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Shear viscosity and diffusion motion of two-dimensional dusty plasma liquids

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Abstract

A molecular dynamics method for studying diffusion motion and shear viscosity is presented for two-dimensional (2D) plasma liquids. The calculations obtained by using the mean-squared displacement (MSD), velocity autocorrelation function (VACF) and the shear autocorrelation function indicate that there is a diffusive motion for the lower coupling range of strongly coupled liquid states. In the MSD test, both states of a transition phase from normal diffusion to superdiffusion, and the extreme superdiffusion at intermediate coupling strength are dependent on screening strengths. The simulation data show that the position of extreme superdiffusion shifts towards higher coupling with an increase in screening strength, and the superdiffusion is nearly in a constant motion for higher coupling. A smooth transition from normal diffusion to superdiffusion exhibits the existence of superdiffusion at intermediate coupling strengths in the VACF test. A valid shear viscosity exists only at the intermediate and higher coupling parameters. It seems that the present calculations cannot establish a coupling between the viscosity and diffusion in 2D Yukawa liquids.

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(Some figures may appear in color only in the online journal)

1. Introduction

Transport parameters like diffusion and shear viscosity describe the material properties of fluids within the framework of the continuum of fluid dynamics. They are essential in many engineering and science applications. On the other hand, the behavior of the transport parameters in various situations can give an insight into the fundamental processes that occur at the atomistic level. The two-dimensional (2D) Yukawa systems can be regarded as models which cover both systems with long- and short-range interactions. These models play a significant role in many physical, chemical and biological systems [1]. A wide range of charged particle systems can be modeled as Yukawa systems in the liquid state: these include colloidal suspensions [2], high-energy density matter [3], strongly coupled dusty plasmas [4, 5], dusty plasmas levitated in a monolayer [6] and a structural analysis of symmetric and asymmetric plasma crystals [7].
The shear viscosity and diffusion of a solid or a liquid can be measured experimentally. These experiments, however, can only be performed at a macroscopic scale and cannot resolve the details of the transport processes at a microscopic level [19]. Recently, the superdiffusive motion of dust particles in 2D DPLs (monolayer) and quasi-2D has been frequently claimed in many experiments [20–24]. These observations were supported by recent MD simulations with 2D and quasi-2D DPLs [10–12, 24–28]. However, another experimental group [6] with 2D monolayer dusty plasma investigated the diffusive motion for a wide range of the Coulomb coupling parameter and observed a subdiffusive process near the melting point. These conclusions were enhanced by the recent MD simulations [11], and more recent Langevin dynamics (LD) and equilibrium MD simulations for 2D DPLs [24, 27, 28]. Liu et al [24] performed the MD and LD simulations to investigate diffusion motion and reported the results that the most extreme superdiffusion exists at intermediate coupling strength without any significant non-Gaussian statistics. Subsequently, Ott and Bonitz [28] performed the LD simulations and claimed that subdiffusion is possible at sufficiently large friction, and in the long time limit, anomalous diffusion vanishes and the system returns to normal diffusion for dissipative as well as for frictionless systems. However, they did not observe a monotonic increase of superdiffusion with an increase in \( \kappa \) (stiffness of interactions) which is our first motivation for this work.

For shear viscosity, the earlier MD simulations [29] motivated by an experiment on shear viscosity using a 2D dusty plasma monolayer [30] showed a fast decay of the SACF. Nonequilibrium MD simulations with 2D Yukawa liquids [31] explored the viscosity coefficients, and the results obtained from this method did not depend significantly on system size. Recently, the MD simulations [11] showed that a transport coefficient exists for diffusion at low Coulomb strength and for viscosity at high Coulomb strength, but not in the opposite limits. The conditions for self-diffusion and shear viscosity in 2D DPLs are different, as the literature includes both simulation and experimental studies. A minimum possible value of shear viscosity may exist during the course of maximum value of superdiffusion [10]. The second motivation for this work is the observation of minimum possible values of shear viscosity with a variation of \( \kappa \).

Studies of transport coefficients in such 2D DPLs are especially interesting due to doubts about the existence of contradictory observations in both experiments and theoretical grounds. A majority of authors have reported significant deviations from normal diffusion and fast decay of the SACF. The strength of irregular diffusion can be usually computed by the differences of the values of slope \( \alpha \). The source of these differences is unknown, and even the existence of transport coefficients is being debated. Possible causes of deviation lie in differences in the complex plasma states such as screening strength \( \kappa \) and coupling strength \( \Gamma \).

This work is also motivated by a long-standing controversy over these transport observations in the recent 2D DPLs, with conflicting experimental and simulation conclusions. Our aim is to carry out a systematic study of the effects of coupling and screening strengths of dust particle interaction on superdiffusion and to investigate the existence of related transport coefficients of 2D DPLs by using extensive numerical simulations.

2. Method of numerical simulation

The present 2D Yukawa liquid simulation is based on the equilibrium MD method [32, 33], and it is similar to the 2D monolayer dusty plasma experiments [6, 20, 22] conducted in equilibrium conditions unlike some experiments that are driven by dissipation [19, 23, 30]. This equilibrium MD simulation offers a frictionless atomic system with applied periodic boundary conditions (PBCs) to model an infinite system, which makes it different from dissipative experiments. The Yukawa system is a statistical ensemble of charged particles interacting through the Yukawa pair potential given by

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

where \( Q \) is the charge on a dust particle, \( r \) is the interparticle distance and \( \lambda_D \) is the Debye screening length. In thermodynamic equilibrium, such a Yukawa system can be fully characterized by the two parameters [8, 9]: the Coulomb coupling parameter \( \Gamma = (Q^2/4\pi \varepsilon_0)/(1/ak_B T) \) and screening parameter \( \kappa = a/\lambda_D \). Here, \( T \) is particle kinetic temperature (in energy units), \( a = (n \pi)^{-1/2} \) is the Wigner–Seitz radius [34] and \( n \) is the equilibrium dust number density. Time scales of interest are characterized by an 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.

In the present simulation, particle motion is modeled by Newton’s equations. A fifth-order predictor–corrector algorithm [33] is used to integrate the normalized equations of motion of the N Yukawa dust particles. The particle number in the microcanonical MD simulation is \( N = 1024–18225 \), placed in a computational cell with edge lengths of \( L_x/L_y = 2/\sqrt{3} \). In order to simulate the infinite system, PBCs are imposed on the computational cell of the Yukawa system with a size of \( L/a \). The imposed periodicity needs to be consistent with the fact that the ground state at low temperatures is a triangular lattice [35]. When the number of dust particles satisfies \( N = (\text{integer})^2 \), or is equal to the number of unit cells, then the periodicity satisfies this condition. The Ewald sums method is used to take care of the long-range interaction between the Yukawa dust particles. In the Ewald summation method, the interaction potential is divided into two parts, one converges rapidly in the real-space sum and the other converges rapidly in the reciprocal space sum. For higher screening values of \( \kappa \), the real-space sum part alone exhibits enough performance and precision. Pairwise Yukawa interparticle forces are summed over a \( \kappa \)-dependent cut-off radius [31, 36]. As there is no thermostat used in the simulation and the required system temperature is attained by periodically rescaling the velocities of the particles in the initialization phase of the simulation that precedes the thermodynamical equilibrium of the system. Once the system reaches thermodynamical equilibrium, the periodic rescaling of particle velocities continues and allows the system to
progress under constant energy conditions. The simulation time step, \(0.001 \leq \Delta t \leq 0.003 \omega_p^{-1}\), takes the large cell size of the system into account and allows it to calculate the important data at long times [10, 11]. Thus, the system size and the dust sound speed [34] decide the present maximum independent observation times, \(t_{\text{obs}}\), to be 306 \(\omega_p^{-1}\), 598 \(\omega_p^{-1}\) and 1086 \(\omega_p^{-1}\), for \(\kappa = 1, 2\) and 3, respectively. This observation time \(t_{\text{obs}} \leq L/v_s\), where \(v_s\) is the sound speed of the fastest mode, is limited by the condition that no collective oscillations (sound waves) should be able to traverse the simulation box of length \(L\) during measurement [11]. All runs are evolved for \(15 \times 10^3 \omega_p^{-1}\) time units. To further reduce statistical noise, four independent MD simulation runs are carried out with arbitrarily chosen configurations of the particle positions for each target temperature \(T\), and then averaging these measurements to improve the statistics. In this paper, it is reported that the diffusive motion of 2D Yukawa system is in the domain of plasma parameters, \(1 \leq \Gamma \leq 300\) and \(1 \leq \kappa \leq 3\), and for shear viscosity it is, \(40 \leq \Gamma \leq 300\) and \(\kappa = 2\).

2.1. Diagnostic methods

Two familiar diagnostic methods, mean-squared displacement (MSD) and VACF, are used to characterize dust particle motion. First, the most important quantity is the MSD of particles

\[
\text{MSD}(t) = \langle [\mathbf{r}_j(t) - \mathbf{r}_j(t_0)]^2 \rangle, \tag{2}
\]

where \(\mathbf{r}_j(t) - \mathbf{r}_j(t_0)\) is a time series of the squared displacement, \(\mathbf{r}_j(t)\) represents the position of the \(j\)th particle, and \(\langle \cdot \cdot \cdot \rangle\) denotes an ensemble average over all particles. Anomalous diffusive motion is randomly characterized by a deviation from \(\alpha = 1\) as

\[
\text{MSD}(t) = D(\Delta t)^\alpha, \tag{3}
\]

where normal diffusion is identified when the diffusion exponent approaches unity (\(\alpha = 1\)), when \(t \to \infty\). The suitable diffusion coefficient \(D\) is determined by the MSD through the Einstein relation, \(D = \lim_{t \to \infty} \text{MSD}(t)/4t\). In contrast, superdiffusion and subdiffusion have larger and smaller diffusion exponents than unity, respectively. The second analysis is based on the VACF and SACF for diffusive motion and shear viscosity, respectively. For the equilibrium Yukawa systems, the transport coefficients are calculated using the Green–Kubo formulae. For designing the two tests of the VACF and the SACF, the transport coefficients are given as follows [11].

For diffusive motion and coefficient \(D\)

\[
D = \frac{1}{2} \int_0^\infty Z_D(t) \, dt, \quad Z_D(t) = \langle v_j(t) \cdot v_j(t_0) \rangle. \tag{4}
\]

The integrand \(Z_D(t)\) is the VACF and it is an ensemble average of the product of particle velocities at time \(t\) and an initial time \(t_0\). For diffusive motion, the \(|Z_D(t)|\) decays faster than \(t^{-1}\), when \(t \to \infty\), and a meaningful diffusion coefficient \(D\) can be obtained with equation (4). In contrast, if the \(|Z_D(t)|\) decays slower than \(t^{-1}\) and the integral diverges, when \(t \to \infty\), it is an indication of superdiffusion behavior, and the motion is subdiffusive, \(|Z_D(t)|\) oscillates and the integral has zero value, when \(t \to \infty\) [10].

3. Results and discussion

In order to classify the motion as diffusive or nondiffusive, a first series of simulations is carried out for the long time behavior of the MSD. For a better understanding of diffusive motion, an indicator of MSD(t)/t is used in this paper. The MSD(t)/t data are plotted in figures 1–3 for \(\kappa = 1, 2\) and 3, respectively, covering from nonideal state (\(\Gamma = 1\)) to a strongly coupled liquid. Figures 1–3 (log–log scale) illustrate asymptotic behaviors at short \(\omega_p t \leq 2\) and long \(\omega_p t > 2\) time windows. A ballistic motion displays constant value of motion is subdiffusive, 

\[
\langle \mathbf{r}_j(t) - \mathbf{r}_j(t_0) \rangle = \langle \mathbf{r}_j(t_0) \rangle - \langle \mathbf{r}_j(t) \rangle, \quad \text{for } t \to \infty.
\]

\[
\text{MSD}(t)/t = D/\kappa - \omega_p^2 t^2, \quad \text{for } t \to \infty.
\]

\[
\text{MSD}(t)/t = D/\kappa - \omega_p^2 t^2, \quad \text{for } t \to \infty.
\]

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\text{MSD}(t)/t = D/\kappa - \omega_p^2 t^2, \quad \text{for } t \to \infty.
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\[
\text{MSD}(t)/t = D/\kappa - \omega_p^2 t^2, \quad \text{for } t \to \infty.
\]
show that the dotted lines that the maximum value of slope is that the overall diffusion results for five or six different starting and ending times to choose suitable MSD time series data and generate our final intervals used in selecting the MSD simulation data to fit. We than unity because the system is under binary interactions, calculated values. It is observed that for nonideal gaseous states (lower coupling), the slope is only slightly larger than unity because the system is under binary interactions, and the motion is diffusive for lower coupling at long time values. But when the coupling strength increases towards intermediate coupling, the superdiffusion is most extreme because the collective property dominates in the system. It is found from figure 1 that a maximum value of slope is $\alpha \approx 0.13$ at $\Gamma = 40$ for $\kappa = 1$ and then the slope becomes nearly constant with an increase in $\Gamma$. The superdiffusion exists for an intermediate Coulomb coupling strength, confirming the earlier simulations [10, 24, 28], but contrary to the simulation results of Donko et al [11], where the superdiffusion was found at higher $\Gamma \geq 100$. The present simulation data show that there is a peak value of $\alpha$ at $\Gamma = 40$, which is higher than that reported in the previous MD simulations [10], in which the peak occurs at $\Gamma = 18$ with a value of $\alpha \approx 0.3$. It can be observed that $\alpha$ of the present calculation ($\approx 0.13$) is slightly lower than and the Coulomb coupling value ($\Gamma = 40$) lies closer to those reported in the previous MD work ($\alpha \approx 0.18$ at $\Gamma = 44$) of Liu et al [24] and the LD results ($\alpha \approx 0.20$ at $\Gamma \approx 34$) of Ott and Bonitz [28]. The present intermediate $\Gamma$ value is nearly at twice the value as reported in [10], which indicates the maximum value of superdiffusion where the earlier viscosity [29, 31] has minimum value. Clearly, this tendency predicts the existence of minimum possible value of shear viscosity at intermediate $\Gamma$, which will be illustrated in figure 5. It is noted from Figures 2 and 3 that the maximum values of slope are $\alpha \approx 0.15$ ($\Gamma = 60$), and $\alpha \approx 0.19$ ($\Gamma = 80$) for $\kappa = 2$ and $\kappa = 3$, respectively.

It is examined from figures 1–3 that the overall diffusion trends are found and depend on $\kappa$ in the 2D DPLs for lower $\Gamma$, and these trends agree well with the earlier results reported in the MD [11] and the LD [28] simulations, but the results for $\Gamma < 20$ in the MD simulation were not reported. The superdiffusion is dependent on the Coulomb coupling strengths in the 2D DPLs, confirming the earlier simulations [28], and it is also systematically dependent on $\kappa$ for all $\Gamma$. Moreover, the present data indicate that the extreme value of the superdiffusion increases with an increase in $\kappa$, and then nearly a constant superdiffusion motion occurs with an increase in $\Gamma$. These observations show that superdiffusion exists at intermediate and higher $\Gamma$. This important behavior agrees well with the earlier results reported for the DPLs at higher $\Gamma$ [11]. The overall shapes of all the curves in Figures 1–3 are same for $\kappa = 1$, 2 and 3 but the main advancement is that the state for extreme superdiffusion shifts towards higher $\Gamma$ with an increase in $\kappa$. Overall anomalous diffusive motion is dependent on both the $\Gamma$ and range $\kappa$ of pair interaction.

The results of the VACFs $(t)$ for six Coulomb coupling strengths are shown in figure 4. It is very important to consider a large $\kappa = 2$ value because the sound speed diminishes rapidly with $\kappa$ [11]. The absolute values of the VACFs are used because the systems may be under caged motion of particles even at early times. In the most common test of diffusion (or superdiffusion), here we find that the long time tail in the VACF decays faster than $1/t$ (or slow decay of $1/t$). The data fitting procedure for our VACFs time series simulation data is the same as described in [11] for the correlation functions. Fit the VACFs data for an appropriate time interval to a power-law decay, $\log[Z(t)] = \alpha \log(t) + \text{intercept}$. This data fitting form has been used to represent the long time tail in the VACF.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{MSD$(t)/t$ of the Yukawa liquids for different $\Gamma$ at $\kappa = 2$. For details, see the caption of figure 1.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{MSD$(t)/t$ of the Yukawa liquids for different $\Gamma$ at $\kappa = 3$. For details, see the caption of figure 1.}
\end{figure}
decays of 2D Yukawa DPLs [10, 11, 24]. The data fitting form is directly fitted to the simulation measurements with five or six different starting and ending time intervals, for each value of Γ. Figure 4 shows that different decays with the long time tails in the VACFs indicate the anomalous diffusive motions. A fast decay of \( t^{-1.46} \) and a slow decay of \( t^{-1} \) appear at \( \Gamma = 1 \) and \( \Gamma = 60 \), respectively, and these fast to slow decays indicate a smooth transition from normal diffusion to superdiffusion. The first three and last three curves follow roughly about \( t^{-1.46} \) and \( 1/t \), respectively. These trends are contrary to those in [11] where the superdiffusion at the intermediate Coulomb coupling was not noticed, however, the trends are same as observed in the previous MD simulations of Liu and Goree [10]. The analysis of the VACFs test indicates that superdiffusion exists at intermediate coupling in the 2D DPLs. It can predict that the minimum possible viscosity may have a unique value at intermediate coupling and its existence is presented in the SACFs test.

Figure 5 shows the long time behavior of the SACFs in the same conditions as in the figure for VACFs, and the simulation data are for a large system size. The results for the second series of the MD simulations of a 2D Yukawa liquid are observations of the shear viscosity together with the indication of the superdiffusive motion. It can be noted from the SACFs that the long time behavior will determine whether the transport coefficient is unique or not. It can be seen from figure 5 that the SACFs are for the three values of coupling \( \Gamma = 40, \Gamma = 60 \) and \( \Gamma = 300 \), and here the second value is regarded as the maximum value of superdiffusion and the third one is the value at higher \( \Gamma \). Various starting and ending times in the simulation data analysis of the SACFs, normalized by \( \omega_0 \), are tested for each value of \( \Gamma \) with the same procedure as for the VACFs. The thick line is a power-law fit to \( \Gamma = 40 \) and indicates a slow decay, \( t^{-0.56} \), which shows that shear viscosity does not exist for 2D YDPLs at \( \Gamma < 60 \), and the rapid decays appear for the other two \( \Gamma \) values. The start time = \( 10000t \) and end time = \( 55000t \) for the fit to the curve \( \Gamma = 40 \). The curves for \( \Gamma = 60 \) and \( \Gamma = 300 \) follow roughly the decays of \( t^{-1.2} \) and \( t^{-1.3} \), respectively, and these behaviors show the rapid decays faster than a power law. This tendency is significant because it predicts the minimum possible value of \( \eta_0 \) at \( \Gamma = 60 \) where the superdiffusion reported in the earlier literature had a maximum value [10, 24, 28]. However, this behavior is unlike the earlier results of Donkó et al [11], and the possible reason for the difference is that they did not observe the superdiffusion at intermediate \( \Gamma \) in their simulations. The minimum possible value of \( \eta_0 \) exists at twice the value of \( \Gamma \) as compared with the previous simulations [29, 31]. From figure 5, it can also be observed that shear viscosity definitely exists at higher Coulomb coupling (\( \Gamma = 300 \)), confirming the earlier results [11]. This long time analysis helps to calculate finite viscosity coefficients using the Green–Kubo relations in 2D YDPLs.

4. Summary

The equilibrium MD simulation method is applied to determine shear viscosity and to understand the anomalous diffusive motion for 2D YDPLs over a wide range of plasma parameters of \( \Gamma \) and \( \kappa \). The first contribution of the present simulation is that it provides an understanding of the diffusion motion in Yukawa liquids. The overall diffusion motion is analyzed at the long time limit in 2D DPLs for lower \( \Gamma \). The extreme superdiffusion of charged dust particles is observed for intermediate \( \Gamma \) and it depends on \( \kappa \). The present simulations indicate that superdiffusion occurs only at intermediate and higher \( \Gamma \). For \( \kappa = 2 \), the long time decays of the VACFs indicate a smooth transition from normal diffusion to superdiffusion, showing that superdiffusion exists at intermediate coupling strengths. These examinations show that superdiffusion depends on \( \Gamma \) and a finite value of shear viscosity occurs after the transition phase from normal diffusion to superdiffusion (at intermediate and higher \( \Gamma \)), and it does not exist before this transition phase (at lower \( \Gamma \)).

The present simulations provide more reliable data for the existence of the valid Yukawa shear viscosity than the earlier
results. These calculations confirm that the minimum possible value of shear viscosity exists, signifying the most extreme superdiffusion. It seems that the prediction of minimum value of shear viscosity can help in understanding the fundamental superdiffusion behavior in 2D Yukawa dusty plasma systems. The long time of stress SACFs verify the validity of the shear viscosity results. For $\kappa = 2$, the decays of the SACF curves at the intermediate ($\Gamma = 60$, where maximum superdiffusion exists) and higher ($\Gamma = 300$) coupling follow roughly the fast decays, indicating the finite shear viscosity coefficients. However, at coupling $\Gamma < 60$, a slow decay of the SACF indicates that the valid shear viscosity coefficient does not exist. The present simulation analysis shows that viscosity cannot couple with diffusion and it depends on $\kappa$ and $\Gamma$. All these observations suggest that anomalous diffusive motion in the 2D dusty plasma is dependent both on Coulomb coupling and on screening strengths.

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