastic components of the complex response of matter to oscillating shear stress as $\eta(\omega)$, was computed for 3D Yukawa liquids in [16].

Here we combine and extend previous numerical efforts, with our latest dusty plasma experiment [17] by performing systematic simulations addressing the complex shear viscosity of 2D Yukawa systems in a wide range of shear rate and excitation frequency parameters. We aim to explore the dependence of the features of the system on these parameters and to identify the underlying phenomena.

Our simulations are based on a non-equilibrium molecular dynamics method, with an applied oscillatory shear, using the Gaussian thermostated SLLOD equations of motion in planar Couette flow, in conjunction with Lees-Edwards periodic boundary conditions [18]. The computation of the complex shear viscosity is based on the evaluation of the off-diagonal element of the pressure tensor as it is described in detail in [16]. We perform the simulations for $N = 11400$ particles, in a wide range of shear rates (1), for a series of perturbation frequencies

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(2) and Coulomb coupling parameters (3), with a Yukawa screening parameter $\kappa = 1$:

$$\bar{\gamma} = \frac{\dot{\gamma}}{\dot{\gamma}_0} = \frac{\partial v_x}{\partial y}\frac{a}{v_{\text{therm}}} = 0.04...4.0, \text{ where } \quad a = 1/\sqrt{\pi n} \tag{1}$$

$$\bar{\omega} = \omega_{\text{shear}}/\omega_p = 0.05...1, \text{ where } \quad \omega_p^2 = nQ^2/(2\varepsilon_0 m a) \tag{2}$$

$$\Gamma = \frac{Q^2}{4\pi\varepsilon_0}\frac{1}{ak_BT} = 100,\ 200,\ 500 \tag{3}$$

The principal investigated quantities are the real (viscous dissipative) and imaginary (elastic) parts of the complex viscosity, the energy absorbed by the thermostat (equivalent to the energy absorbed by the particle ensemble from the external perturbation), the density and current fluctuation spectra, and the pair correlation function.

In the small shear limit our simulation results are in qualitative agreement with 3D simulation results [19]. Compared to our previous dusty plasma experiment [17] we obtain good agreement for: (i) the shear rate dependence of the viscosity at static shear and (ii) the frequency dependence of the viscosity at intermediate shear rates (see Fig. 1). This comparison serves as an experimental verification of our simulations and supports its validity in parameter regimes not yet explored experimentally.

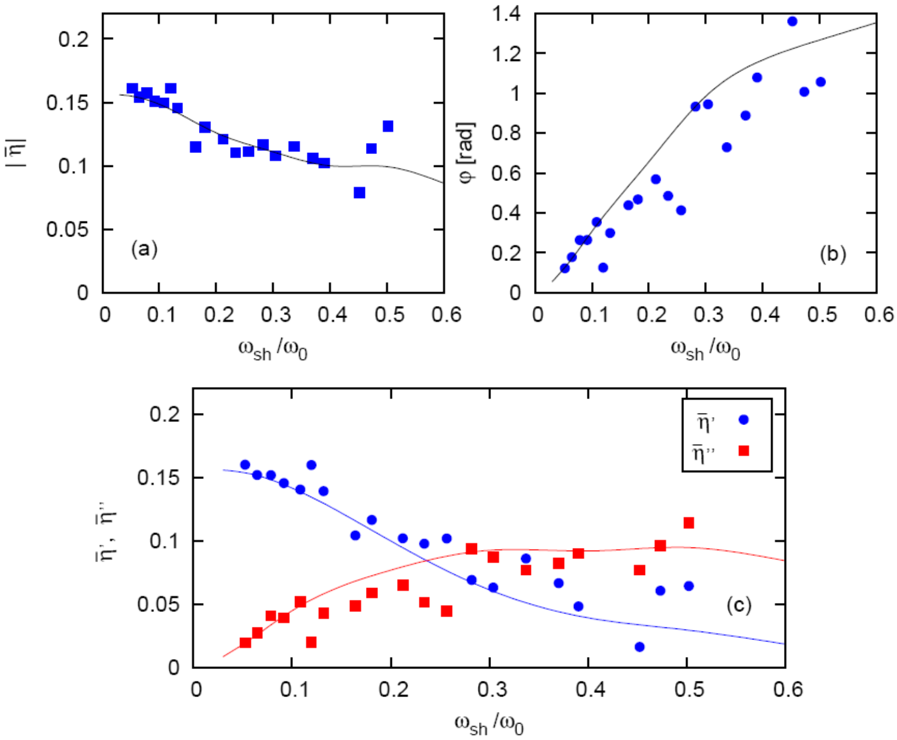

Fig. 1 Frequency dependence of the shear viscosity. (a) Magnitude $|\eta(\omega)|$, (b) complex phase angle $\varphi(\omega)$, (c) real and imaginary parts $\eta'(\omega), \eta''(\omega)$. The symbols are experimental data values, lines show MD simulation results for $\Gamma = 200$. For details of the experiment see [17].

First we focus on the complex shear viscosity and its real–imaginary decomposition. In Fig. 2(a) one can observe the same non-monotonicity in the frequency dependence at intermediate shear rates ($\sqrt{\bar{\gamma}} \approx 1...1.5$) as it was found in the experiment as shown in Fig. 1(a), which is a result of the crossover of the real and imaginary contributions as it can be seen in Fig. 2(c) and (d).

To gain more insight into the microscopic processes dominating the viscosity we have measured the amount of energy absorbed by the Gaussian thermostat acting on the system. Fig. 3 reveals, that at $\omega/\omega_p \approx 0.4 - 0.5$ some kind of resonance develops in the systems at moderate shear rates, and that at $\omega/\omega_p \approx 0.7$ and higher shear rates the system does absorb relatively small amount of energy from the external shearing forces.

A possible explanation for the resonance is, that a 2D Yukawa system with $\kappa = 1$ in the strongly coupled liquid phase has a characteristic Einstein frequency of $\omega_E/\omega_p \approx 0.5$ as studied in [20]. The Einstein frequency is the frequency of oscillation of a single particle around its equilibrium position in the immobilized frozen environment of the other particles of the system, thus it represents single particle excitation, which is enhanced by the periodic external forces in case of frequency matching.

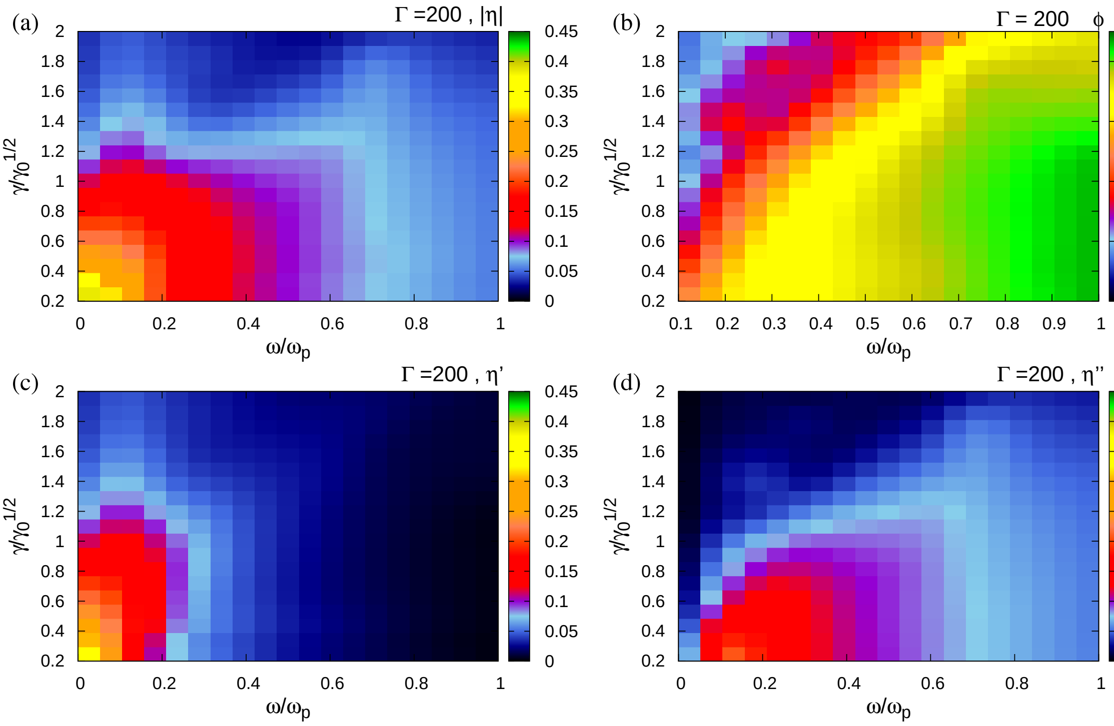

Fig. 2 Shear rate and frequency dependence of the shear viscosity: (a) magnitude $|\eta(\omega)|$, (b) complex argument $\phi(\omega)$, (c) real and (d) imaginary parts $\eta'(\omega), \eta''(\omega)$ for $\Gamma = 200$.

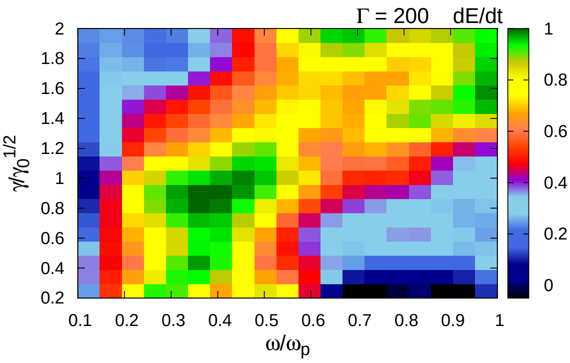

Fig. 3 The normalized average energy absorbed by the thermostat (equivalent to the energy absorbed by the particle ensemble from the external perturbation).

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The local minimum in the absorbed energy seems to coincide with the the plateau frequency of the longitudinal wave dispersion of the system ($\omega_L/\omega_p \approx 0.74$). Fig. 4 shows the peak intensities of the $L(k, \omega)$ longitudinal current fluctuation spectra, as described in [20] in the solid phase at $\Gamma = 500$ for better visibility.

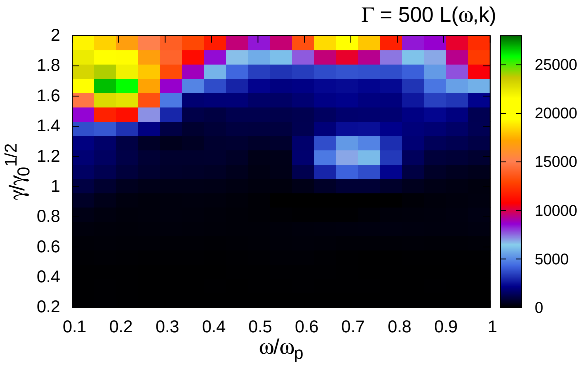

Fig. 4 Peak amplitude (in arb. units) of the longitudinal current fluctuation spectra in the solid phase at $\Gamma = 500$.

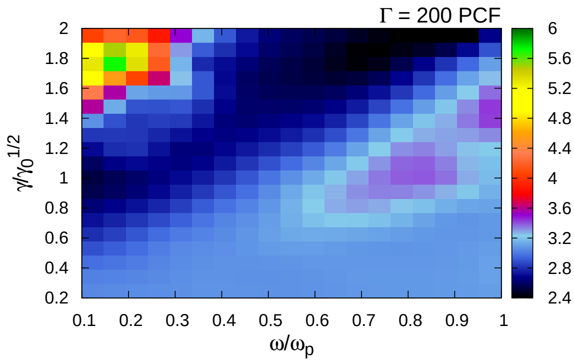

Fig. 5 First peak of the pair correlation function.

An enhanced collective wave activity is observed, when the excitation frequency and shear rate are in the vicinity of the observed absorbance minimum, indicating the long living nature and large amplitude of the excited collective modes (waves) in the system.

To describe positional structure in the systems we show in Fig. 5 the amplitude of the first peak of the pair correlation function (PCF).

A complex behavior is observed with a few competing trends. At lower shear rates the PCF increases with frequency, while at high frequencies a maximum of the PCF appears as the shear rate increases. The extremely high and fluctuating values at small frequencies and high shear rates are subjects of further investigations.

In conclusion, we have shown, that for 2D Yukawa systems (1) the non-monotonicity of the frequency dependence of the complex shear viscosity appears due to the competition of dissipative and elastic deformations, (2) single particle excitations are responsible for rapid heating at moderate frequencies, (3) collective wave excitations dominate at higher frequencies, and (4) the external shearing forces can enhance structural order in the system.

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