Dynamical Properties of Two-Dimensional Yukawa Liquids: A Molecular Dynamics Study

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The dynamical structure factor and the spectrum of the momentum-density fluctuations of 2D Yukawa liquids are analyzed in the domain of weak and intermediate coupling and screening parameters. The dispersion relations of the longitudinal and transverse collective excitations are obtained and compared with the random phase approximation (RPA) and harmonic approximation for triangular lattice.

1. INTRODUCTION

Yukawa system is a statistical ensemble of charged particles interacting through Yukawa potential given by

$$ U(r) = \frac{Q^2}{r} \exp(-r/\lambda), \quad (1) $$

which may serve as a model for dust grains immersed in plasma (dusty plasma)[1] or colloidal particles in electrolytes[2]. Here, $Q$ is the charge on the dust grain, $r$ is the separation between two dust grains, and $\lambda$ is the screening length due to Debye shielding by the background medium.

In dusty plasma experiments, we often observe two-dimensional Yukawa systems as well as three-dimensional ones. A typical example of two-dimensional Yukawa system is the single layer of micrometer-sized dust grains suspended in the sheath of a low-pressure rf-discharge. These two-dimensional systems provide us with clear examples of the lattice of charged particles which can be observed by CCD cameras or naked eyes and also serve as a probe to estimate physical parameters of grains and environmental plasmas[3, 4].

The dynamical properties of Yukawa system in the domain of strong coupling, including the longitudinal and transverse modes, have been studied theoretically[5-7], experimentally[8, 9], and by numerical simulations[10, 11]. Since the properties of two-dimensional (2D) systems may be different from those of three-dimensional (3D) because of reduced dimensionality, it is interesting to explore the properties of 2D Yukawa systems whose 3D counterparts have recently been given considerable attention. The information on dynamical properties will also greatly help us to determine physical parameters related to dust particles and environmental plasma in experiments.

When in thermodynamic equilibrium at the temperature $T$, Yukawa system is characterized by two dimensionless parameters: The coupling parameter

$$ \Gamma = \frac{Q^2}{ak_B T} \quad (2) $$

and the screening strength

$$ \xi = a/\lambda. \quad (3) $$
Here $a$ is the mean distance between particles defined by $a = (\pi n)^{-1/2}$, $n$ being the areal density. Sometimes the effective coupling parameter $\Gamma^* = \Gamma \exp(-\zeta)$ is used but the properties of our system cannot be scaled by this combination only.

In this paper, we report the dynamical properties of two-dimensional Yukawa system in the domain of Yukawa plasma parameters $5 \leq \Gamma \leq 100$ and $1 \leq \xi \leq 2$. The spectra of the density and current fluctuations are computed, and the dispersion relations of the longitudinal and transverse collective excitations are obtained and compared with the random phase approximation (RPA) and harmonic phonons in a triangular (hexagonal) lattice.

2. NUMERICAL METHOD

We use microcanonical molecular dynamics (MD) method for $N = 900$ Yukawa particles with mass $m$ interacting through Yukawa potential (1) to study the dynamical properties of 2D Yukawa system. In order to simulate the infinite system, we impose the periodic boundary conditions in $x$- and $y$-directions with periods $L_x$ and $L_y$, respectively, the aspect ratio being $L_x/L_y = 2/\sqrt{3}$. The imposed periodicity needs to be consistent with the fact that the ground state at low temperatures is the triangular lattice. When the number of particles satisfies $N = (\text{integer})^2$, or is equal to the number of unit cells, our periodicity satisfies this condition. We use the Ewald method to take care of the long range interaction between particles.

The normalized equation of motion is integrated using velocity Verlet algorithm. We adopted a time step around $0.005\omega_p^{-1}$ which guarantees 7 digits accuracy in the energy conservation after several tens of thousands steps. Here

$$\omega_p = (2\pi n Q^2/ma)^{1/2}$$

is the typical frequency of 2D plasma oscillation[12].

To attain a given value of the temperature or $\Gamma$, we renormalize the particle velocities periodically, monitoring the kinetic energy. Once the kinetic energy take on the expected value, the microcanonical evolution of the system is followed. The average is taken over a sufficiently long time after the system has reached thermodynamical equilibrium. The actual values of $\Gamma$ are determined by the average kinetic energy over microcanonical periods at thermal equilibrium.

3. DYNAMICAL FLUCTUATION SPECTRA

3.1 Dynamic Structure Factor

Longitudinal properties of many-body system are clearly seen from the dynamic structure factor which is defined as

$$S(k, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt A(k, t)e^{i\omega t},$$

where

$$A(k, t) = \frac{1}{N} \langle \rho_k(t) \rho_{-k}(0) \rangle$$

is the density-density correlation function and $\rho_k(t)$ is the density fluctuation

$$\rho_k(t) = \sum_{i=1}^{N} \exp[-ik \cdot r_i(t)].$$

When the system is in the liquid state, the dynamic form factor depends only on the magnitude of the wave number,

$$S(k, \omega) = S(k, |\omega|).$$

Since our data are given in a finite time interval $\tau$ in this work, we compute $\langle \rho_k(t) \rho_{-k}(0) \rangle$ as the time average over $\tau$, expanding $\rho_k(t)$ into a Fourier series as[12]

$$\langle \rho_k(t) \rho_{-k}(0) \rangle = \frac{1}{\tau} \int_{0}^{\tau} dt' \rho_k(t + t') \rho_{-k}(t')$$

$$= \frac{1}{\tau^2} \sum_{\omega_n} |\rho_k(\omega_n)|^2 \exp(-i\omega_n t),$$

where $\omega_n = (2\pi/\tau)n$, $n = 0, \pm 1, \pm 2, \pm 3, ..., n$ and obtain

$$S(k, \omega) = (2\pi\tau)^{-1} |\rho_k(\omega_n)|^2.$$ 

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Here we note the relation \( \sum \omega_n \sim (\tau/2\pi) \int d\omega \) for \( \tau \to \infty \). We also note that, due to periodicity of our system, the values of wave number in our analyses are restricted to the ones given by

\[
\mathbf{k} = \frac{2\pi}{L} \left( n_x, \frac{2n_y}{\sqrt{3}} \right),
\]

where \( n_x \) and \( n_y \) are integers.

The dynamic structure factor, \( \omega_p S(k, \omega) \), obtained for several wave numbers are shown in Fig.1 for \( \xi = 1 \) and \( \Gamma = 50 \). For small wave numbers, the dynamic structure factor is dominated by the contribution of the collective mode. The collective peak broadens with increase in wave number and finally merges into the continuous spectrum of excitations which is monotone.

### 3.2 Dispersion relation of longitudinal collective mode

Before presenting the results obtained from the structure factor, we may make simple expectations for the dispersion based on the random phase approximation (RPA) and lattice dynamics. These two would give limiting cases of weak and strong coupling.

In the random phase approximation which is expected to work in the domain of weak coupling, the dielectric response function is given by

\[
\varepsilon(k, \omega) = 1 + \frac{K_D}{(k^2 + 1/\lambda^2)^{1/2}} W \left\{ \omega \left( \frac{m}{k_B T} \right)^{1/2} \right\}.
\]

Here we note that the Fourier transform of the Yukawa potential is given by \( 2\pi Q^2/(k^2 + 1/\lambda^2)^{1/2} \) and define \( K_D \) and \( W(z) \) by

\[
K_D = \frac{2\pi n Q^2}{k_B T},
\]

and

\[
W(z) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dx \frac{x \exp(-x^2/2)}{x - z - i0},
\]

respectively. From the asymptotic expansion of \( W(z) \) for \( |z| \to \infty \), we have the collective mode given as the solution for \( \varepsilon(k, \omega) = 0 \) as

\[
\omega(k) \sim \omega_p \frac{k \sqrt{a}}{(k^2 + 1/\lambda^2)^{1/4}} \left[ 1 + \frac{3}{2} \left( \frac{k^2 + 1/\lambda^2}{K_D} \right)^{1/2} \right],
\]

for \( k \ll K_D \). We may expect that the RPA dispersion will be applicable when the coupling is weak.

When particles form the triangular lattice, the phonon dispersions within harmonic approximation are obtained as the eigenmodes of the dynamical matrix. We expect that the dispersion obtained by our simulations may approach to these phonons when the coupling is strong enough. The RPA and lattice results are compared in Fig. 2.

The dispersion relation obtained from the peaks in the dynamic structure factor for given values of \( k \) are depicted in Fig.3 for \( \xi = 1 \) and \( \Gamma = 100.09 \). The positions of the peaks representing the collective excitations are plotted.

These dispersions are to be compared with the results of RPA and the harmonic lattice. When the coupling is not so strong, our results have the tendency to follow the RPA values and approach those of phonons when the coupling is strong so that \( \Gamma \geq 20 \) for \( \xi \leq 2 \).
In conclusion, the spectra of the fluctuations in the density and the momentum current are

\[ C_t(k, \omega) = \frac{1}{2\pi \tau} \left\langle \left| \frac{k}{k} \times \mathbf{g}_k(\omega) \right|^2 \right\rangle, \quad (20) \]

and

\[ g_k(\omega) = \int_0^\tau dt g_k(t) \exp(i\omega t), \quad (21) \]

for \( \omega = \omega_n \). The spectrum of longitudinal current fluctuation \( C_l(k, \omega) \) is connected to the dynamic structure factor \( S(k, \omega) \) through

\[ C_l(k, \omega) = (\omega/k)^2 S(k, \omega). \quad (22) \]

We have obtained the longitudinal and transverse current fluctuation spectra from our molecular dynamics simulations. We have confirmed that the relation between the longitudinal component and the dynamic form factor (22) is satisfied with sufficient accuracy. Examples of transverse spectra are shown in Fig. 4 for \( \xi = 1 \), for some values of wave numbers. We observe that the transverse collective mode is well defined only in the case of strong coupling such that \( \Gamma \geq 100 \) for only small domain of the wave number \( 1 \leq k \alpha \leq 2 \) for \( \xi = 1 \).

The position of the peak of the transverse spectrum, representing transverse mode dispersion, is plotted in Fig. 5 as an example. The result is compared with that of the transverse branch of harmonic phonons in hexagonal lattice at \( T = 0 \). For a fixed wave number, the minimum and maximum of the frequency are attained for the propagations in the directions \([10] \) and \([1\frac{1}{2}] \), respectively. We observe that the transverse collective mode is well-defined in a wider domain of wave number for \( \xi = 1 \) than for \( \xi = 2 \).

4. CONCLUSION

In conclusion, the spectra of the fluctuations in the density and the momentum current are
FIG. 4: Some examples of transverse spectrum for $\xi=1.0$ and $\Gamma = 100.09$.

FIG. 5: Dispersion relation of transverse mode for $\xi=1.0$ and $\Gamma = 100.09$. Solid line is the transverse branch of harmonic phonons in hexagonal lattice.