Journal of Physics: Conference Series

PAPER • OPEN ACCESS

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To cite this article: L A Mistryukova *et al* 2019 *J. Phys.: Conf. Ser.* **1348** 012097

Journal of Physics: Conference Series **1348** (2019) 012097 doi:10.1088/1742-6596/1348/1/012097

Collective excitations in two-dimensional fluid with dipole-like repulsive interactions

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Abstract. Collective excitations in a two-dimensional fluid with repulsive dipole-like interactions are systematically studied by molecular dynamics simulations. A two-oscillator model is used to reconstruct dispersion curves and to measure q-gap boundary values in the dispersion relation of the transverse (shear) mode. Functional form for the dependence of the q-gap boundary value on the coupling parameter is suggested. The results obtained can be used in future investigations of collective excitations in fluids, especially in two-dimensional cases.

1. Introduction

Two- and quasi-two-dimensional (2D) systems are widespread in nature. Atomic, molecular or colloidal monolayers on interface surfaces, vortices in thin-film semiconductors, two-dimensional electron gas on the surface of liquid helium are typical examples of such systems. Another well-known quasi-two-dimensional system is a complex (dusty) plasma [1, 2] in ground-based conditions. Various 2D systems play an important role in a wide range of phenomena occurring on various interfaces. For example, colloidal systems at interfaces can play a crucial role in many important technical and biological processes like system stabilization [3–5], synthesis [6, 7] or catalysis [8]. Moreover, some microswimmers [9] or even more complex multiagent systems [10–12] can be treated as two-dimensional systems of interacting particles. In many cases, such systems form a fluid-like phase.

Establishing interrelations between the pair interaction and various properties (dynamic, structure and thermodynamic) is one of the key tasks of modern condensed matter physics. In the case of crystals, this problem is almost solved by lattice dynamics theory [13] and some other approaches [14, 15] where collective excitations (phonons) play a central role. For fluids it is not so, and the role of collective excitations is still poorly understood. Unlike crystals, not all transverse (shear) excitations are present in fluids [16–19]. The domain of wave-vectors corresponding to the absence of transverse excitations is located in the long-wavelength regime and is often called the "q-gap". Understanding the q-gap behaviour across coupling regimes is important for a detailed understanding of fluid properties and to the elaboration of corresponding theories. However, as far as we know the q-gap behaviour in various fluids is poorly studied especially in cases of two-dimensional systems.

In the present paper, we systematically study the q-gap behavior in a two-dimensional fluid consisting of particles interacting with a repulsive dipole-like potential $\propto 1/r^3$ by molecular dynamics (MD) simulations. This type of interactions is also known as inverse-power-law potential (IPLk where k denotes the exponent) and is relatively well studied theoretically [18, 20, 21]. Moreover, repulsive IPL3 interaction is intrinsic to various real two-dimensional systems, where it appears due to different effects: the occurrence of parallel dipole moments in systems at interfaces [22–25] induced by external electric/magnetic fields [26–30] or by nonequilibrium environment flows [31, 32]. In particular, it should be mentioned that colloidal systems on interfaces (with the IPL3 interaction) allowed to experimentally investigate [24, 27, 33] the famous Berezinsky-Kosterlitz-Thouless-HalperinNelson-Young (BKTHNY) scenario of two-dimensional melting [34, 35]. The results obtained in the present work can be useful in future studies of collective excitations in 2D fluids.

2. Methods

We performed MD simulations of the classical 2D system interacting with IPL3 potential:

$$\phi(r) = \epsilon(\sigma/r)^3, \tag{1}$$

where ϵ and σ are the energy and length scales of the interaction. We considered two dimensional systems consisting of $N = 10^4$ particles of masses m in the NVT ensemble with Nose-Hoover thermostat. The cut-off radius for interactions was chosen as $r_c = 25\rho^{-1/2}$ where $\rho = N/V$ is the areal density. Numerical timestep was chosen as $\Delta t = 2.4 \times 10^{-4}\sqrt{ma^2\Gamma/\epsilon}$ where $a = (\pi\rho)^{-1/2}$ is 2D Wigner-Seitz radius and $\Gamma = \epsilon(\sigma/a)^3/T$ is dimensionless interaction (coupling) parameter. All the calculations were performed using the LAMMPS package [36].

In accordance with the standard approach [18, 37, 38] the longitudinal and transverse current correlation spectra can be calculated in the following way:

$$C_{\mathrm{L,T}}(\mathbf{q},\omega) \propto \mathrm{Re}\int dt\ \langle j_{\mathrm{L,T}}(\mathbf{q},t) j_{\mathrm{L,T}}(-\mathbf{q},0)\rangle\, e^{i\omega t}, \tag{2}$$

where $j_{\mathrm{L}}(\mathbf{q},\omega)$ and $j_{\mathrm{T}}(\mathbf{q},\omega)$ are the longitudinal and transverse components of velocity current $\mathbf{j}(\mathbf{q},t) \propto \sum_i \mathbf{v}_i(t)\exp[i\mathbf{q}\mathbf{r}_i(t)]$, $\mathbf{v}_i(t)$ is the velocity of i-th particle with the radius-vector $\mathbf{r}_i(t)$ and summation is performed over all particles in the system. Due to isotropy of fluids we can average $C_{\mathrm{L,T}}(\mathbf{q},\omega)$ over all directions of the wave vector $\mathbf{q}$ in order to get the dependence on $q = |\mathbf{q}|$.

We used the two-oscillator model [39, 40] to extract dispersion curves from calculated intensity distributions $C_{\mathrm{L,T}}(\mathbf{q},\omega)$. In accordance with this approach the full amplitude $C_q(q,\omega) = C_{\mathrm{L}}(q,\omega) + C_{\mathrm{T}}(q,\omega)$ should be approximated by the function:

$$f(q,\omega) = A\left[f_{\mathrm{L}}(q,\omega) + f_{\mathrm{T}}(q,\omega)\right], \tag{3}$$

where A is a normalization constant, $f_{\mathrm{L}}(q,\omega)$ and $f_{\mathrm{T}}(q,\omega)$ correspond to the contributions of the (longitudinal) high- and (transverse) low- frequency modes respectively, each having a double-Lorentzian shape:

$$f_{\mathrm{L,T}}(\omega) = \gamma_{\mathrm{L,T}}\left[\frac{1}{(\omega-\omega_{\mathrm{L,T}})^2+\gamma_{\mathrm{L,T}}^2} + \frac{1}{(\omega+\omega_{\mathrm{L,T}})^2+\gamma_{\mathrm{L,T}}^2}\right]. \tag{4}$$

Optimization for each value of q allows to obtain dispersion relations $\omega_{\mathrm{L}}(q)$ and $\omega_{\mathrm{T}}(q)$ of high- and low- frequencies modes respectively with the corresponding $\gamma_{\mathrm{L,T}}(q)$ values and the normalization constant $A(q)$.

3. Results

An example of the collective excitation spectra in a 2D IPL3 fluid with $\Gamma = 31.8$ is shown in Figure 1(a). Excitation spectra amplitudes $C_q(\omega)$ are shown in color-coded format. The blue and red circles correspond to high- and low-frequency modes, respectively, obtained based on the two-oscillator model. The black circles denote maxima positions of $f_{\mathrm{T}}(\omega)$. In the long-wavelength regime some deviations between the two approaches were noted. In both sets of red and black points, there is a long-wavelength domain in which the frequency is zero (corresponding to the q-gap). Due to non-zero γ_{T} values, the black points are systematically lower than the red ones, which also follows from Eq. (4). Moreover, if $\gamma_{\mathrm{T}}/\omega_{\mathrm{T}} \gtrsim \sqrt{3}$, then the maximum of $f_{\mathrm{T}}(q,\omega)$ is located at $\omega = 0$, even though ω_{T} itself is non-zero. Therefore, the q-gap boundary value q_g measured using the two-oscillator model (red points) is lower than q_* value measured from the maxima of $f_{\mathrm{T}}(\omega)$. The difference between q_g and q_* values has been already briefly discussed in the context of three-dimensional Yukawa and Coulomb systems [41]. The numerically obtained amplitudes $C_q(\omega)$ along with the corresponding fits by the two-oscillator model for the two given values of the wave vector q are shown in Figures 1(b) and 1(c). Good agreement both at moderate and short wavelengths is observed.

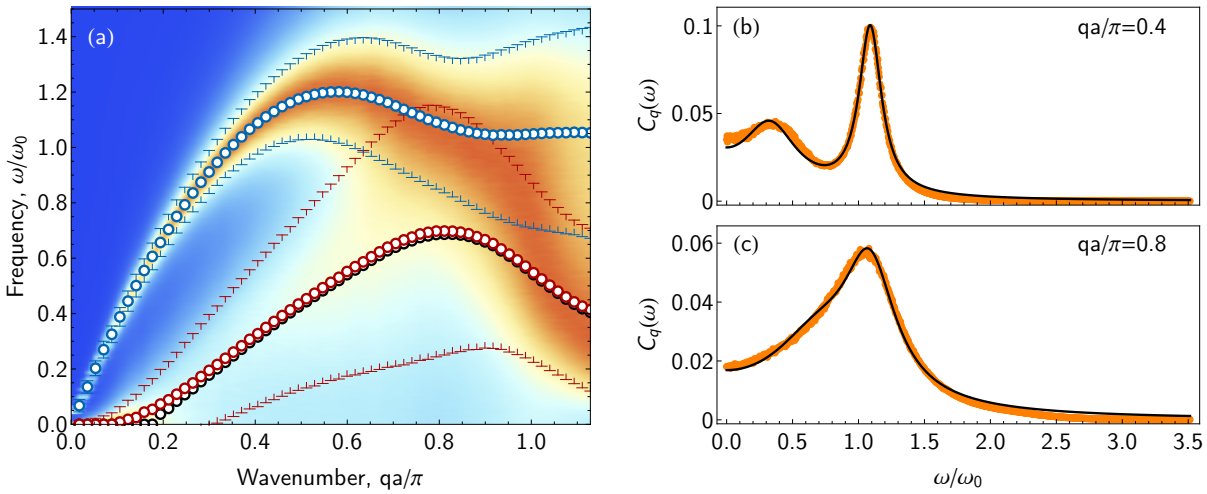

Figure 1. The collective excitation spectra in the 2D IPL3 system at $\Gamma = 31.8$. The normalized amplitudes $C_q(\omega)$ at each given q in color-coded format, dispersion curves $\omega_{\mathrm{T}}(q)$ (red circles) and $\omega_{\mathrm{L}}(q)$ (blue circles) obtained based on the two-oscillator model, the values $\omega_{\mathrm{L,T}} \pm \gamma_{\mathrm{L,T}}$ which are marked by symbols $\top$/ $\perp$ of the corresponding color are shown in Panel (a). Black circles correspond to maxima of $f_{\mathrm{T}}(q,\omega)$. Frequencies are expressed in units of 2D plasma frequency $\omega_0 = \sqrt{2\pi\rho\epsilon\sigma^3/ma^3}$. The numerically obtained amplitudes $C_q(\omega)$ (orange points) and the corresponding fits using Eq. (3) (black curves) for wave numbers qa/π equal to 0.4 and 0.8, respectively are shown in Panels (b) and (c).

The values of the q-gap boundary, q_*, can be easily detected from the maxima of $f_{\mathrm{T}}(\omega)$ since the maxima locations ω_{m} exhibit an explicit jump from zero to finite values at q_*. Analysis using the two-oscillator model can lead to the presence of some (small) noise at low ω_{T} values and therefore the accurate determination of q_g is somewhat more complicated. The dependence of ω_{T} on q obtained by the two-oscillator model for $\Gamma = 42.7$ is shown on Fig. 2(a). In this strongly coupled regime, $\omega_{\mathrm{T}}(q)$ behaves as a linear function in the vicinity of the q_g value. The latter can be measured by fitting $\omega_{\mathrm{T}}(q)$ data with the help of the function

$$\omega_{\mathrm{T}}(q) \approx c_{\mathrm{T}}(q - q_g)\theta(q - q_g), \tag{5}$$

where c_{T} and q_g are fitting parameters and $\theta(q)$ is the Heaviside function. However, in the 2D IPL3 system far from the fluid-solid phase transition (lower Γ), the dependence $\omega_{\mathrm{T}}(q)$ becomes

non-linear in the vicinity of q_g as demonstrated in Fig. 2(b). The question about the exact origin of this $\omega_{\rm T}(q)$ behaviour (obtained based on the two-oscillator model) is beyond the scope of the present paper and should be considered separately. We just note that the dependence $\omega_{\rm T}(q)$ can be reasonably well described by the function of the form

$$\omega_{\rm T}(q) \approx \left[c_{\rm T}(q-q_g) + c_2(q-q_g)^2\right]\theta(q-q_g), \tag{6}$$

where $c_{\rm T}$, c_2 and q_g are fitting parameters. Example of such a fit is shown in Fig. 2(b). It should be noted that such a strong deviation from the linear behavior of $\omega_{\rm T}(q)$ near q_g is not observed in 3D system even for the case of one-component plasma (corresponding to the very soft and long-ranged interaction limit) [41]. The results of q_* and q_g measurements are presented in Figure 2(c). Black points correspond to q_* values obtained using the maxima $\omega_{\rm m}(q)$. Orange and red symbols correspond to q_g values obtained from the fits of MD data for $\omega_{\rm T}(q)$ using Eqs. (5) and (6), respectively. Black and orange points on Fig.2(c) can be well approximated by the functional form

$$q_g(\Gamma) \approx A + B\Gamma + C\exp(-D\Gamma), \tag{7}$$

where A, B, C and D are constants. At the same time, the behavior of red points is more simple and can be approximated by a linear function. Note that the obtained dependencies can also be fitted by $q_g \propto \Gamma^{-n}$ (where n is a constant) in a moderate range of Γ values, which has been observed in a 2D one-component plasma previously [42].

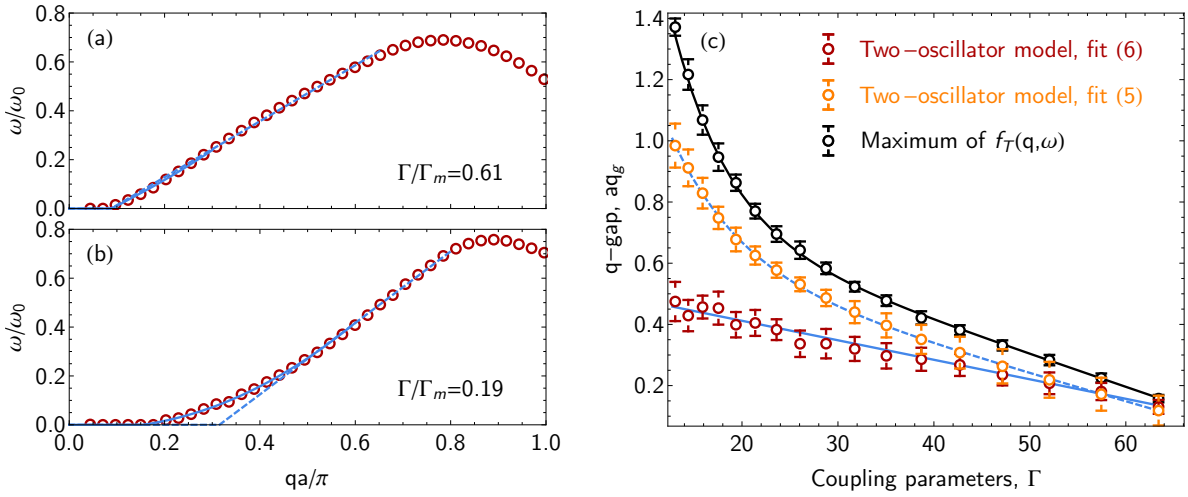

Figure 2. The q-gap behaviour in the 2D IPL3 system. The panels (a) and (b) show the dependence $\omega_{\rm T}(q)$ for $\Gamma = 42.7$ and $\Gamma = 13$, respectively. Red symbols correspond to results obtained by the two-oscillator model, dashed and solid blue curves are fits by Eq. (5) and Eq. (6), respectively. The summarized results of the q-gap boundary measurements are shown in Panel (c). Black symbols correspond to q_* values obtained from the maxima $\omega_{\rm m}(q)$. Orange and red symbols are q_g values obtained using $\omega_{\rm T}$ data fitted by Eq. (5) and Eq. (6), respectively. Black solid ($q_*a \approx 0.84 + 5.83\exp*(-0.17\Gamma) - 10.7\times10^{-3}\Gamma$) and blue dashed ($q_g a \approx 0.69 + 2.52\exp(-0.14\Gamma) - 9.1\times10^{-1}\Gamma$) curves are fits by Eq. (7) and the blue solid curve corresponds to a linear fit ($q_g a \approx 0.54 - 6.4\times10^{-3}\Gamma$).

4. Conclusion

In this paper, the behaviour of the q-gap in the two-dimensional system with repulsive dipole-like interactions was systematically studied . The value of q-gap boundary has been obtained from the maxima positions of the transverse correlation spectra as well as from the two-oscillator

model. It is demonstrated that when moving away from the melting point, the dependence of $\omega_T(q)$ becomes strongly non-linear in the vicinity of the transverse wave onset (q-gap boundary). We have suggested a functional form, which fits well the dependence of the q-gap boundary on the coupling parameter in a wide range of coupling strength. The obtained results can be used in future studies of collective excitations in fluids, especially in cases of two-dimensional systems.

Acknowledgements
The study was supported by Russian Science Foundation (RSF) Grant No. 17-19-01691.

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