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Ground State Configurations of Two-dimensional Plasma Crystals under Long-range Attractive Particle Interaction Force

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Abstract

The configurational properties of two-dimensional clusters of charged dust particles in dusty plasma interacting with each other via a model potential with a short-range repulsion and a long-range attraction are investigated through the Monte Carlo simulation technique. The particles are confined by a harmonic potential. For the small number of particles, a hexagonal structure of the ground state changes into a shell configuration with increasing value of the attraction parameter α. For larger clusters, the increased attraction changes the defect locations and more particles energetically suit in the center of the cluster.

1. Introduction

Dusts in plasmas have been of interest in astrophysics for many decades [1,2]. Typically, dusty plasmas are multi-component plasmas consisting of charged micro-sized particles, electrons, ions, and neutral atoms or molecules. The dust grains are usually negatively charged because of the much higher mobility of electrons as compared to that of ions. The interaction between highly charged particles can lead to their structural ordering, e.g., "plasma condensation" and crystallization. This ordered solid phase of dusty plasmas was first predicted theoretically by Ikezi [3]. Since then different states of complex plasmas ranging from "gaseous plasmas" to "liquid plasmas" and "plasma crystals" were experimentally observed [4–9]. The latter can serve as an easily observable macroscopic model of similar structures on the atomic level. In a gas discharged plasma, the dusty grains can be electrically suspended in the sheath above the electrodes, where the gravity is exactly balanced by the electric force. In experiments, negatively biased electrodes are usually placed in order to keep dust grains from running away horizontally. In this way, under appropriate conditions, one can have a monolayer finite two-dimensional (2D) dusty plasma crystals [9–11]. In an infinite 2D crystal, the triangular lattice is the basic stable structure. The opposite case corresponds to a relatively small number of dusty grains. This type of classical systems consisting of a small number of grains interacting through repulsive interactions can be classified as the strongly coupled atom-like clusters. The structure of these finite 2D dusty plasma crystals has been analyzed in Refs. [10–15]. The spectral properties of 2D dusty clusters were investigated in Refs. [15–17]. The excitation of normal modes of 2D Yukawa system in laboratory complex plasmas was recently observed [18] and good agreement with the theoretical work was found [15].

The interdust interaction can be characterized by the repulsive Yukawa potential

$$U(r) = \frac{q^2}{4\pi\varepsilon_0 r}\exp\left(-\frac{r}{r_d}\right),$$

where q is the grain charge and r_d is the Debye length. The screened Yukawa potential $U(r)$ is believed to be a reasonable approximation when the distance between two grains is not large. However, one notes that if the entire system is neutral, then dust grains, which can contain a significant proportion of the negative charge of the system, necessarily see a highly positive background of ions, electrons, and neutral particles. The possible forces of attraction between dust grains may occur, e.g., due to direct bombardment by plasma, Coulomb scattering of plasma fluxes and neutral fluxes [19]. Taking the mutual attraction between dust grains into account, an analytical model can be used to investigate the behavior of a finite 2D dusty plasma crystals (or clusters) confined by a parabolic potential [17]. Even without external confinement, the attraction between dust grains may lead to 2D self-organized dust clusters by Molecular Dynamics (MD) simulation [20]. The structure of cluster of small number of dust grains was analytically studied in Ref. [17]. Thus it is of interest to extend this work to the case of a large number of dust grains to study how the attractive force affects the structure of dust crystals. To fulfill this purpose, we introduce a general potential function containing the long-range attraction [17],

$$U_{\text{new}}(r) = \frac{q^2}{4\pi\varepsilon_0 r}\exp\left(-\frac{r}{r_d}\right) - \alpha\frac{q^2}{4\pi\varepsilon_0 r}, \tag{1}$$

where α denotes the attraction strength.

In the present paper, we will study the structure of a finite 2D dust system with interaction potential U_{new} and external parabolic confinement by employing the method used in Refs. [18,21]. By comparing the energy of different configurations found, we investigate the structure of the ground state for different number of dust particles in the cluster.

2. Model system

The model system consists of N identically charged dust grains interacting through a model potential given in Eq. (1)

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and moving in a 2D plane where they are confined by a parabolic potential. The Hamiltonian is given as

$$H = \sum_{i>j}^{N} U_{\text{new}}(\boldsymbol{r}_{ij}) + \sum_{i}^{N} U_{\text{conf}}(\boldsymbol{r}_i), \tag{2}$$

where the confinement potential $U_{\text{conf}}(r) = \frac{1}{2} m\omega_0^2 r^2$ is circular symmetric and parabolic (m is the mass of the grain, ω_0 is the radial confinement frequency), r_i is the distance of ith grain from the center of the potential well and r_{ij} denotes the relative distance between grains i and j. Here the motion of the grains is restricted to (x, y) plane.

By normalizing the energy to E_0 and the distances to r_0 with

$$E_0 = \left[\frac{m\omega_0^2}{2}\left(\frac{q^2}{4\pi\varepsilon_0}\right)^2\right]^{1/3},$$

and

$$r_0 = \left(\frac{2}{m\omega_0^2}\frac{q^2}{4\pi\varepsilon_0}\right)^{1/3},$$

the Hamiltonian can be rewritten in a simple dimensionless form as [18]

$$H = \sum_{i=1}^{N} r_i^2 + \sum_{i>j}^{N}\left[\frac{\exp(-r_{ij}\kappa)}{r_{ij}} - \frac{\alpha}{r_{ij}}\right], \tag{3}$$

where $\kappa = r_0/r_d$ is the screening strength. For convenience, $\kappa = 5$ will be applied in all calculations and used throughout the article. Therefore, at zero temperature the behavior of this system is completely characterized by the number of particles N and the attraction strength α.

3. Numerical approach and results

Due to the presence of the confinement energy and the very complex inter-grain interaction, a complete description of the cluster system is complicated and cannot be obtained analytically. Therefore, we use the standard Metropolis algorithm for Monte Carlo simulation [22]. We start the calculation from the random initial distribution of the particles, and the real ground state configurations are then obtained during the MC equilibration run at zero temperature. In order to surely achieve the global minimum, the annealing process is utilized, i.e., the system was heated up and cooled down again at zero temperature.

The dusty cluster has a shell structure with the repelling particles held together by a circular harmonic potential [23]. The configuration is determined by these two competing effects, namely circular symmetry and triangular structure (Wigner lattice). In a finite system there is a competition between the bulk triangular lattice and the circular confinement potential which tries to force the particles into a ring like configuration. As we know, in Yukawa system, when $\kappa > 4$, the system transforms into a Wigner crystal and forms the triangular structure [14,15]. In this paper we will present the ground state configurations with the more general potential function containing the short-range repulsion and the long-range attraction.

For a small cluster (with small number of particles N), grains are packed into concentric shells. Depending on the total number of grains, the confining potential's detailed form, and mutual repulsion and attraction, a complicated structure with the inner triangular cores surrounded by the outer circular shells can be observed [24]. Table I shows the packing sequences of the ground states for $\kappa = 5$ and different attraction strength α for $N = 4 - 30$ particles. The parameter α was varied from 0 to 0.3. Here $\alpha = 0$ means that the particles interact through pure Yukawa potential, without the attractive force. The state (N_1, N_2, N_3, ...) corresponds to the state with occupation number N_i in the ith shell from the center. Steady increase number of particles causes the variation of N_i. Certain saturation number of particles for each shell exists and new shell appears when the existing shells are "full".

For $N = 3, 4$ and 5, polygons are formed. For $N = 6$, a grain appears at the center of the pentagon to minimize the energy and forms the two–shell structure. The states with (1,6), (1,7), (2,7) and (3,7) structures are found as N increases from 7 to 10. For small N, the attraction doesn't take effect on the packing of dust grains since the confinement dictates the favorable configuration. Comparing our results with those of Refs. [14,15], one can find that they coincide for $N \in \{3, 9\}$, but different when $N = 10$, probably due to the different screening strength κ. Table I clearly shows that the structure of the dust cluster with $N \leq 13$ is independent of the attraction strength α. Even when α becomes as high as 0.3, the structure of dust cluster is exactly the same as that for the case of $\alpha = 0$. This can be explained as follows: when N is small, the distance between any two dust grains is smaller than a critical value for which the attraction becomes comparable to the Yukawa repulsion. However, when N increases further, this critical distance can be

Table 1. *Mendeleev table for the particle packing sequences for* $N = 4-30$, *for different attraction parameter* α. *Here* α *is varied from 0 to 0.3 while Yukawa parameter* κ *equals 5.*

	$\alpha=0$	$\alpha=0.1$	$\alpha=0.2$	$\alpha=0.3$
$N=4$	4	4	4	4
$N=5$	5	5	5	5
$N=6$	(1,5)	(1,5)	(1,5)	(1,5)
$N=7$	(1,6)	(1,6)	(1,6)	(1,6)
$N=8$	(1,7)	(1,7)	(1,7)	(1,7)
$N=9$	(2,7)	(2,7)	(2,7)	(2,7)
$N=10$	(3,7)	(3,7)	(3,7)	(3,7)
$N=11$	(3,8)	(3,8)	(3,8)	(3,8)
$N=12$	(4,8)	(4,8)	(4,8)	(4,8)
$N=13$	(4,9)	(4,9)	(4,9)	(4,9)
$N=14$	(4,10)	(4,10)	(5,9)	(5,9)
$N=15$	(5,10)	(5,10)	(5,10)	(1,5,9)
$N=16$	(1,5,10)	(1,5,10)	(1,5,10)	(1,5,10)
$N=17$	(1,6,10)	(1,6,10)	(1,6,10)	(1,6,10)
$N=18$	(1,6,11)	(1,6,11)	(1,6,11)	(1,6,11)
$N=19$	(1,6,12)	(1,7,11)	(1,7,11)	(1,7,11)
$N=20$	(1,7,12)	(1,7,12)	(2,7,11)	(2,7,11)
$N=21$	(2,7,12)	(2,7,12)	(2,7,12)	(2,7,12)
$N=22$	(2,8,12)	(2,8,12)	(2,8,12)	(2,8,12)
$N=23$	(3,8,12)	(3,8,12)	(3,8,12)	(3,8,12)
$N=24$	(3,8,13)	(3,9,12)	(3,9,12)	(3,9,12)
$N=25$	(3,9,13)	(3,9,13)	(3,9,13)	(3,9,13)
$N=26$	(4,9,13)	(4,9,13)	(4,9,13)	(4,9,13)
$N=27$	(4,10,13)	(4,10,13)	(4,10,13)	(4,10,13)
$N=28$	(4,10,14)	(4,10,14)	(4,10,14)	(4,10,14)
$N=29$	(5,10,14)	(5,10,14)	(5,10,14)	(1,5,10,13)
$N=30$	(1,5,10,14)	(1,5,10,14)	(1,6,11,12)	(1,6,11,12)

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achieved in the α-range we investigate. For $N = 14, 15$ particles the ground state configuration will change when increasing α (see Table I). The situation changes again for $N = 16$–18, since those configurations are very stable because of symmetry and cannot be influenced by increased attraction. For $N \in \{19, 20, 24, 29, 30\}$, the parameter α alters again the configurations, but $N = 21$–23 and 25–28 are the "magic" numbers and the stable symmetric structures are not changed by the attractive force.

To summarize the Table I, the attraction parameter α can influence and change only the configurations with non-magic number of particles. The ground state is changed in a way that the hexagonal lattice rounds–up into a more shell-like structure, and the radius of the system decreases due to the attraction between the particles. This transition is illustrated in Fig. 1 for $N = 19$ particles. In Fig. 1(a), when α is zero, one can see the perfect hexagonal structure, which is in agreement with Ref. [15]. This structure resembles the Wigner lattice which is formed by the strongly coupled interaction. When increasing α, the size of the system reduces, the triangular lattice is replaced by a ring structure and one particle from the outer shell fits in the central region, changing the configuration, size and the shape of the cluster in the ground state (see Fig. 1(b–c)).

Figure 2 shows that the energy and the radius of the cluster (see the inset) for $N = 19$, as a function of the attraction parameter α. As explained before, the radius monotonically decreases with increased attractive force. Since the distance between particles decreases, one could naively expect that the short-range Yukawa repulsion should prevail and that the total energy should be positive. However, the attraction increases faster with increasing α than the repulsion and the total energy decreases almost linearly (see Fig. 2).

For the larger systems, we use the defect theory to get a better understanding of the topological nature of the cluster structure. When $\alpha = 0$ the configuration is similar to the case of pure Coulomb system ($\kappa = 0$ and $\alpha = 0$), and the cluster has the hexagonal structure in the central region with the ring structure on the edge [23]. We make use of the Voronoi construction [25] for the cluster structure (for detailed description see Ref. [24]). We observed two kinds of defects in the Yukawa system, i.e. dislocations and disclinations. A dislocation is a pair of two disclinations consisting of a defect with 5-fold (−) and a defect with 7-fold (+) coordination number. The net topological charge

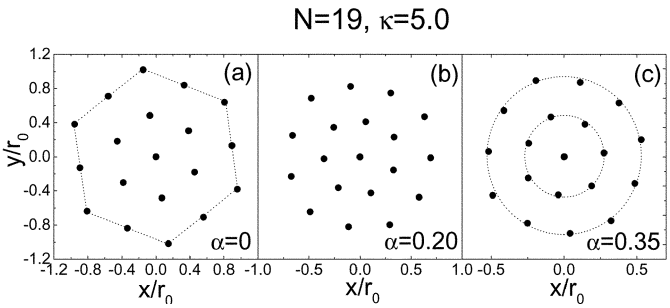

Fig. 1. The ground state configurations for $N = 19$ particles with increasing attraction between the particles, for attraction parameter (a) $\alpha = 0$, (b) $\alpha = 0.2$, and (c) $\alpha = 0.35$. The dotted curves are guides for illustrating the hexagonal (shell) structure of the ground state.

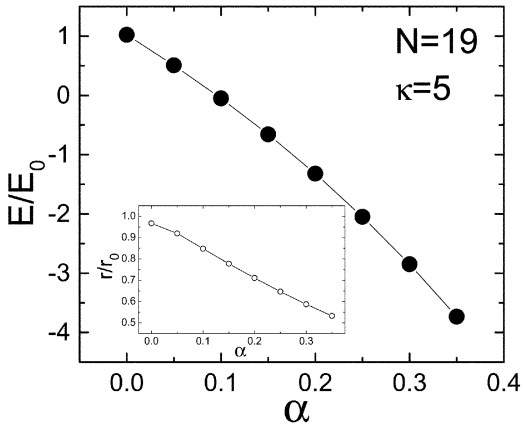

Fig. 2. The energy and the radius of the $N = 19$ cluster as function of the attraction parameter α.

$N_- - N_+$ always equals six, as was already demonstrated in Refs. [14,24].

In Fig. 3, the Voronoi structures are shown for $N = 100$ for different α values. Figs. 3(a,b) show the structure of the ground state for $\alpha = 0$ and $\alpha = 0.1$, respectively. In both cases, six geometry-induced defects appear in those configurations, and they are not influenced by attraction between particles, except for the fact that the system is reduced. Only six 5-fold disclinations are present, since the outermost ring contains 24 particles, which is a multiple of the topological charge. This situation has been investigated earlier in the pure Coulomb system [24]. However, for $\alpha > 0.1$, the location of defects is strongly influenced by increase of the attraction. For Yukawa system ($\alpha = 0$), the defects are located in the transition region between the triangular lattice in the center of the cluster and the shell structure at the edge. Now, for increased α, defects move towards the center as result of three competing forces, namely, confinement, Yukawa repulsion and α-attraction. The cluster patterns are determined by the need to balance the tendency to form a triangular lattice against the formation of a compact circular shape. When $\alpha = 0.2$, one can see the

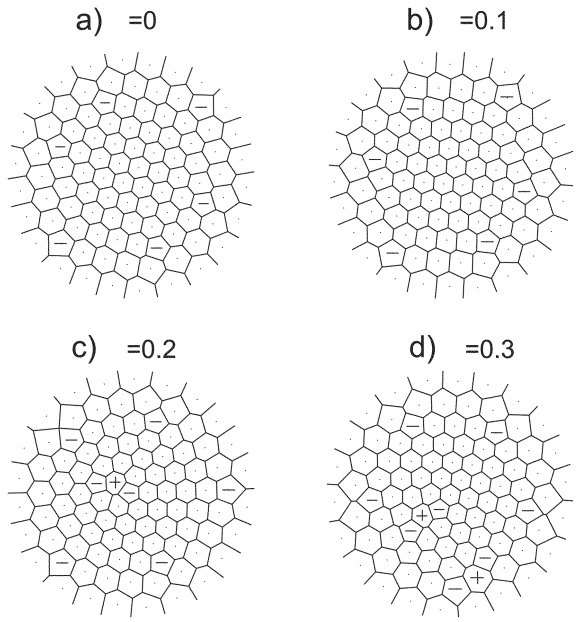

Fig. 3. The ground state configurations for $N = 100$ particles for different values of α. The Voronoi structure is shown and the defects (i.e., disclinations) are indicated by "+ for a 7-fold", and by "− for a 5-fold", coordination number. The dots indicate the positions of the particles.

appearance of defects not only at the edge but also in the central region (see Fig. 3(c)). In recent theoretical studies, the center of the cluster was shown to be a forbidden defect area [14,24] when the long-range attraction between particles is not taken into account. It should be noted that the number of particles in the outermost ring changes from 24 to 23, which also jeopardizes the theory of geometrically induced defects in the case of purely repulsive particle interactions. One particle moves to the center because of the attractive force which increases the total number of disclinations to 8. For $\alpha = 0.3$, one more particle energetically suits to the central region, the outmost ring has only 22 particles, one more dislocation appears, increasing the total number of defects to 10.

4. Conclusion

We presented the ground state configurations of two-dimensional (2D) clusters of charged dust grains in dust plasma. The results were obtained numerically, using a model in which the dust particles are confined by a harmonic potential and interact with each other via the Yukawa potential with the short-range repulsion and the long-range attraction (with control-parameter α). With increased attractive force, different structures are found and analyzed. When increasing α, in the case of small clusters, particles change their formation from the triangular lattice to the shell structure. For larger cluster, the attractive force fits more particles in the central region which increases the number of dislocations and more defects energetically suit further from the edge of the cluster.

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