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A comparative study between effects of shadowing potential and ODS on Coulomb crystal formation

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Abstract. In dusty plasma, the overlapping Debye spheres around dust grains produce an attractive force. Shadowing force is exerted between neighboring particles because of mutual distortion of ion or neutral flux to the particles. A comparative study has been made on the role of these two forces on 2D structure of dusty system. Radial distribution function for the particles is a comparative study between the effect of the coupled Yukawa-shadowing potential and the coupled Yukawa-Overlapping Debye Sphere (ODS) potential on 2D dust crystal formation, which has been performed by using molecular dynamics simulation. The structure of the system is investigated by calculating the radial distribution function ($g(r)$) for different values of Γ, κ and dust number densities n_d. It is seen from our study that the Coulomb coupling parameter does not have significant effect on both ODS and shadowing forces. The attractive shadowing force is more dominant for grains with large screening parameter. However, the ODS force becomes dominant with the increasing value of the dust number density. The results for the Yukawa-Shadowing and the ODS potential are also compared with experimental results and a close agreement is obtained for attractive shadowing force.

1. Introduction

The formation of dust crystal is a well-known phenomenon in dusty plasma physics. On account of large negative charge, dust particles immersed in plasma can turn plasma into a strongly coupled system. Ikezi [1] pointed out that dust particles present in low temperature strongly coupled plasma may lead to formation of Coulomb crystals, if the Coulomb coupling parameter exceeds a critical value. Ikezi's prediction was experimentally demonstrated by several researchers [2–6]. The discovery of plasma crystals has encouraged the plasma physics community to work in this area. It gives a platform to condensed matter physicist to study about phase transition, melting process etc. Plasma crystal may be used as a model system to study involved dynamical processes. Plasma crystal offers ideal tool to observe phase transition at kinetic level because of two factors: direct visualization of individual particles and short restoring time required by the particles to reach equilibrium after perturbation.

One outstanding problem of dust crystal is that the average interaction potential between two dust particles is not known precisely. The shielding of dust particle

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and resulting interaction potential are not explored properly. It is usually assumed that the average interaction potential between two dust particles is of the Debye–Hückel or the Yukawa type. It is now well established that dust particles form Coulomb crystal in presence of strong repulsion forces [7–8]. However, a question generally arises regarding the existence of any attractive force between the grains. The mechanism of interaction among grains in plasma is a complex phenomenon and needs substantial amount of research both at theoretical and experimental levels to understand it. For system where inter-particle distance is larger than the Debye length, it may not be sufficient to consider the Debye–Hückel potential as the interaction potential among the dust grains. The effect of attractive force like shadow force or the overlapping Debye sphere can not be ignored in such cases. The existence of an attractive component in the force between dust particles was experimentally studied and verified by several methods [9–11]. It was suggested by Tsytovich et al. [12] that the grains create flux of plasma particles toward their surface and the shadow of the plasma flux to one of the interacting grains by another grain creates an attractive force. Since these forces are not screened, they can dominate Coulomb repulsion force at distances larger than the ion Debye screening length. This attractive force may play a major role in the formation of dust crystal. Ramazanov et al. [13] investigated the interaction between dust particles in a plasma on the basis of experimental pair correlation function. They confirmed existence of an attractive component in the interaction potential of dust particles. Nambu et al. [14] in their pioneering paper have shown that charged particulates with same polarity can attract each other due to collective interactions involving dust acoustic waves. They have also theoretically shown that the wake potential involving resonant collective interaction of moving grains with dusty plasma modes may explain the presence of periodic attractive forces along the line of motion of dust particles [14–16]. Takahashi et al. [17] have experimentally demonstrated the role of wake potential in the formation of Coulomb crystal.

Shukla and Rao [18] have discussed the possibility of Coulomb crystallization under an attractive force between charged dust grains in a multi-component dusty plasma whose constituents are tenuous electrons, streaming ions and negatively charged dust grains. They have shown that these could be a far-field non-Coulombean potential that may be responsible for bringing the like particulates together that leads to microscopic Coulomb crystallization in dusty plasma. Quasi-lattice structures may be formed under such attractive forces between like polarity dust grains. Resendes et al. [19] have suggested a static screening mechanism for the formation of plasma molecules in the bulk plasma and the plasma sheath. They identified correlation Coulomb energy as the mechanism responsible for plasma crystals. They suggested that each grain is correlated with its own Debye sheath and the interaction takes place between the dressed grains.

Tsytovich [20] has pointed out that the observed values of the critical coupling constant in most of the experiments are not consistent with the physical and theoretical estimates of this quantity. He suggested a new physical model for phase transition in a dusty plasma. He has shown that the balance between nonlinear screening at short distances and collective attraction at large distances determine the mean inter-particle distances corresponding to the values observed in the transition to the crystalline state.

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Ishira et al. [21] have shown that a like-charge attraction could align dust particles along the equipotential line on a void boundary perpendicular to the ion flow in the complex plasma.

Tsytovich et al. [22] have reported about some of their interesting results regarding helical dust structures. They have performed molecular dynamics (MD) simulations to demonstrate that a random distribution of grains, interacting via a potential with shadow attractive well forms spherical grain crystals.

Very recently Hou et al. [23] have used MD simulation to study the effect of the overlapping Debye sphere on structure of 2D dusty plasma. For this, they have made a comparison between the normal Yukawa potential and potential due to the overlapping Debye spheres. Their results show a clear difference between the two potentials for large screening parameter κ or at low dust density.

Although there exist different theories about attractive interactions among dust grains in plasma, a clear understanding of the mechanism is still lacking. There are few experimental studies that investigate about the interactions among the particles. Melzer et al. [24] performed an experiment where they had demonstrated that attractive net binding forces exist between the negatively charged dust. They found by laser manipulation of dust particles that net forces between the particles can be reversibly changed between attraction and repulsion.

In this paper, a MD code is developed to study phase transition of 2D Coulomb crystals in presence of shadowing and the overlapping Debye sphere (ODS) potentials. The study has shown some interesting results. Both shadowing and ODS have distinct roles to play for different parameter regimes of the dusty system.

2. Theoretical modeling and simulation

We consider a 2D dusty plasma system of identical, spherical particles of mass m_d and charge Q immersed in a neutralizing background plasma. It is assumed that the average inter-particle potential between two dust particles separated by a distance r_{ij} is of the Debye–Hüchel or the Yukawa type that is given by

$$\Phi(r_{ij}) = \frac{Q_d^2}{4\pi\epsilon_0 r_{ij}} exp(-r_{ij}/\lambda_D), \tag{2.1}$$

where λ_D is the Debye length of plasma defined as

$$\lambda_D = \left(\frac{q_i^2 \bar{n}_i}{\epsilon_0 K_B T_i} + \frac{e^2 \bar{n}_e}{\epsilon_0 K_B T_e} \right)^{-\frac{1}{2}},$$

where q_i, $-e$, $\bar{n}_i$, $\bar{n}_e$, T_i and T_e denote the ion charge, charge of electron, ion mean density, electron mean density, temperature of ions and electrons, respectively. The ratio of average Coulomb potential energy to the average kinetic energy can be written as $\Gamma = \frac{Q_d^2}{4\pi\epsilon_0 a K_B T_d}$, where $a = (\frac{3}{4\pi n_d})^{\frac{1}{3}}$ is the mean inter-particle distance and T_d is the temperature of the dust grains. On account of large charge on dust particles, dusty plasma easily attains strongly coupled regime. When Γ exceeds a certain critical value, the dust pericles may crystalize into solid-like structure. The phase transition of such a system is determined by two basic parameters: Γ and screening parameter, $\kappa = a/\lambda_D$.

It has been already discussed that role of attractive force in forming plasma crystal cannot be ignored. Tsytovich et al. [12] suggested that there may exist shadowing

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force between two dust grains immersed in sea of plasma particles, which is given as

$$F_{\text{shadow}} = -\frac{3}{8}\frac{r_d^2}{\lambda_{Di}^2}\frac{Z_d^2 e^2}{r_{ij}^2}, \tag{2.2}$$

where r_d, Z_d, λ_{Di} and r_{ij} represent the grain size, number of charges residing on the dust grain surface, the ion Debye screening length and inter-particle distance, respectively. The shadow force arises due to asymmetric ion flow toward- the dust grains. For a single, isolated grain, net momentum transfer due to ion flow to the grain is zero. However, if the flow of ions gets obstructed due to the grains, then the net momentum transfer may not be zero. This results in an effective attractive force between two isolated grains, which is given by the above equation. The shadow force is a relatively weak force and smaller than the bare Coulomb force by a factor $(3r_d^2/8\lambda_{Di}^2)$. This force is, however, not screened and can dominate the Coulomb repulsion forces at distance larger than the Debye screening length $\lambda_D \approx \lambda_{Di}$ and can affect dust crystal formation if the inter-dust distance is larger than the ion Debye screening length.

The ODS around dust grains produce an attractive force [19, 25, 26]. The interaction energy of the sheath of one grain with the bare charge of the other grain is

$$\Phi_{\text{ODS}}(r_{ij}) = -\frac{Q_d^2}{4\pi\epsilon_0 2\lambda_D} exp(-r_{ij}/\lambda_D). \tag{2.3}$$

The result of this potential is strong repulsion at short distance and a weak attraction at larger distances (beyond a critical radius $r_c = 2.73\lambda_D$).

In this paper, we intend to have a comparative study between effects of the shadowing potential and the ODS potential on Coulomb crystal formation. It is interesting to find out regimes of dominance of the two attractive potentials.

We examine the effect of the usual Debye–Hückel and the ODS potentials

$$\Phi_{Yu,\text{ODS}}(r_{ij}) = \frac{Q_d^2}{4\pi\epsilon_0 r_{ij}} exp(-r_{ij}/\lambda_D) - \frac{Q_d^2}{4\pi\epsilon_0 2\lambda_D} exp(-r_{ij}/\lambda_D) \tag{2.4}$$

on pair correlation function of the dusty system. The first term in the above expression is the Debye–Hückel potential, and the second term arises due to interaction of sheath of one grain with the bare charge of the other.

Here a MD code is developed to study 2D crystal formation. The combined potentials, the Yukawa-ODS and the Yukawa-shadow, have been incorporated to derive the interacting force among the particles. Simulations have been performed for a wide range of parameters, such as the Coulomb coupling parameter Γ, screening constant κ, dust density n_d and dust radius r_d. The simulations are performed with 900 particles for face centered cubic (FCC) crystal structure for the following plasma parameters: $n_i = (1.5 \times 10^{14} - 4.0 \times 10^{14})$ m^{-3}, $T_e = 2320$ K, $T_i = 300$ K, $T_d = 40$ to 1000 K. This lattice is used as an initial condition. Each grain is assigned an initial velocity (random in magnitude and direction) such that the average kinetic energy corresponds to the chosen temperature T_d.

Newton's equation of motion is solved numerically using the velocity Verlet algorithm for interaction potentials mentioned above. In MD scaling, Newton's equation for the two cases takes the following form:

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Yukawa-shadowing

$$\frac{d^2r'_i}{dt'^2} = \Gamma\kappa\left[\left(1+\frac{1}{r'_{ij}}\right)\frac{1}{r'_{ij}}exp(-r'_{ij}) - \left(\frac{3}{8}\right)\left(\frac{r'^2_d}{\lambda'^2_{Di}r'^2_{ij}}\right)\right], \tag{2.5}$$

Yukawa-ODS

$$\frac{d^2r'_i}{dt'^2} = \Gamma\kappa\, exp(-r'_{ij})\left[\frac{1}{r'_{ij}}\left(1+\frac{1}{r'_{ij}}\right) - \frac{1}{2}\right], \tag{2.6}$$

where $r'_{ij} = r_{ij}/\lambda_D$, $r'_d = r_d/\lambda_D$ and $\lambda'_{Di} = \lambda_{Di}/\lambda_D$. From these results pair correlation may be calculated that gives a picture of the structure of particles. The pair-correlation function in 2D is defined as

$$g(r) = \frac{A}{N}\frac{N(r,\Delta)}{2\pi r\Delta}, \tag{2.7}$$

where A is the area of the simulated region, N is the number of simulated particles and $N(r,\Delta)$ is the number of particles located in a circle of infinitesimal thickness Δ from $r-\Delta/2$ and $r+\Delta/2$. One may study the solid, liquid and gaseous phases of the system under different conditions from the above simulation.

3. Results and discussion

It has been mentioned that both Coulomb parameter Γ and screening constant κ control the formation of Coulomb crystal. A comparative study has been done between the shadowing potential and the ODS potential, keeping basic interaction as because of the Yukawa potential, for different values of Γ. The results are plotted in Fig. 1.

It is well known that the Yukawa system-like dust particles described here transit from organized crystalline state to fluid state as the value of Coulomb parameter Γ increases. Figure 1 shows variation of $g(r)$ with Γ. It is seen that larger the value of Γ, more pronounced are the peaks of Radial Distribution Function (RDF) plot. The effect of both ODS and shadow is to increase the height and sharpness of the RDF peaks. For almost all the values of Γ, the contributions of the shadow and the ODS forces almost overlap with each other. However, it is seen that the shadow force is slightly more dominating than the ODS force and results in even sharper peaks with the rise in the value of Γ. For large values of Γ, the difference in the peak heights for the two cases is almost negligible.

Figure 2 shows the RDF plots both for shadow and ODS forces for different values of screening constant κ. The simulations are performed keeping the value of Γ fixed at 6.409×10^3. For $\kappa = 1.66$, the two plots of RDF almost overlap with each other. The dust particles with this value of κ arrange themselves in crystalline state. With increase in the value of κ, a drastic change appears in the RDF plots. The contribution of the shadow force is no longer the same as that of ODS. It is seen that the shadow force is not that affected with increase in the value of κ. The shielding does not have much effect on the shadow force. However, the ODS potential has the tendency to take the system to gaseous state. For larger values of κ, the difference in both peak height and shape for the two cases, *i.e.* shadow and ODS is quite prominent. While the contribution of the shadow force is still to maintain the crystalline state, that of ODS is completely opposite.

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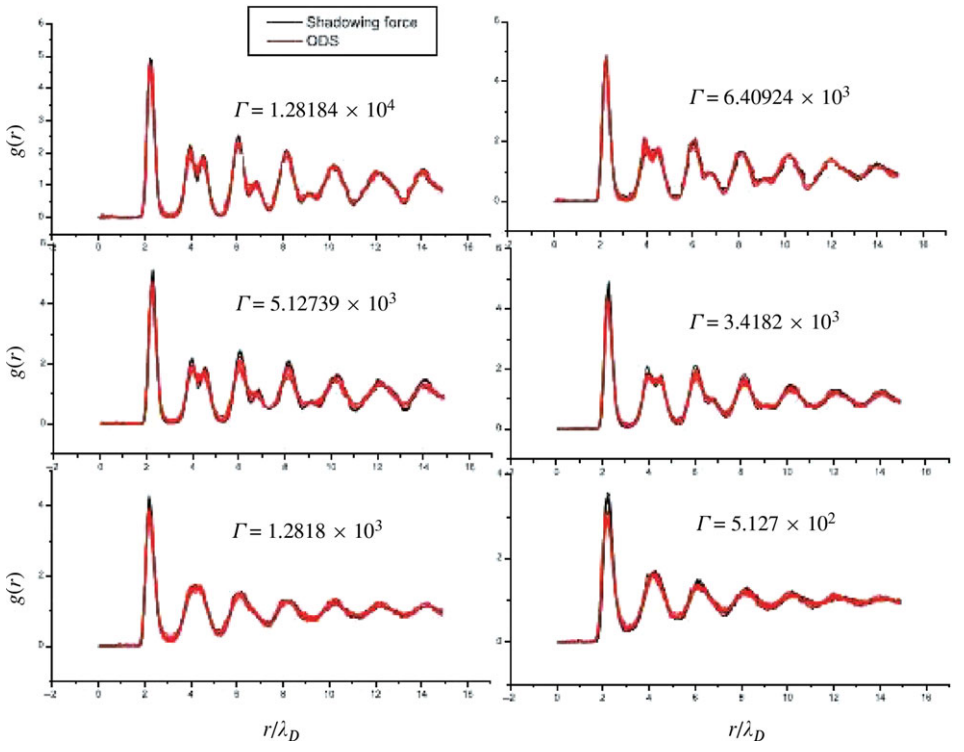


Figure 1. (Colour online) Plot of $g(r)$ vs. r/λ_D for shadowing force and ODS for different values of Γ taking $\kappa = 1.66$.

It is clear from these results that both shadow and ODS facilitate the formation of Coulomb crystal for $\kappa < 2$. The increase in κ results in reduction in the values of shielding length λ_D. In the ODS term, the exponential factor $exp(-r_{ij}/\lambda_D)$ dominates over the term $Q_d^2/2\lambda_D$ for small λ_D. The result is that the ODS potential decreases very sharply with the decrease in the value of λ_D. Owing to screening effect, the Yukawa potential also decreases with the rise in κ. The effect of the combined Yukawa and ODS potentials is to cause phase transition of the crystalline state of dust particles to disordered gaseous state for large values of κ.

A reverse effect is observed for the combined Yukawa and shadow forces. Although with the rise in the value of κ, the Yukawa potential decreases exponentially, the combined Yukawa and shadow forces still maintain the crystalline pattern. The absolute value of the shadow force increases with the rise in κ and the term due to this force plays a dominating role.

Thus, it is seen that up to mean inter-particle distance $a = 1.608173 \times 10^{-4}$ m ($\lambda_D = 5.72927 \times 10^{-5}$ m, $\kappa = 1.66$), the combined Yukawa-shadow and Yukawa-ODS overlap with each other and facilitate equally the process of crystallization. With the increase in inter-particle distance, the ODS effect becomes gradually weak. However, even then shadow effect predominates and crystallization is possible with this term. It may be concluded that for large κ ($\kappa > 2$), crystallization is possible only due to the effect of the shadow force. The role of attractive force thus can not be neglected in dust crystal formation.

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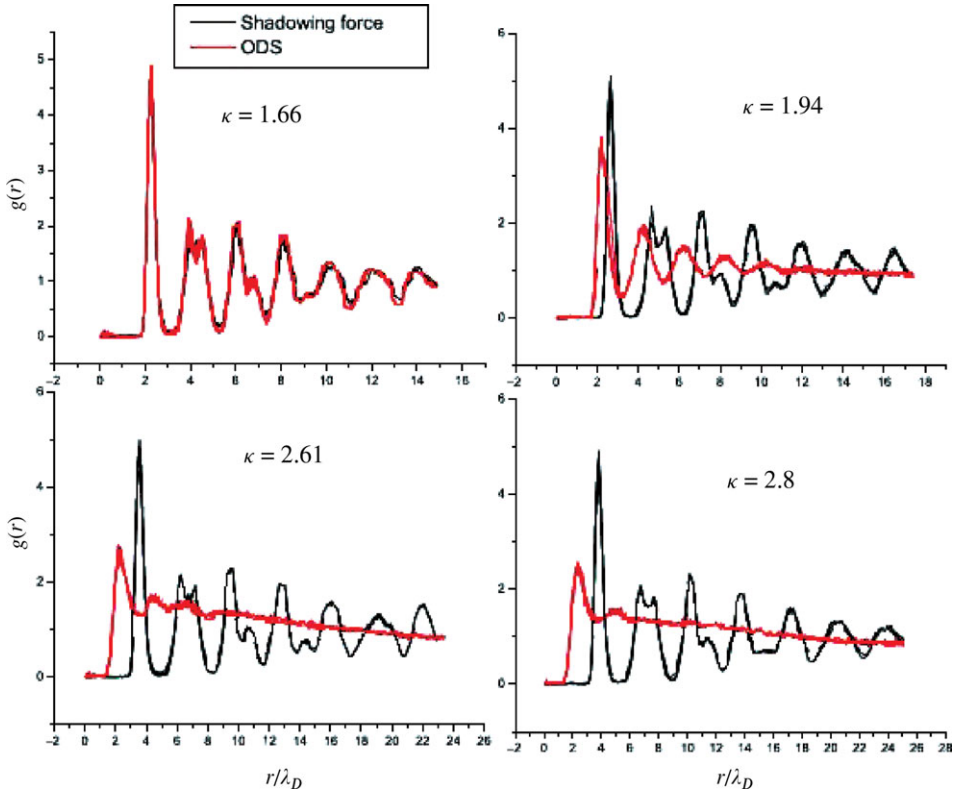


Figure 2. (Colour online) Plot of $g(r)$ vs. r/λ_D for different values of κ, with $\Gamma = 6.40924 \times 10^3$.

Figure 3 shows the comparison of RDFs for the combined Yukawa-shadow and Yukawa-ODS for four different values of dust density $n_d = 2.74 \times 10^{10}$ m^{-3}, 3.74×10^{10} m^{-3}, 4.74×10^{10} m^{-3} and 5.74×10^{10} m^{-3}, respectively. It is known from earlier studies that higher the values of dust density, more is the probability of crystal formation. For large values of n_d ($> 4 \times 10^{10}$ m^{-3}), the effects due to shadow and ODS almost overlap with each other. Large values of dust density usually facilitate the process of crystallization. For relatively small values of dust density, the peak heights and positions for the two cases differ from each other. The shadow force shows sharper and prominent peaks with peak height higher than that of ODS. It is also seen that the peaks due to the combined Yukawa-ODS shift toward smaller inter-particle distance. The dust particles attain gaseous state for the Yukawa-ODS potential, whereas it is still showing crystalline pattern for the Yukawa-shadow force. For small values of n_d, the contribution because of the shadow force is very strong compared to the ODS force.

When dust density is small, the particles are far apart from each other. Although the Coulomb force is screened, shadowing force can still be significant for distances larger than the Coulomb field screening length. The effect of the combined Yukawa-shadowing force is very strong to maintain the crystalline state of the particle. For ODS, on the otherhand, closer the particles, more effective is the overlapping and hence the attractive force. It is clear from the expression for ODS that small

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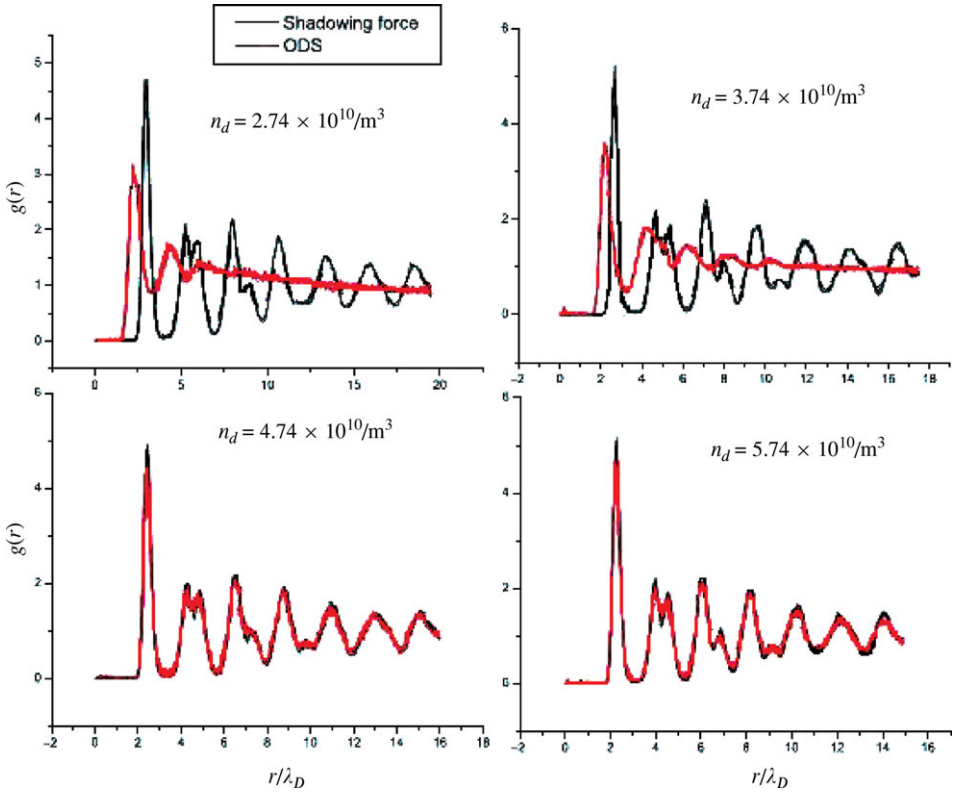


Figure 3. (Colour online) Plot of $g(r)$ vs. r/λ_D for different values of dust number density.

value of n_d results in large inter-particle distance and hence the small Yukawa-ODS potential. Simulation results also show that the average inter-particle distance for the case $n_d = 5.74 \times 10^{10}$ m^{-3} is 1.6×10^{-4} m. It may be inferred that beyond $a = 1.6 \times 10^{-4}$ m, shadow force dominates over ODS and becomes effective in Coulomb crystal formation. Both shadow and ODS potentials are very sensitive to the change in dust density.

Results of our simulation have been compared with the RDF plots obtained experimentally by Ramazanov et al. [13]. They determined RDF from experiments carried out in a DC glow discharge setup. The experimental curves by Ramazanov et al. have been compared with RDFs obtained for the normal Yukawa potential and the Yukawa-shadowing and ODS potentials in our simulation and results are plotted in Figs. 4(a)–(d).

The experimental data, on the basis of which simulations are performed, have been listed in Table 1.

From Figs. 4(a)–(d) it is clearly seen that RDF due to the Yukawa-shadowing potential is closer to the experimental curve than the curves due to the ODS potential or the Yukawa potential. The curve due to the Yukawa-shadowing potential is almost within the experimental errors (10–15 %) mentioned in Pamazanov's plots. It is also seen that for relatively small values of Γ and κ, the curves corresponding to experiment, the shadowing and ODS potentials almost overlap with each other.

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Table 1. Summary of simulational data.

Z_d	Dust number density	Electron number density	Ion temperature	Coulomb coupling parameter Γ	Screening constant κ
$Z_d = 2.1 \times 10^4$	$n_d = 1.4300 \times 10^{10}\text{m}^{-3}$	$n_e = 2.96 \times 10^{16}$ m^{-3}	$T_i = 203$ K	121	1.79
$Z_d = 2.1 \times 10^4$	$n_d = 3.940 \times 10^{10}$ m^{-3}	$n_e = 2.1 \times 10^{16}$ m^{-3}	$T_i = 168$ K	239	2.67
$Z_d = 2.1 \times 10^4$	$n_d = 1.0712 \times 10^{10}$ m^{-3}	$n_e = 2.4 \times 10^{16}$ m^{-3}	$T_i = 221$ K	68.50	1.69
$Z_d = 2.1 \times 10^4$	$n_d = 2.0995 \times 10^{10}$ m^{-3}	$n_e = 2.4 \times 10^{16}$ m^{-3}	$T_i = 240$ K	40.67	1.49

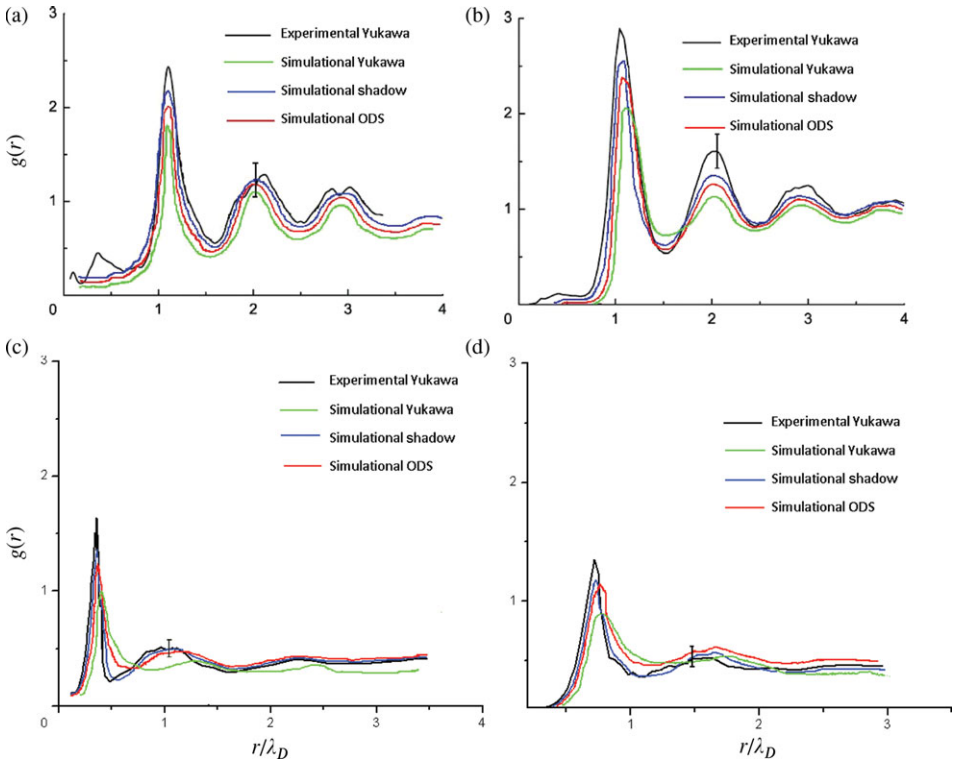


Figure 4. (Colour online) (a) Experimental and simulational $g(r)$ vs. r/λ_D. Plot for $\Gamma = 121$, $\kappa = 1.79$, $n_d = 14300$ cm^{-3}, $n_e = 2.96\text{e}^{10}$ cm^{-3}, $Z_d = 2.1\text{e}^4$, (b) Experimental and simulational $g(r)$ vs. r/λ_D. Plot for $\Gamma = 239, \kappa = 2.67, n_d = 3940$ cm^{-3}, $n_e = 2.1\text{e}^{10}$ cm^{-3}, $Z_d = 2.1\text{e}^4$, (c) Experimental and simulational $g(r)$ vs. r/λ_D plot for $\Gamma = 68.50, \kappa = 1.68, n_d = 10712$ cm^{-3}, $n_e = 2.4\text{e}^{10}$ cm^{-3}, $Z_d = 2.1\text{e}^4$, (d) Experimental and simulational $g(r)$ vs. r/λ_D plot for $\Gamma = 40.67, \kappa = 1.48, n_d = 20995$ cm^{-3} $n_e = 2.4\text{e}^{10}$ cm^{-3}, $Z_d = 2.1\text{e}^4$.

The deviation from the experimental curve is maximum for pure Yukawa potential. For $\gamma = 239$ and $\kappa = 2.67$, the deviation from experimental curve is found to be maximum (Fig. 4(b)). However, in almost all the cases, the results due to the Yukawa-shadowing potential agree with the experimental results. From this analysis it is clear that attractive potentials, like shadowing and ODS potentials, play a major role in determining crystal structure. Consideration of the Yukawa-shadowing potential or

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the ODS potential leads to better agreement with the experimental results rather than mere the Yukawa potential.

4. Conclusions

In this paper, we have compared the effect of attractive ODS and shadowing potentials on structure of 2D strongly coupled dusty plasma. Our results have clearly showed that both ODS and shadowing potentials equally dominate for small values of screening parameter κ and large values of dust density n_d. On the other hand, the shadowing potential plays a dominating role over the ODS potential for large values of screening parameter κ and small values of dust density n_d. For relatively large values of κ, the shadowing potential can dominate the Yukawa repulsive potential and the ODS attractive potential. For a dusty system considered here, it is seen that crystal structure is no longer maintained beyond an inter-particle distance $r_{ij} = 1.6029 \times 10^{-6}$m with Yukawa-ODS as the interaction potential. On the other hand, the Yukawa-shadowing potential maintains the crystal structure even beyond this distance. For longer inter-particle distance, shadowing attractive potential becomes more effective and cannot be ignored. The comparison between our simulation results and the experimental observations clearly reveal that the Yukawa-shadowing force is close to the real situation.

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