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Collective excitations in a two-dimensional dipole system

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Abstract

We address the question of collective excitations in two-dimensional (2D) dipolar systems. The main issue is that such systems have no Hartree and no random-phase-approximation (RPA) limits and calculations have to include particle correlations from the outset. We focus on the longitudinal collective mode representing the density oscillations of the dipoles and on the transverse collective mode representing shear waves. Our theoretical approach is based on the quasi-localized charge approximation (QLCA) adapted to point-dipole systems interacting through a $1/r^3$ potential. Our analytical calculation is accompanied by classical molecular dynamics (MD) simulation. At long wavelengths, the longitudinal and transverse collective excitations exhibit acoustic behaviors with phase velocities that vary linearly with the dipole strength and are wholly maintained by particle correlations. At finite wavenumbers, the mode dispersion resulting from our classical MD simulations shows a roton-like behavior. Comparison with the quantum Monte Carlo dispersion generated through the Feynman relation (Astrakharchik *et al* 2007 *Phys. Rev. Lett.* **98** 060405) shows a remarkably good quantitative agreement between the two.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The two-dimensional (2D) point-dipole system (2DDS), where the particles interact via a $1/r^3$ potential, is receiving a great deal of attention these days, primarily because it can serve as a useful model for the closely spaced electron–hole bilayer (EHB) in its excitonic phase [1–4], and because the 2DDS is a fascinating system in and of itself. The system can be described as a collection of N point dipoles, each of mass $m = m_e + m_h$, occupying the large but bounded area A; $n = N/A$ is the average density. The dipoles are free to move in the xy-plane with dipolar moment oriented in the z-direction. The interaction potential is accordingly given by $\phi_D(r) = p^2/r^3$, where p is the electric dipole strength. The coupling strength in the 2DDS is characterized at arbitrary degeneracy by $\tilde{\Gamma}_D = p^2/a^3\,\langle E_{\rm kin}\rangle$, which, with $\langle E_{\rm kin}\rangle = 1/\beta$, becomes $\Gamma_D = \beta p^2/a^3$ in the high-temperature classical domain; $a = 1/\sqrt{\pi n}$ is the average inter-particle distance and $\beta^{-1} = k_B T$ is the thermal energy. Note that at zero temperature, $\langle E_{\rm kin}\rangle = \langle P^2/2m\rangle = \hbar^2/2ma^2$ and $\tilde{\Gamma}_D = 2r_D = 2r_0/a$ is the appropriate measure of the coupling strength; the characteristic length $r_0 = mp^2/\hbar^2$ is the dipole equivalent of the Bohr radius. Here we focus on the strong coupling regime $\Gamma_D \gg 1$ in the classical domain. In section 3, where we compare our MD-generated dispersion data with those generated from the quantum MC simulations of [5], the correspondence is taken to be $\Gamma_D \Leftrightarrow r_D$.

The approximation that replaces the bound electron–hole excitons in the EHB by the 2DDS model has been considered by a number of investigators [5–8] and most recently by the authors [9] in a combined analytical/molecular dynamics (MD) study of collective excitations in the strongly coupled 2DDS. The main findings of this work can be summarized as follows: (i) the 2DDS acoustic phase velocity is very nearly identical to that of the EHB in-phase mode in its strongly coupled excitonic liquid phase [4]. (ii) The architecture of the 2DDS acoustic phase velocity, which is wholly maintained by particle correlations, is formally invariant over the entire classical to quantum domains all the way down to zero temperature; the corresponding acoustic dispersion is calculated in the quasi-localized charge approximation (QLCA) [10] as

$$\omega^2(q \to 0) = \frac{33}{16}\omega_D^2 \bar{q}^2 J(\tilde{\Gamma}_D), \tag{1}$$

$$J(\tilde{\Gamma}_D) = \int \mathrm{d}^2\bar{r}\,\frac{1}{\bar{r}^3}g(r) = \int_0^\infty \mathrm{d}\bar{r}\,\frac{1}{\bar{r}^2}g(\bar{r}) \tag{2}$$

($\bar{q} = qa$, $\bar{r} = r/a$, $\omega_D = \sqrt{2\pi np^2/ma^3}$ is a characteristic dipole oscillation frequency, and $g(\bar{r})$ is the pair distribution function). (iii) The theoretical values of the acoustic phase velocity inferred from equations (1) and (2), as a function of coupling strength, are in very good agreement both with the MD data and with the corresponding values of the thermodynamic sound speed in the classical and zero-temperature quantum domains.

It should be emphasized that the very fact that the dispersion is acoustic is not a trivial conclusion: claims based on seemingly reasonable assumptions have led to erroneous [$\omega(q \to 0) \propto q^{3/2}$] results [11].

The convergence of the $J(\tilde{\Gamma}_D)$ integral (2) is guaranteed by observing that $g(\bar{r} \to 0) \propto \exp(-\Gamma_D/\bar{r}^3)$ at high temperatures and $g(\bar{r} \to 0) \propto \sqrt{\bar{r}/r_D}\exp(-4\sqrt{r_D/\bar{r}})$ at zero temperature [9]; at large $\bar{r}$, with $g(\bar{r} \to \infty) \to 1$, the integrand drops off as $1/\bar{r}^2$.

As already pointed out in [9], the appearance of the pair distribution function $g(r)$ in equation (2) is crucial. The 2DDS with its $1/r^3$ dipole potential, because of its $r \to 0$ strong singularity, admits neither a Hartree limit nor a random-phase approximation (RPA) description of the collective excitations. Hence, the longitudinal density and transverse current response functions can be calculated only through the introduction of correlations in the formalism,

vis-à-vis the pair distribution function $g(r)$, from the outset. This is why it is required to rely on a nonperturbative calculational method, such as QLCA equation (2). Thus, any attempt to recover the RPA limit by asserting that $g(\bar{r})$ can be set equal to unity in (2) for all $\bar{r}$ is an act of futility since it would result in a divergent average Hartree field.

The goal of this paper is to extend the long-wavelength analysis of [9] both to the analysis of the longitudinal dipole density oscillation mode at finite wave numbers and to the analysis of the transverse shear mode dispersion. We propose to calculate the collective mode dispersion by invoking the QLCA developed some time ago by Kalman and Golden [10] for a variety of strongly coupled charged-particle systems and subsequently adapted to the 2DDS [9]. Here, our combined QLCA/MD treatment will be entirely classical. However, as far as collective excitations are concerned, it is expected that the classical treatment at least qualitatively provides a reasonably good description of the collective mode dispersion of the 2DDS liquid phase at arbitrary degeneracy. As we will see later in this paper, this expectation is borne out by the close agreement between our classical MD dispersion data and those generated from the Feynman relation with input of quantum Monte Carlo (MC) static structure factor data [5].

In section 2 we formulate the QLCA tensorial equation of motion and from it the general formulae for the longitudinal and transverse collective mode dispersion in a strongly coupled 2D classical dipole liquid. In section 3, we analyze the 2DDS dispersion at finite wavenumbers making comparisons between our own classical MD-generated dispersion data and those generated from quantum MC structure factor data via the Feynman relation [5]; we also compare our MD dispersion data with sample QLCA longitudinal dispersion curves. In section 4, we display a sample QLCA transverse shear mode dispersion curve, and we compare it with the corresponding classical MD data. Conclusions are drawn in section 5.

As to representing the behavior of the quantum system through a classical simulation, there remains one open question, namely, whether the formation of a Bose–Einstein condensate would affect the mode dispersion. That this may indeed be the case is known from the Bogoliubov analysis of the excitation spectrum of weakly interacting bosons. Here, however, the condensate fraction can be considered to be negligibly small since strong dipole–dipole correlations tend to destroy coherence. This observation is borne out by the quantum MC simulation of [5].

2. QLCA formalism and collective mode formulae

Over the years, the QLCA method has been successfully applied to a variety of strongly coupled charged-particle systems. Here we follow the paradigm of the original derivation, focusing on the differences that distinguish the point-dipole system from a system of point charged particles. Similarly to what has been established for charged-particle systems, the observation that serves as the basis of the QLC theory is that the dominating feature of the physical state of a classical dipolar liquid with coupling parameter $\Gamma_D = \beta p^2/a^3 \gg 1$ is the quasi-localization of the point dipoles. The ensuing model closely resembles a disordered solid where the dipoles occupy randomly located sites and undergo small-amplitude oscillations about them. However, the site positions also change and a continuous rearrangement of the underlying quasi-equilibrium configuration takes place. Inherent in the model is the assumption that the two time scales are well separated and that it is sufficient to consider the time average (converted into ensemble average) of the drifting quasi-equilibrium configuration.

The steps leading to the QLCA equation of motion for the 2DDS are detailed in [9] and it suffices to quote the result here

$$[\omega^2 \delta_{\mu\nu} - C_{\mu\nu}(\mathbf{q})]\xi_{\mathbf{q},\nu}(\omega) = -\frac{n}{\sqrt{mN}} F_{\mu}^{\text{ext}}(\mathbf{q}, \omega), \tag{3}$$

where the dynamical tensor $C_{\mu\nu}(\mathbf{q})$ is given by

$$C_{\mu\nu}(\mathbf{q}) = \frac{3np^2}{m}\int \mathrm{d}^2 r \frac{1}{r^5} g(r)[\exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r}) - 1]\left[\delta_{\mu\nu} - 5\frac{r_\mu r_\nu}{r^2}\right]; \tag{4}$$

$F^{\mathrm{ext}}_{\mu}(\mathbf{q}, t)$ is a weak external force, and the Fourier representation

$$\xi_{i,\mu}(t) = \frac{1}{\sqrt{mN}}\sum_{\mathbf{q}} \xi_{\mathbf{q},\mu}(t)\exp(\mathrm{i}\mathbf{q}\cdot\mathbf{x}_i) \tag{5}$$

links the collective coordinates $\xi_{\mathbf{q}}(t)$ to the perturbed amplitude $\xi_i(t)$ of the small excursion of the ith particle about its equilibrium quasi-site position $\mathbf{x}_i$. The longitudinal (L) and transverse (T) elements of the dynamical tensor (4) are readily calculated to be

$$C_L(\mathbf{q}) = \frac{3}{2}\omega_D^2 \int_0^\infty \mathrm{d}\bar{r}\frac{1}{\bar{r}^4} g(\bar{r})\,[3 - 3J_0(\overline{qr}) + 5J_2(\overline{qr})], \tag{6}$$

$$C_T(\mathbf{q}) = \frac{3}{2}\omega_D^2 \int_0^\infty \mathrm{d}\bar{r}\frac{1}{\bar{r}^4} g(\bar{r})\,[3 - 3J_0(\overline{qr}) - 5J_2(\overline{qr})]. \tag{7}$$

The collective oscillation mode frequencies

$$\omega_L^2(\mathbf{q}) = C_L(\mathbf{q}), \tag{8}$$

$$\omega_T^2(\mathbf{q}) = C_T(\mathbf{q}) \tag{9}$$

readily follow from equation (3) with the external force $F^{\mathrm{ext}}_{\mu}(\mathbf{q}, \omega)$ turned off. We consider first the small-q behavior, deferring the finite-q analysis of the longitudinal and transverse modes to sections 3 and 4. At long wavelengths, the QLCA equations (8) and (9) further simplify to the longitudinal dipole density oscillation frequency (1) (with $\tilde{\Gamma}_D$ therein replaced by the classical Γ_D coupling parameter) and to its transverse shear mode counterpart, reported here for the first time

$$\omega_T^2(q \to 0) = \tfrac{3}{16}\omega_D^2 \bar{q}^2 J(\Gamma_D); \tag{10}$$

the $J(\Gamma_D)$ values are computed from equation (2) with input from our MD-generated $g(r)$ data. Independently of Γ_D, we observe that the transverse phase velocity corresponding to equation (10) is $1/11$th times smaller than that corresponding to equation (1). Equations (1) and (10) can be identified as the QLCA in-phase longitudinal and transverse acoustic modes in the closely spaced EHB [4, 9].

3. Longitudinal collective mode dispersion at finite wave numbers

We turn now to the analysis of the longitudinal collective mode at finite wave numbers. To further make the case that the classical 2DDS reasonably well emulates the dispersion at arbitrary degeneracy, we have generated figure 1 which compares our MD-generated dispersion curve for the classical 2DDS with that from [5], generated from the Feynman relation with the input of quantum MC static structure factor data for the zero-temperature bosonic dipole system. In making the comparison, we invoke the reasonable correspondence $\Gamma_D \Leftrightarrow r_D$ based on the correspondence of the average kinetic energies, $kT \Leftrightarrow \hbar^2/ma^2$.

While it is true that the Feynman excitation spectrum constitutes only an upper bound to the actual collective mode dispersion, we can nevertheless note the remarkable agreement between the two sets of data in the strong coupling regime. This agreement becomes somewhat less satisfactory with decreasing coupling. We believe that the agreement at the lower wave

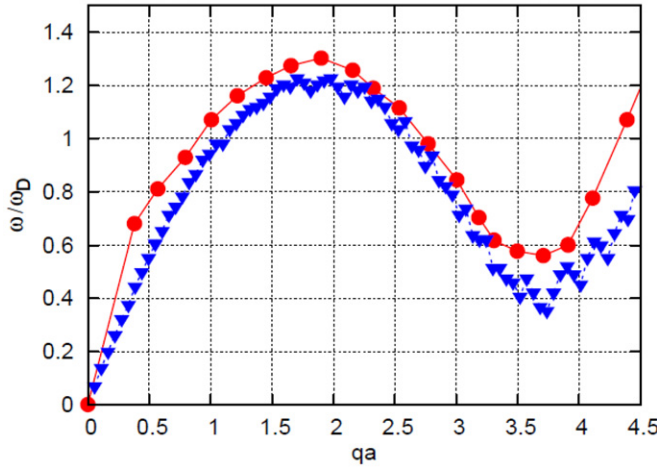

Figure 1. (Color online.) Longitudinal collective mode dispersion curves generated from classical molecular dynamics (MD) simulations (▼) at $\Gamma_D = 30$ and from the reference [5] quantum Monte Carlo (MC) simulations (•) at $r_D = 28.36$.

numbers would be better were it not for possible inaccuracies in the input $S(q \to 0)$ data in [5].

We have evaluated equations (6) and (8) with the input of $g(r)$ data generated from our MD simulations carried out at $\Gamma_D = 15$. The resulting dispersion curve is displayed in figure 2. The extended QLCA (eQLCA) curve is generated from the dispersion relation [9]

$$1 - \frac{m}{nq^2} C_L(\mathbf{q}) \chi_0(\mathbf{q}, \omega) = 0, \tag{11}$$

where the familiar Vlasov density response function

$$\chi_0(\mathbf{q}, \omega) = -\frac{1}{m} \int \mathrm{d}^2 v \frac{\mathbf{q} \cdot \partial F^{(0)}(v)/\partial \mathbf{v}}{\omega - \mathbf{q} \cdot \mathbf{v}} \tag{12}$$

quite naturally emerges in the formalism if one takes account of the effects of random thermal motions of the dipoles [12]. In the zero-temperature *classical* domain, we note that $\chi_0(\mathbf{q}, \omega) = -nq^2/m\omega^2$, so that in this limit, equations (8) and (11) become one and the same. Figure 2 indicates that the QLCA and eQLCA dispersion curves are in excellent agreement with the MD-generated dispersion curves for $qa \leqslant 2$. Beyond $qa = 2$, the agreement between theory and simulations is less satisfactory, with the QLCA devoid of RPA-like thermal effects emerging as the better of the two theoretical descriptions—at least up to $qa \sim 4.5$. The fact that the roton minimum emerges as a result of strong correlations and can be identified from purely classical considerations is remarkable; in fact, it was already emphasized some time ago as an alternate explanation by Nozieres [13].

4. Transverse shear mode dispersion

By now it is well documented that charged-particle systems in the strongly coupled liquid phase can support transverse shear waves [10, 14–26]. This is borne out by numerous MD simulations [14, 15, 18, 19, 21, 23] and by recent laboratory experiments on 2D complex plasmas [26].

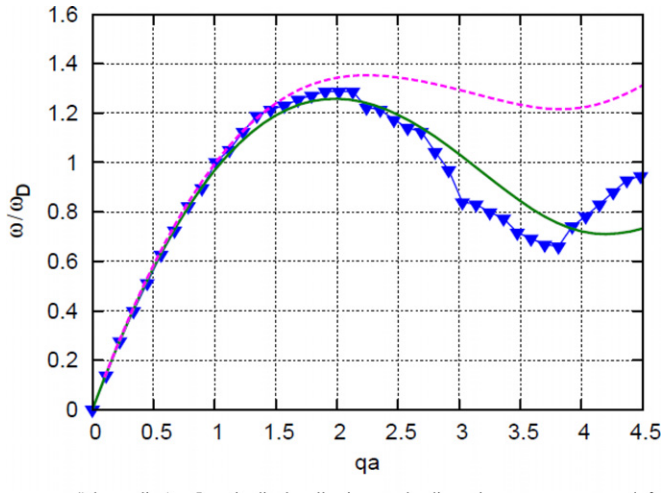

Figure 2. (Color online.) Longitudinal collective mode dispersion curves generated from classical molecular dynamics (MD) simulations (▼) at $\Gamma_D = 15$ and from QLCA (solid line) equations (6) and (8) and eQLCA (dashed line) equations (6), (11) and (12) with the input of MD-generated $g(r)$ data.

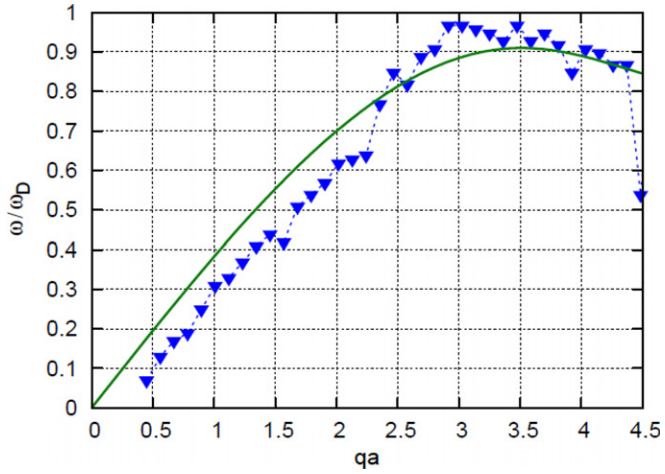

Figure 3. (Color online.) Transverse shear mode dispersion curves generated from classical molecular dynamics (MD) simulations (▼) at $\Gamma_D = 50$ and from QLCA (solid line) equations (7) and (9) with the input of MD-generated $g(r)$ data.

We have generated transverse current correlation spectra from MD simulations of the 2DDS in its strongly coupled liquid phase. The dispersion curve that results is displayed in figure 3, alongside the corresponding QLCA dispersion curve calculated from equations (7) and (9) (no thermal correction is warranted at this high Γ value), with the input of our MD-generated $g(r)$ data. Not surprisingly, our preliminary calculations indicate that agreement between theory and simulation becomes more and more satisfactory with increasing coupling strength. With $J(\Gamma_D = 50) = 0.825$ (taken from table II of [9]b), one can readily verify that the phase velocity in the acoustic regime of figure 3 is well reproduced by equation (10).

The MD data show the emergence of a sharp cutoff $\omega \to 0$ for a finite q. Its existence has also been observed in Yukawa systems [21, 25] and in the in-phase modes of unipolar charged-particle bilayers [18] and electron–hole bilayers [4]. While comparison with the QLCA does show agreement as far as the linear acoustic dispersion is concerned, the QLCA, because it does not take account of damping in the formalism, nevertheless fails to predict this conspicuous finite-q cutoff in the shear mode oscillation frequency.

5. Conclusions

This paper presents an analysis of the collective mode dispersion of a classical two-dimensional dipole system (2DDS) in the strongly coupled liquid phase. The theoretical calculations are based on the quasi-localized charge approximation (QLCA) [10]; as we have emphasized in the introduction, the application of a non-perturbative method such as the QLCA is required for the theoretical treatment of the 2DDS for which no RPA description of the system exists. Our theoretical calculations are complemented by molecular dynamics (MD) simulations. The analysis of this paper extends our recent study [9] of the longitudinal mode at long wavelengths to the finite wave number domain. There we confirmed that the longitudinal dipole oscillation mode in the $q \to 0$ limit exhibits an acoustic behavior and demonstrated that equation (1) describes the acoustic dispersion over the entire classical to quantum domains all the way down to zero temperature. The near-perfect agreement between equation (1) with (2) and our MD dispersion data [9] attests to the accuracy of the QLCA description. This point is further underscored in [9] by the close agreement between the acoustic phase velocities calculated from equation (1) and the thermodynamic sound speeds in the classical and quantum domains.

In the present work, focusing on the finite-q behavior of the dispersion, we observe the closeness between our MD-generated longitudinal dispersion curve for the classical 2DDS and that of [5] generated from the Feynman relation with the input of quantum MC static structure factor data. Quite remarkably, this close resemblance persists for wave numbers q extending beyond the roton minimum $qa \approx 3.6$, suggesting that the roton minimum has a classical origin, rooted in the strong correlations prevailing in the system.

For high Γ_D values both the QLCA calculations and the MD simulations reveal the existence of a shear mode. The MD-generated dispersion, however, shows the ubiquitous sharp finite-$qa \sim 0.3$, $\omega = 0$ cutoff observed as well in the Yukawa systems [21, 25] and in electronic bilayers [4, 18]. Below this q value, the shear mode ceases to exist, since the liquid phase cannot support shear in the long-wavelength limit.

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