Shear viscosity of two-dimensional strongly coupled complex (dusty) plasmas

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Abstract. A molecular dynamics method has been employed of studying shear viscosity for two-dimensional plasma liquids. For the entire range of strongly coupled liquid states, shear autocorrelation functions indicate overall valid viscosity coefficients. A systematic dependence of shear viscosity value on screening strength ($\kappa$) is observed for an intermediate and higher Coulomb coupling strengths ($\Gamma$). The simulation data indicate that the position of the viscosity value shifts towards higher $\Gamma$ as $\kappa$ increases. It is observed that valid viscosity coefficient exists and it is dependent on plasma parameters ($\Gamma$, $\kappa$). A finite minimum viscosity exists nearly at the same value of $\Gamma$ where the most extreme super-diffusion was earlier found and is reported for a wide range of coupling and screening parameters.

1. Introduction

In recent years, the transport problems in non-ideal systems of interacting particles are of significant interest in various fields of science and technology. In some cases, the presence of dust particles can be quite beneficial in the efficiency of solar cell where as an undesirable contaminant that can destroy microchips during their plasma enhanced fabrication. The presence and formation of dust in plasma systems has been widely studied both experimentally and numerically [1,2]. The industrial applications and widespread existence of dusty plasmas, combined with a number of their general and standard thermophysical properties, make dusty plasmas extraordinary attractive and interesting subjects for many researchers. Shear processes play a dominant role in determining dynamical properties of many physical, chemical and biological systems. Shear viscosity is one of dynamical property of fluids required to describe shear flows and damping of waves. Shear viscosity is essential for predicting collective mode properties of strongly coupled complex (dusty) plasmas (SCCDPs) plasma, an issue at the forefront of rapidly evolving field of dusty plasma [3,4].

The thermophysical properties of two and three dimensional SCCDPs have been studied in great detail for many decades [1-9]. This work reviews the outcomes of studies carried out in the last two decades, which facilitate us to understand a picture of the variation in the viscosity coefficient over the whole range of plasma parameters of the SCCDPs. The correlation functions of two dimensional (2D) SCCDPs have recently attracted the particular attention to the researchers for studying dusty plasma [3,10,11]. A slow decay $\propto t^1$ of the velocity autocorrelation function (VACF) was observed in the earlier 2D molecular dynamics (MD) measurements of hard disk liquids, showing no diffusive motion [12]. Similar conclusions have been publicized with an additional argument that this asymptotic
behaviour should also exist in kinetic contributions of the autocorrelation functions for the shear viscosity and thermal conductivity, regardless of the pair potential [13]. Another MD simulation with observed a $t^{-1}$ decay of the shear autocorrelation function (SACF) in the 2D soft disk liquids [14].

Shear viscosity has been experimentally investigated in 2D dusty plasma liquids (DPLs) monolayer of dust particles [2], and these observations were supported by earlier equilibrium MD (EMD) simulations with 2D DPLs [14]. Soon after, nonequilibrium MD simulations (NEMD) were employed with 2D Yukawa liquids [11] and investigated the viscosity coefficients at lower plasma parameters ($\Gamma$). A long standing controversy over these transport observations with conflicting experimental and simulation results in recent 2D Yukawa liquids is our motivation for presented work.

Recently, in a previous paper, the present authors have been studied similar computations with detailed argument on shear stress autocorrelation functions (SACFs) measurements for intermediate and higher Coulomb coupling strengths of 2D SCCDPLs [15]. Our previous results, for SACFs, show that the long time behaviour will determine whether the shear viscosity coefficient is unique or not. In this presented work, we have extend our work for the determination of shear viscosity coefficients ($\eta$) for the whole range of plasma parameters ($\Gamma$, $\kappa$) than those used previously known results for the 2D SCCDPLs [11,14].

The purpose of the presented work is to investigate further all possible dependences of the shear viscosity on the screening and Coulomb coupling strengths ($\Gamma$, $\kappa$), using the same method and the extended set of parameters as in Shahzad and He [15]. Moreover, the aim of this work is to investigate a systematic study of the effects of screening length of the dust particle interaction on shear viscosity and to investigate the existence of the related shear viscosity coefficients of 2D SCCDPLs, by using extensive numerical simulations. This paper is organized as follows: In Section 2, the estimate of the shear viscosity coefficient for Yukawa liquids is analyzed through the equilibrium MD method, and this section also describes the simulation technique. Next, the obtained results are presented and discussed with simulation data reported by other author’s in Section 3. The work is summarized in Section 4.

2. Theory and EMD algorithm

A well known Green-Kubo relation (GKR) is commonly used for the shear viscosity coefficients of uncharged particles [16,17]. Equilibrium MD is used for 2D Yukawa liquid simulations [3,15] and it is similar to the 2D monolayer dusty plasma experiments [2] conducted in equilibrium environments. It has been shown that the standard GKRs of liquids apply to the SCCDPLs [3-9,11,15]. Currently, the Yukawa (screened Coulomb) potential model is the best known model for simulation of the pairwise interactions between dust particles with each other in laboratory plasma of gas discharge and in many physical systems (biology, medicine, physics of polymers, etc.)

$$\phi(|r|) = \frac{Q^2 e^{-|r|/\lambda_D}}{4\pi\varepsilon_0 |r|},$$

(1)

where, $r$ is the interparticle distance, $\lambda_D$ is the Debye screening length and $Q$ is the charge on a dust particle. In thermodynamic limit, such a Yukawa model can be described by two reduced parameters [3,10,11,15]: the Coulomb coupling parameter $\Gamma=(Q^2/4\pi\varepsilon_0)(1/a\lambda_D T)$ and the screening parameter $\kappa=a/\lambda_D$. Here, $T$ is absolute temperature, $a_B$ is Boltzmann’s constant, $a=(n\pi)^{1/2}$ is the Wigner-Seitz radius [7] with $n$ is the equilibrium dust number density. Time scales of interest are regarded as inverse of the plasma frequency $\omega_p=(Q^2/2\pi\varepsilon_0 m a^3)^{1/2}$, where $m$ is the dust particle mass.

To compute the shear viscosity $\eta$, we start from the following usual equations

$$\eta = \frac{1}{Ak_B T} \int_0^\infty Z_\eta(t) dt, \quad Z_\eta(t) = \left\langle P^\eta(t) P^\eta(t_0) \right\rangle,$$

(2)
where $Z_\eta(t)$ is the shear stress autocorrelation function, $A$ is area for a 2D system, $T$ system temperature, and the angular bracket indicates an ensemble average for Yukawa systems. In order to compute the shear viscosity, time series data for the positions $(x_i, y_i)$, velocities $(v_{ix}, v_{iy})$ and off-diagonal elements of pressure tensor $P_{xy}$ are required and given as

$$P^{\eta}(t) = \sum_{i=1}^{N} m v_{ix} v_{iy} - \frac{1}{2} \sum_{i,j}^{N} \frac{x_i y_j - v_{ix} v_{iy}}{r_{ij}} \frac{\partial \phi(r_{ij})}{\partial r_{ij}},$$

where $N$ is the number of particles, $m$ is the dust particle mass and $r_{ij} = \mathbf{r}_i - \mathbf{r}_j$. The first term of Eq. (3) is kinetic contribution, which depends on particle velocities and the second term is a potential contribution, which depends on the Yukawa pair potential given in Eq. (1). In calculating SACF from MD simulation data, it is used a common method of overlapping time segments. Further details of the correlation functions from MD simulation method, were reported in [3]. The 2D viscosity $\eta$ is normalized by $\eta_0 = \frac{m \omega_p a^2}{\eta}$. All time series data are recorded during MD simulation and used Eqs. (2) and (3) to calculate $\eta$.

2.1. Numerical simulation

We start as usual with a system of $N=1024$-18225 particles enclosed in a simulation box with edge lengths $L_x/L_y = 2/\sqrt{3}$, interacting through a pairwise potential of Yukawa type, and the number particle motion is modeled by Newton’s equations. The particle number is chosen large enough to be free of the size effects noted for the present work. It is reported in our earlier equilibrium MD simulation estimations that particle number is sufficient to test such system sizes [15]. Therefore, this particle number $N$ is sufficient for simulations that in order to save computer time. Our MD computations are performed in a microcanonical ensemble and a fifth order predictor-corrector algorithm [1,3] is employed to solve the normalized equation of motion of $N$ Yukawa particles. Periodic boundary conditions (PBCs) are maintained in all directions and the minimum image convention of the $N$ Yukawa particles throughout our numerical experiment, for simulation of an infinite system. The imposed periodicity needs to be consistent with the fact that the ground state at low temperatures is the triangular lattice [3,15,17]. When the number of dust particles satisfies $N = (\text{integer})^2$, or is equal to the number of unit cells, our periodicity satisfies this condition.

We derived the Ewald sums expression of the force, energy and pressure tensor which are implemented in our numerical code. In the Ewald summation method, the interaction potential is divided into two parts, one of which converges rapidly in real space sum and the other converges rapidly in the reciprocal space sum. For higher screening values $\kappa$ the real space sum part alone gives enough performance and precision. Pair wise Yukawa interparticle forces are summed over a $\kappa$-dependent cutoff radius [1,3,7-9]. Additional details of the Ewald sums technique for Yukawa interactions are reported by Shahzad and He [7]. The desired system temperature is attained by periodically synchronize all particles and renormalizes their velocities to the required target value for $T$ and the system reaches thermodynamical equilibrium. Once the system reaches thermodynamical equilibrium, the periodic renormalization of particle velocities is continued and allows the system progress under the constant energy conditions. Production stages are employed between $9.5 \times 10^6/\omega_p$ and $12.5 \times 10^6/\omega_p$ time units in the series of data recording of $\eta_0$. The simulation time step $0.001/\omega_p \leq dt \leq 0.005/\omega_p$ is maintained the large cell size to allow computing the important data at long times [3,15]. In addition, to reduce statistical noise, two independent equilibrium MD calculations runs are carried out with arbitrarily chosen configurations of the particle positions, for each target temperature $\Gamma$, and averaging these measurements to improve the statistics. In this paper, the computations are reported for shear viscosity of 2D SCCDPs over wider range of plasma parameters of $(40 \leq \Gamma \leq 180)$ and $(1 \leq \kappa \leq 3)$. 
3. Results and Discussion

The results obtained for our MD series of simulation of a 2D Yukawa liquid are estimations of shear viscosity showing the indication of superdiffusive motion at intermediate and higher Coulomb coupling parameters, as we earlier reported extreme superdiffusion in Ref [15]. The shear viscosity trends in 2D DPLs depend on both the Coulomb coupling strength and the screening strength $1/\kappa$. These simulation data are for a large system size ($N = 18252$), but with different $\Gamma$, which covers the value of coupling strength, where the viscosity ($\eta_0$) has minimum possible value depends on $\kappa$, [6,15] up to $\Gamma=180$.

Figure 1. Comparison of results for minimum possible values of shear viscosity as a function of Coulomb coupling $\Gamma$ for Yukawa liquid, obtained from Green-Kubo relation defined in Eqs. (2) and (3), at (a) $\kappa=1$; (b) $\kappa=2$ and (c) $\kappa=3$ (c). EMD of Shahzad and He: SH 2D EMD: present results, NEMD of Donkó et al [11]: Donkó et al 2D NEMD, EMD simulation results of Salin and Caillol [4]: SC 3D EMD, EMD calculations of Saigo and Hamaguchi [5]: SH 3D EMD, and Homogenous Shear Algorithm (HSA) and Reverse MD (RMD) of Donko and Hartmann [6]: DH 3D HSA and RMD.

Figure 1 shows the main results obtained from the EMD method for the different plasma states simulated for the Yukawa liquids at $\kappa=1$, 2 and 3, respectively. Parts (a), (b) and (c) of the figure 1 show our calculations for the shear viscosity with $N = 18252$ particles at a long run, as well as the
previous results taken from the NEMD simulations of Donkó et al [11], Green-Kubo EMD of Salin and Caillol [4], EMD work of Saigo and Hamaguchi by using tensor-product spline function [5] and homogenous shear algorithm (HSA) and reverse MD (RMD) of Donko and Hartmann [6]. A first observation is that $\eta_0$ has its minimum possible value, nearly indicating the most extreme superdiffusion, at $\Gamma=40$ for $\kappa=1$, $\Gamma=60$ for $\kappa=2$ and $\Gamma=80$ for $\kappa=3$. The evidence of maximum values of superdiffusion has been discussed in our earlier published work [15]. These results are important because this happens nearly at the same value of $\Gamma$ where the shear viscosity was earlier to have a minimum value [11,14]. There are different factors to be chosen to obtain the best results by the presented equilibrium MD for shear viscosity. We can vary the strength of screening parameter ($\kappa$), system length (run time), the system temperature ($\Gamma$) and system size ($N$) in order to examine how efficiently the EMD algorithm computes the shear viscosities of SCCDPs.

Starting from the values of $\Gamma$ at which $\eta_0$ has lowest values, the present simulations give a definitely lower $\eta_0$, compared to results in Ref. 11. The simulations are carried out with $N=18252$ for $\kappa = 1, 2$ and 3, and it is important that the EMD method gives measurements for $\eta_0$ within the limited statistical uncertainties over the wide range of system sizes. It is observed that the presented results of $\eta_0$ are slightly lower than and lie more close to the earlier NEMD calculations of Donkó et al [11] but our results are slightly higher at region between $180 \leq \Gamma \leq 300$ for the $\kappa=2$ case. These investigations are significant because the results happen at the same values of coupling $\Gamma$ where the $\eta_0 \cong 0.072$ at $\kappa=1$ and $\eta_0 \cong 0.06$ at $\kappa=2$ were earlier shown to have the minimum values of $\eta_0$ [11,14]. The presented results for $40 \leq \Gamma \leq 180$ at $\kappa=1$ and $60 \leq \Gamma \leq 180$ at $\kappa=2$ lie between of data sets of 2D NEMD of Donkó et al [11] and the results of 3D calculations of $\eta_0$ by different authors [4-6]. Our simulation data for viscosity are dependent on the degree of correlations in the 2D system, and the dependence is clearly monotonic. Our second examination from figure 1 is that the $\eta_0$ is dependent on $\kappa$, like 3D simulation [4-6]. The present simulations show that the minimum possible value of $\eta_0$ shifts towards higher $\Gamma$ as $\kappa$ increases. The same shifting behavior was also seen in earlier 3D simulations. The minimum value of $\eta_0$ decreases with increasing $\kappa$. Our simulation trends have a good agreement with the earlier 2D MD of Ref. 14 and NEMD of Ref. 11 simulations. In addition, the presented results are also well matched with the earlier 3D Green-Kubo EMD investigations of Ref. 4, spline function EMD work of Ref. 5 and homogenous shear algorithm (HSA) and reverse MD (RMD) calculations of Ref. 6.

Finally, it is revealed the universal scaling law for the CDPLs. Figure 2 shows the variation of reduced shear viscosity $\eta^*/\eta_*$ (normalized by the Einstein frequency) at different normalized temperatures

![Figure 2. Variation of reduced shear viscosity normalized by Einstein frequency $\eta^*(T^*)$ with reduced temperature $T^*$ for Yukawa system at different $\kappa=1, 2$ and 3. The thick line is obtained using the simple Scaling Law: $\eta^* = AT^* + B/T^* + C$, showing the Universal behaviour.](image)

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\( T^* \) (ratio of the temperature to melting temperature) for \( \kappa = 1, 2 \) and 3. It is shown from figure 2 that the \( \eta^* \) is dependent on both the screening and reduced temperature in the SCCDPs. The results obtained for \( \eta^* \) using EMD method provide the suitable trend nearly for all the plasma state points of \( \kappa \) and \( \Gamma \). The solid line given in figure 2 is obtained using the simple empirical fit of form, \( \eta^* = AT^* + B/T^* + C \), with coefficients: \( A = 0.02287 \), \( B = 1.14437 \), and \( C = -0.15092 \), same as in Ref. 5 and 11. This scaling law is found to reproduce appropriately the shape of \( \eta(T^*) \) curves at three \( \kappa \) values and it gives suitable relationship between \( \eta^* \) and \( T^* \) for nearly the whole plasma state points of \((\Gamma, \kappa)\), confirming the earlier simulation results [8, 11, 17].

4. Conclusion

Equilibrium MD simulation approach has been employed to determine shear viscosity of a 2D SCCDPs over a wide range of plasma parameters of \( \Gamma \) and \( \kappa \). New simulations provide more reliable data for Yukawa shear viscosity than earlier known results. The calculations confirm that the minimum possible value of shear viscosity exists at intermediate and higher Coulomb couplings. It is revealed that the prediction of minimum value of shear viscosity helps to understand the fundamental behavior in 2D Yukawa dusty plasma systems. Our data indicate that the shear viscosity dependent on the screening strength and the degree of correlation in 2D Yukawa liquids. Our simulations show that the minimum possible value of viscosity shifts towards higher Coulomb coupling as screening parameter increases. Our shear viscosity calculations illustrate a fair agreement with earlier MD and NEMD simulations. In future work, it will also be of highly interest for analysis to see how quantum effects influence viscosity in 3D and 2D SCCDPs and it is suggested a need for an experiment or simulation.

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