Collective Modes in Two-Dimensional One-Component-Plasma with Logarithmic Interaction

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Collective modes of a two-dimensional one-component-plasma (2D OCP) with the repulsive logarithmic interaction between the particles are analyzed using the quasi-crystalline approximation (QCA) combined with the molecular dynamic simulation of the equilibrium structural properties. It is found that the dispersion curves in the strongly coupled regime are virtually independent of the coupling strength. Arguments based on the excluded volume consideration for the radial distribution function allow us to derive very simple expressions for the dispersion relations, which show excellent agreement with the exact QCA dispersion over the entire domain of wavelengths.

FORMULATION

The system considered in this paper represents a collection of point-like particles moving on a two-dimensional surface and interacting via a pairwise repulsive logarithmic potential of the form $V(r)=-\varepsilon\ln(r/a)$, where ε is the energy scale and r/a is the reduced distance between a pair of particles. This interaction potential corresponds to the solution of the 2D Poisson equation and represents the interaction between infinite charged filaments. In the conventional notation $\varepsilon = Q^2$ and $a=(\pi n)^{-1/2}$. The considered system has been employed to model vortices in thin-film semiconductors and has some relevance in the context of the anomalous quantum Hall effect. The system is characterized by ultra-soft interactions between the particles and is of interest from the fundamental point of view as an opposite limit of the celebrated hard sphere (hard disc in 2D) model. Below we apply the quasi-crystalline approximation (QCA) to obtain the dispersion relations of the longitudinal and transverse modes at strong coupling.

IMPLEMENTATION OF THE QCA

The quasi-crystalline approximation was proposed by Hubbard and Beeby (1969). This theoretical approach can be regarded as a generalization of the phonon theory of solids. In the simplest version, the particles forming liquid are assumed stationary, but the system is characterized by a liquid-like order, measured in terms of the isotropic radial distribution function (RDF) $g(r)$. The linear response of such disordered system can be approximately calculated and related to the frequencies of the collective modes. The theory becomes exact in the special case of a cold crystalline solid. In this sense, the term "quasi-crystalline approximation" appears adequate, and we employ it here. In the context of plasma physics, similar approach is known as the quasilocalized charge approximation (QLCA). In the QCA model, the dispersion relations are related to the inter-particle interaction potential *V(r)* and the equilibrium radial distribution function $g(r)$ of strongly interacting particles. The compact QCA expressions for the longitudinal and transverse modes in neutral fluids are

$$\omega_L^2=\frac{n}{m}\int\frac{\partial^2 V(r)}{\partial z^2}g(r)[1-\cos(kz)]d^2r,\qquad \omega_T^2=\frac{n}{m}\int\frac{\partial^2 V(r)}{\partial y^2}g(r)[1-\cos(kz)]d^2r.$$

Adopted to the 2D situation (particles are confined to the yz plane) and to the presence of the neutralizing background, these expressions yield for the logarithmic potential

$$\omega_L^2=\omega_p^2+\omega_p^2\int_0^\infty\frac{h(x)J_2(qx)}{x}dx,\qquad \omega_T^2=-\omega_p^2\int_0^\infty\frac{h(x)J_2(qx)}{x}dx.$$

Here, $\omega_p=(2\pi Q^2 n/m)^{1/2}$ is the 2D OCP plasma frequency, $x=r/a$ is the reduced distance, $h(x)=g(x)-1$ is the pair correlation function, $q=ka$ is the reduced wave number, and $J_2(x)$ is the Bessel function of the first kind. From these equations immediately follows that

$$\omega_L^2+\omega_T^2=\omega_p^2,$$

which represents the two-dimensional version of the Kohn's sum rule.

In the long-wavelength (small q) limit, we use the series expansion of $J_2(x)$ combined with the fist sum rules to obtain for the longitudinal mode

$$\frac{\omega_L^2}{\omega_p^2}\cong 1-\frac{q^2}{16}+\frac{q^4}{96\Gamma}-\frac{q^6(4-\Gamma)}{16\Gamma^2}+O(q^8).$$

The first two terms coincide with the harmonic solid analysis by Alastuey and Jancovici (1981). Note that they are independent of Γ. This provides preliminary indication that the dispersion relations may not be very sensitive to Γ in this normalization, the point that will be further discussed below.

In the short-wavelength limit (large q), the longitudinal and transverse frequencies approach the common asymptote, the Einstein frequency $\omega_E=\omega_p/\sqrt{2}$.

SIMULATIONS

Standard molecular dynamics simulations with the Verlet velocity algorithm and Langevin thermostat have been performed. Initially, $N=4800$ pointlike particles are randomly distributed over the unit sphere (to eliminate the periodic boundary conditions), and equilibrated (at a given Γ) configurations are then used to calculate $g(x)$ [and hence $h(x)$] and to provide the Voronoi tessellation. Some results of the simulations are presented in Fig. 1, where typical configurations of particles (color-coded via the number of nearest neighbors) are shown for the three values of Γ (Γ = 40, 80 and 150). The ground state of the 2D OCP with the logarithmic interaction is well known to be hexagonal, so that blue (five-fold) and red (seven-fold) particles are the topological defects. The defects abundance, $\delta_d=(N_{5\text{fold}}+N_{7\text{fold}})/N$, drops down as Γ increases. For the configurations shown in Fig. 1, these abundances are about 0.41 (Γ = 40), 0.30 (Γ = 80), and 0.22 (Γ = 150).

Using the obtained RDFs $g(x)$ (plotted in the inset of Fig. 2), the dispersion curves of the longitudinal and transverse modes, within the QCA approach, have been calculated. The results are shown in Fig. 2 by symbols. It is evident that in the considered regime of strong coupling, the dispersion relations are very insensitive to the exact value of Γ, although the variations in RDFs are significant. The symbols are all falling on the two distinct curves (L-mode and T-mode), and no signature of any systematic deviations can be detected. The black curves correspond to the simplified version of the QCA. The agreement between these curves and the location of the symbols is excellent.

SIMPLIFIED QCA

Recently, we have proposed a useful simplification of the QCA (or, equivalently, QLCA) formalism for 3D OCP. In this simplified version, the excluded volume arguments suggest to use a simplest toy step-wise model of RDF: $g(x)=\theta(x-R)$, where θ(x) is the Heaviside step function. The distance R (measured in units of a) characterizes the radius of an excluded sphere around each particle due to a strong (repulsive) inter-particle interaction. To estimate this quantity, energy and pressure equations have been used, which are also expressed as certain integrals over $g(x)$, or $h(x)$ in the present case. For the single component Yukawa systems, it was demonstrated that the results are not particularly sensitive to whether the energy or pressure equation is used to determine R. The obtained dispersion relations are in very good agreement with the conventional QLCA in the long wavelength regime and correctly predict the approach to the Einstein frequency in the short-wavelength limit.

In the present case, there is a natural way to determine R, by requiring the perfect screening condition to be satisfied (in this way, we also get the exact result for the excess pressure, but not for the excess energy). This results in $R=1$ and, hence,

$$\frac{\omega_L^2}{\omega_p^2}\cong\frac{1}{2}+\frac{J_1(q)}{q},\qquad \frac{\omega_T^2}{\omega_p^2}\cong\frac{1}{2}-\frac{J_1(q)}{q}$$

This shows excellent agreement with the conventional (full) QCA (or QLCA) formalism in the entire domain of q (see Fig. 2), much better than in the case of 3D Yukawa systems. The agreement is too impressive that one may think of a mathematical identity involved. This is, however, not the case, because the low-q limit of the conventional QCA does contain some (although vanishingly small) dependence on Γ, while the first of these equations does not.

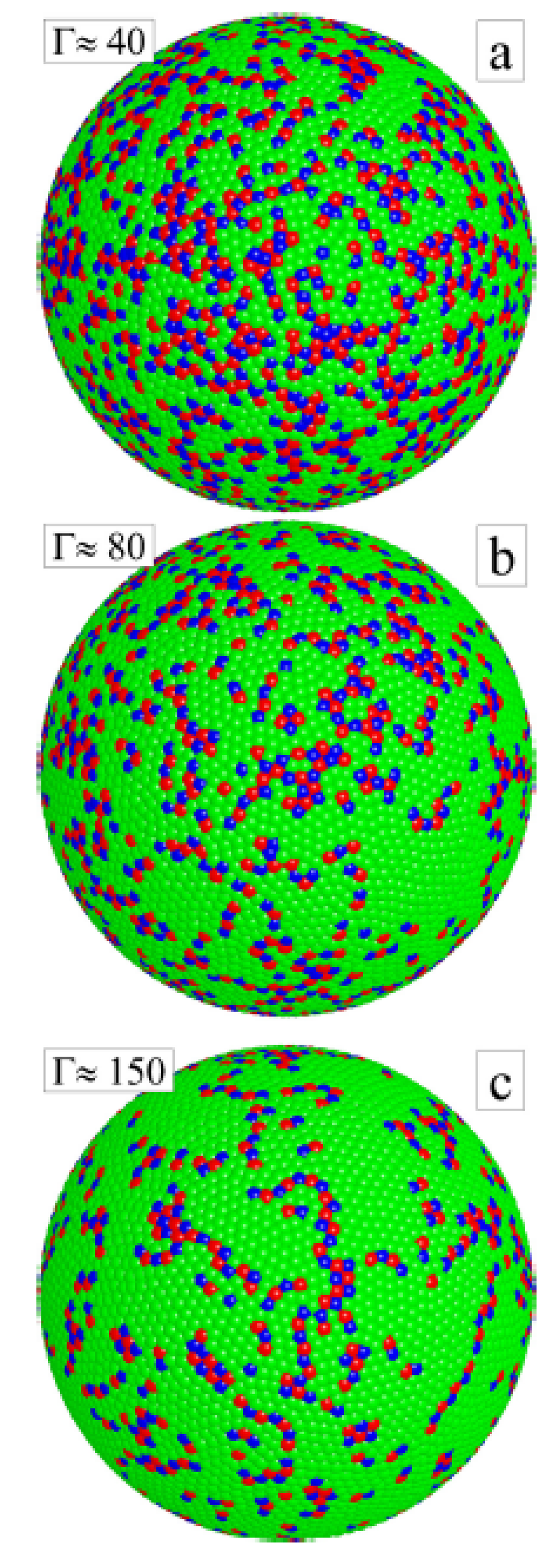

Fig. 1. Structure of the 2D OCP with the logarithmic interaction for different coupling values (indicated on the plot) as modelled on a sphere. Particles are color-coded via the number of nearest neighbors defined from the Voronoi analysis: five-fold (blue), six-fold (green), and seven-fold (red).

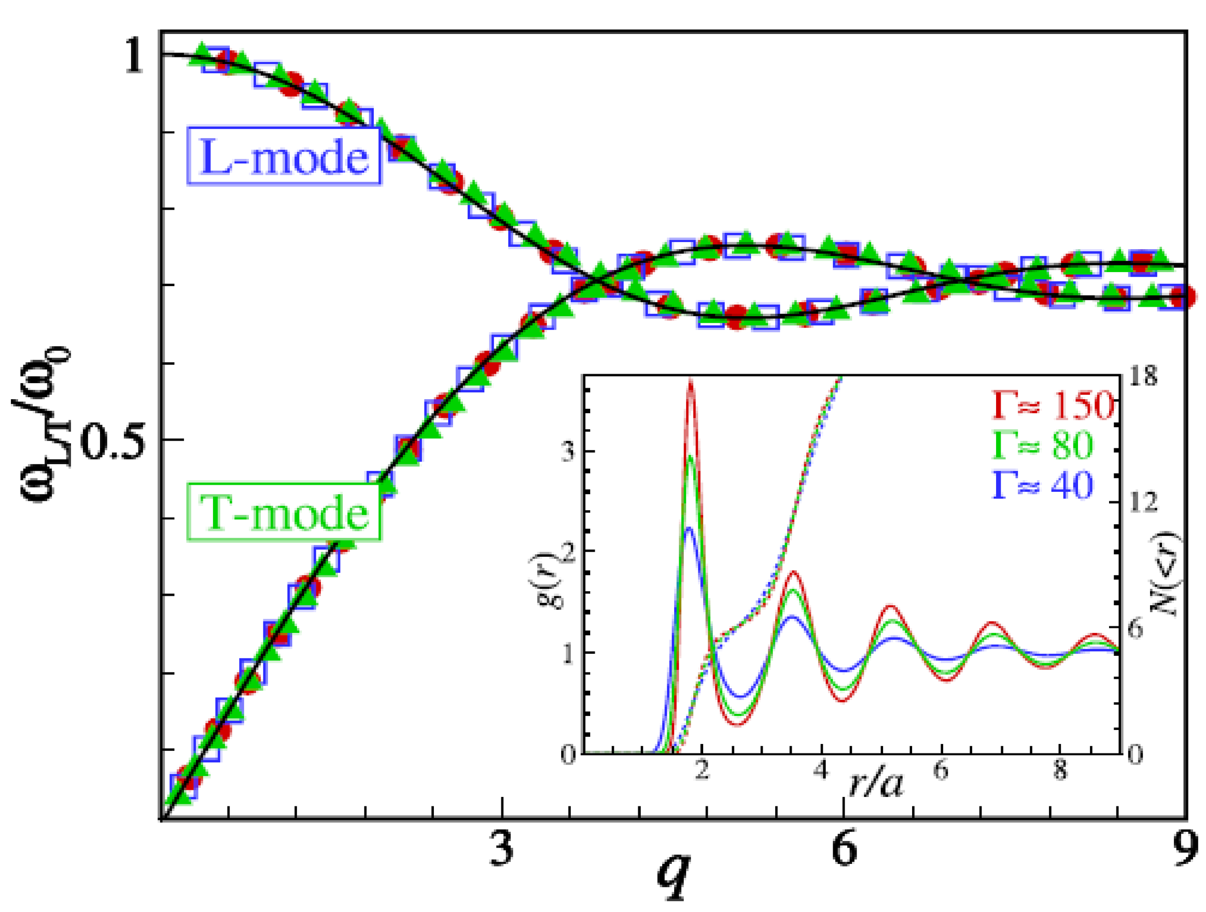

Fig.2. Dispersion relations of the longitudinal (L) and transverse (T) waves in strongly coupled 2D OCP. The solid black curves correspond to the simplified QCA. Symbols correspond to the conventional QCA with *g(r)* obtained via the direct MD simulations: red, green, and blue colors correspond to coupling parameter Γ = 150, 80, and 40. The corresponding RDFs are shown in the inset. The cumulative functions *N*(<*r*) of g(r) are also plotted in the inset.

ONSET OF NEGATIVE DISPERSION

The QCA (QLCA) approach, describing elastic waves in fluids in a manner analogous to phonons in solids, is the theory for the strongly coupled state. It neglects the kinetic effects and, as a result, cannot reproduce the transition from positive to negative dispersion (which refers to dω/d*k* < 0 at k -> 0; note that the dispersion is always negative within QCA) at moderate coupling. Recently, it was suggested that in the long-wavelength limit the kinetic and correlational effects appears in the dispersion relation as a simple superposition and, hence, the OCP dispersion relation can be written as

$$\omega^2=\omega_p^2+3k^2v_T^2+(\Delta K_\infty/nm)k^2.$$

Here ΔK$_\infty$ is the high-frequency or instantaneous bulk modulus (taking into account the character of plasmon dispersion). For the considered 2D OCP system $\Delta K_\infty^{2D}=P_{\rm ex}$ and $P_{\rm ex}=-\frac{1}{4}nT\Gamma$, which results in

$$\omega^2=\omega_p^2+k^2v_T^2(3-\Gamma/4)$$

The transition from negative to positive dispersion occurs at Γ = 12, which is close to the condition derived previously by Hansen (1981) using different arguments. In the limit Γ >> 1 this yields $\frac{\omega_L^2}{\omega_p^2}\cong 1-\frac{q^2}{8}$, which is different from the QCA result, but coincides with the conventional fluid approach.

CONCLUSION

To summarize, we have discussed the collective modes behaviour in the 2D OCP fluid with the logarithmic interaction between the particles. The dispersion relations in the strong coupling regime were obtained using the QCA (or QLCA) method coupled to the MD simulations on a sphere, to get information about the system structural properties. The simplified QCA approach based on a toy model for the RDF, which accounts for the excluded volume effects, yields analytic expressions which are in excellent agreement with those from the conventional QCA. The condition for the onset of negative dispersion has been estimated. This work was supported by the A*MIDEX project (No. ANR-11-IDEX-0001-02) funded by the French Government "Investissements d'Avenir" program managed by ANR.

Further details can be found in Phys. Plasmas **23**, 052115 (2016) and Phys. Plasmas **23**, 104506 (2016).