Properties of two-dimensional dusty plasma clusters.

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Two-dimensional classical cluster of particles interacting through a screened Coulomb potential is studied. This system can be used as a model for “dusty particles” in high-frequency discharge plasma. For systems consisting of \( N = 2 - 40 \) particles and confined by a harmonic potential we find ground-state configurations, eigenfrequencies and eigenvectors for the normal modes as a function of the Debye screening length \( R_D \) in plasma. Variations in \( R_D \) cause changes in the ground-state structure of clusters, each structural rearrangement can be considered as a phase transition of first or second order (with respect to parameter \( R_D \)). Monte Carlo and molecular dynamics are used to study in detail the melting of the clusters as the temperature is increased. By varying the density and the temperature of plasma, to which the particles are immersed, one can modulate thermodynamical properties of the system, transforming it in a controllable way to an ordered (crystal-like), orientationalally disordered or totally disordered (liquid-like) states. The possibility of dynamical coexistence phenomena in small clusters is discussed.

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I. INTRODUCTION

Small charged particles of ”dust” are rather common systems, and are observed on different scales and in different environments: clusters of dust in the interstellar medium, charged colloidal suspensions, ordered structures in the gas discharge used in thermal processing of materials are examples of such systems. At present much attention is paid to experimental investigation of the properties of ”dusty plasma” which is a system of small micrometer particles in a high frequency gas discharge. One of the main reasons of this attention paid to the artificial objects like this one is the ability of a direct observation of their static and dynamical properties. The study of dusty plasma crystals and liquids ”in vitro” which is being carried out in a number of laboratories around the world is of a great importance for understanding the plasma properties and is a powerful tool for the examination of melting, annealing and formation of defects of different kinds.

Small particles immersed in a plasma may acquire large (up to \( 10^5e \)) charges \( Ze \) due to high mobility of plasma electrons. The presence of plasma screening modifies the Coulomb interparticle interaction and, with a good precision, the system can be described as a system of particles interacting with a Yukava-type pair potential. Here we consider two-dimensional (2D) clusters of dusty particles confined by an external harmonic potential of strength \( \alpha \). It is obvious that it is 2D system that realizes when one consider particles of ‘dust’ immersed in a plasma discharge cloud with the transverse dimension higher than the Debye screening length. The energy of the system has the form:

\[
E = \left( Ze \right)^2 \sum_{i<j}^N \frac{\exp(-|r_{ij}|/R_D)}{|r_{ij}|} + \alpha \sum_{i=1}^N |r_i|^2
\]

The Debye screening length in plasma is determined as \( R_D = (4\pi q_i^2 n_i/k_b T_i + 4\pi e^2 n_e/k_b T_e)^{-1/2} \) where \( q_i, n_i \) and \( T_i \) are the charge, mean density and temperature of plasma ions and \( e, n_e, T_e \) are that of plasma electrons respectively.

The energy of a cluster, being written in dimensionless units \( r_0 = (Ze)^{2/3}/\alpha^{1/3} \) for distances and \( E_0 = \alpha r_0^2 \) for energies becomes:

\[
E = \sum_{i<j}^N \frac{\exp(-\gamma |r_{ij}|)}{|r_{ij}|^3} + \sum_{i=1}^N |r_i|^2
\]

where the dimensionless parameter \( \gamma = r_0/R_D \) defines the range of the pair interaction potential. From (2) one can see that the thermodynamic state of a cluster of a given number of particles is determined by two dimensionless parameters: the inverse dimensionless screening length \( \gamma \) and the dimensionless temperature of ”dusty” grains \( \Theta = k_b T/E_0 \). The range of interaction between particles in a cluster \( 1/\gamma = r/R_D \) is controlled by the density and the temperature of a plasma (see above).

In this paper we consider the properties of two-dimensional (2D) clusters as a function of the number of particles \( N < 40 \), the screening length \( 1/\gamma \) and the temperature \( \Theta \). We show (see Sec. I) that the change in the screening length (i.e. in parameter \( \gamma \)) causes rearrangements of the ground-state structure of the cluster at a set of points \( \gamma^* \),
such structural transitions can be treated as phase transitions of the first or the second order with respect to parameter γ. In Sec. II we apply molecular dynamics (MD) and Monte Carlo (MC) simulations in a canonical ensemble in order to study the thermodynamic properties of small clusters. We show that in clusters of rather a small number of particles and at a small enough plasma screening (at γ < 10), as the temperature is increased, the orientational disordering happens first, i.e. shells rotate with respect to each other by losing their mutual orientation order. At more higher temperatures a total disordering of cluster shells takes place.

II. GROUND-STATE CONFIGURATIONS

Ground-state configurations (see Table 1 and Fig. 1-3) of the system (2) have been found with the help of the following methods: 1) The modified Newton method [8]; 2) The combination of ”random search” and ”gradient search” methods [9]. For the results to be more reliable, all configurations discussed below have been independently obtained by both of these methods. Of course, no one of the present methods of the minimization of a multidimensional function is able to guarantee that the configuration obtained is a global minimum one. To overcome this difficulty we have used up to 200 randomly distributed initial configurations. This approach have also enabled us to investigate both the local minima and their caption regions (i.e. ”specific weights” of local minima).

At γ ≪ 1 model (2) describes the Coulomb cluster in a harmonic trap, the system that have been actively studied both experimentally [10,11] and with the use of computer simulations [12], [8,13]. In particular, the calculations carried out before have revealed that particles in small finite systems arrange themselves into shells. An analysis of shell structures for different number of particles N carried out before have revealed that particles in small finite systems arrange themselves into shells. An analysis of shell structures for different number of particles N carried out before have revealed that particles in small finite systems arrange themselves into shells. An analysis of shell structures for different number of particles N carried out before have revealed that particles in small finite systems arrange themselves into shells. An analysis of shell structures for different number of particles N carried out before have revealed that particles in small finite systems arrange themselves into shells.

The presence of parameter γ which determines the range of the pair potential enables one to investigate the influence of this range on the structures and properties of clusters. The fact that cluster structure depends on the range of interaction potential becomes obvious from Table 1 in which some ground-state configurations for 2D clusters in a harmonic trap are presented.

As the value of parameter γ changes, rearrangements of ground-state structure take place, each point γ* of any of these changes can be treated as a point of phase transition of one kind or another. Following by the approach used in work [13], the order of these phase transitions can be determined from the plot of the ground-state energy E(γ), the discontinuity in the n-th derivative of E(γ) with respect to parameter γ corresponds to the phase transition of n-th order. Another way to determine the order of the phase transition is to analyse the behaviour of eigenfrequencies ωi(γ), i = 1,2N for the normal modes: first order transition takes place at the point γ* at which any of the eigenfrequencies exhibits a jump while softening of any of the eigenfrequencies (when it becomes zero) testifies about second order phase transition.

The eigenfrequencies of the cluster of N = 10 particles vs. screening parameter γ ∈ [0, 10] are presented in Fig. 1. At points γ ≈ 1.4 and γ ≈ 8.2 of first order transitions the eigenfrequencies exhibit jumps that are clearly seen. From Fig. 1b one can see that with a decrease in the interaction range first, at γ ≈ 1.4, the distribution of particles throughout shells changes and the configuration typical for the Coulomb interaction is replaced by one appropriate to the dipole cluster of 10 particles (\{2,8\} → \{3,7\}). Further reduction in the screening radius transforms (at γ ≈ 8.2) the cluster to the most ”packed” state \{2,8\} which is characteristic of a system of hard spheres.

The point of the first order phase transition γ* can be determined as the point, where the energies of ground-state configurations for 2D clusters in a harmonic trap are presented. The point of the first order phase transition γ* can be determined as the point, where the energies of ground-state configurations for 2D clusters in a harmonic trap are presented. The point of the first order phase transition γ* can be determined as the point, where the energies of ground-state configurations for 2D clusters in a harmonic trap are presented.

In Fig. 2 the ground-state energy of a cluster of 33 particles are given. At γ ≈ 3.751 the first derivative of the ground-state energy with respect to parameter γ is discontinuous (see inset of Fig. 2a). Investigation of cluster configurations shows that the numbers of particles in two outer shells change here as \{1,6,11,15\} → \{1,6,12,14\}. In the vicinity of the transition point γ* ≈ 3.751. From this figure one can see that the configuration of the global minimum at γ < γ* corresponds to a local one at γ > γ*.

One can see that in the cluster of 37 dipole particles one of the particles is between the second and the third shell to form an interstitial (analogous to the Frenkel defect in crystals) and to make the division of the ground-state configuration into shells ambiguous [8]. The 'dusty' cluster of 37 particles is supposed to exhibit a rich variety of structural rearrangements while varying γ. The investigation of this cluster at different values of screening strength has revealed four phase transitions in the region γ ∈ [0,1.6] (see Fig. 3a), namely two second order transitions (at γ ≈ 0.78 and γ ≈ 1.22) and two first order transitions (at γ ≈ 0.52 and γ ≈ 1.34).

From Fig. 3a on can see that the number of particles in the outer shells changes at γ ≈ 0.52. It is worth while to note that a distinctive feature of the first order phase transition is the abrupt change in the cluster structure,
Usually, this peculiarity exhibits as the change in the distribution of particles throughout shells (like that one can observe for the clusters of 10 and 33 particles, see Fig. 1,2). This very change takes place at $\gamma = 0.52$ for the cluster involved. However no apparent changes in structure of the cluster are seen at the point $\gamma \approx 1.34$ of the first order phase transition. More detailed study have shown that at this point there exist a rotation of the third shell with respect to the fourth one. This is illustrated in Fig. 3b which presents the mutual orientational order parameter $g_{s_1s_2}$ of different pairs of shells $\{s_1, s_2\}$, the value which is very sensitive to the changes in mutual orientation of cluster shells.

Subsequent increase in the parameter $\gamma$ leads to the realization of two other first order transitions which are depicted in Fig. 3b. In the first of them (at $\gamma \approx 7.015$) one of the particles implants between the second and the third shells (see Table 1 and the discussion above). The corresponding transition can be written as $\{1,7,13,16\} \rightarrow \{1,6,11,12,17\}$. At $\gamma > 19$ the cluster becomes well - faceted and has the most symmetrical structure $\{1,6,12,18\}$. Note that in this region of $\gamma$ the minimal nonzero eigenfrequency $\omega_{\min}$ corresponds to twofold degenerate vibrations of the whole cluster in the harmonic trap with the frequency $\omega_{\min} = \sqrt{2}$. Further decreasing in the range of the pair potential does not lead to any structural rearrangements.

The study of Coulomb and dipole clusters have shown that the basis for most configurations is provided by different parts of 2D hexagonal lattice $\mathbb{Z}^2$. When describing and analyzing the properties of such configurations it is suitable to introduce into consideration the ”crystal shells” $Cr_i$ that are concentric groups of nodes of ideal 2D crystal with $c$ nodes placed in the center of these groups. Obviously, in view of the axial symmetry of the confinement potential, we can concentrate on a finite number of the most symmetrical crystal shells which, by the number of particles in the center of the system, can be divided into the following groups: $Cr_1$, $Cr_2$, $Cr_3$, $Cr_4$. With the help of the crystal shell concept we have found that changes in the ground state structure of “dusty” clusters, as parameter $\gamma$ is increased, comes in such a way, as to fill the maximal number of crystal shells.

III. PHASE TRANSITIONS

One of the distinctive peculiarities of small clusters is the existence of two stages of their disordering: an intershell (orientational melting of shells $s_1$ and $s_2$ at the temperature $\Theta_{s_1s_2}$) and a radial disordering (total melting at temperature $\Theta_f$). The analysis of eigenfrequencies shows that the clusters with the small values of lowest nonzero eigenfrequencies $\omega_{\min}$ have the eigenvectors corresponding to mutual rotations of shell clusters. Such clusters have low temperatures $\Theta_{s_1s_2}$ of intershell disordering. It is obvious that changes in the cluster structure caused by variations in the control parameter $\gamma$ lead to the modulation of the temperatures of both orientational $\Theta_{s_1s_2}$ and total $\Theta_f$ disordering. Moreover, the phenomenon of the orientational disordering may disappear at all if the cluster has a well packed structure. The results of our simulations have proved this suggestion.

The dependencies of the mutual orientational order parameter $g_{21}(\Theta)$ for two-shell cluster of $N = 10$ particles at several values of parameter $\gamma$ are given in Fig. 4a. It is evident that $g_{s_1s_2}$ drops to zero at the point of relative disordering (mutual rotation of shells $s_1$ and $s_2$) $\{3\}$. One can see from Fig. 4a that the change in the system configuration $\{2,8\} \rightarrow \{3,7\}$ which occurs at $\gamma \approx 1.4$ (see Fig. 1) leads to a sharp decrease in the orientational disordering temperature: $\Theta_{21}(\gamma < 1.4) \approx 1.3 \cdot 10^{-4} \rightarrow \Theta_{21}(\gamma > 1.4) \approx 0.7 \cdot 10^{-5}$.

The cluster is well - packed in the region $\gamma > 8.2$ (see Fig. 1) and that is why it does not experience the orientational melting, when an increase in the temperature leads directly to the interchange of particles between shells at $\Theta \approx 10^{-3}$. This can be seen from the analysis of radial square deviations $u_\gamma^2$:

$$u_\gamma^2 = \frac{1}{N} \sum_i \left[ \langle |r_i|^2 \rangle - \langle |r_i| \rangle^2 \right]$$

(3)

The dependence $u_\gamma^2(\Theta)$ is given in Fig. 4b, also shown are analogous curves at $\gamma = 1$ and $\gamma = 2$. One can see that even the slightest variation in the value of control parameter $\gamma$ may change the temperature of the total melting up to orders.

The changes in the interaction potential lead to the modification of the structure of the energy surface which determines the type and the distinctive features of the phase transitions. For this reason, one can suppose that at some values of the parameter $\gamma$ the system can have very interesting thermodynamic properties. In Fig. 5a the dependence of the radial square deviations $\{3\}$ of four - shell cluster of $N = 33$ particles at $\gamma = 3.76$ is given. The graph has a number of plateaus located in different temperature intervals. A detailed investigation has shown that the regions of a sharp increase in $u_\gamma^2$ correspond to the radial disordering of different pairs of shells: particles start to interchange between the third and the fourth shell at temperature $\Theta_{34}^I \approx 5 \cdot 10^{-4}$ and between the second and the third – at $\Theta_{23}^I \approx 0.005$. The total melting of the cluster takes place at $\Theta_f^I \approx 0.01$. 

3
Some useful information about the character of the disordering considered can be obtained by exploring the local minima distribution $\rho(E_{\text{loc}})$. In order to estimate this histogram, at each measurement time point we have performed several hundreds of gradient search iterations to find the nearest local minimum with the energy $E_{\text{loc}}$.

In Fig. 5b the local minima distribution of the system of 33 particles at $\gamma = 3.76$, $\Theta = 10^{-4}$, $\Theta = 8 \cdot 10^{-3}$ is shown. In an entirely ordered state (at $\Theta = 10^{-4}$) the system lives in the vicinity of the global minimum (with energy $E = 64.795946$ and the structure $\{1, 6, 12, 14\}$). At $\Theta = 8 \cdot 10^{-3}$ the cluster can be also found at the lowest local minima distribution $E^{(1)} = 64.795975$ with the configuration $\{1, 6, 11, 15\}$ (see Fig. 2b).

Considering the results stated above one can conclude that the first disordering seen in the temperature interval $[10^{-4}, 10^{-3}]$ (see Fig. 2) corresponds to the nonzero probability of the cluster to be found in the state $\{1, 6, 11, 15\}$ which is metastable at the given value of the parameter $\gamma$. Such changes in the distribution of particles throughout shells demand the overcoming of potential barrier that, knowing about large specific weights of both "ground" and "excited" states, allows one to treat this temperature interval as that of the dynamical coexistence of two cluster forms $\{1, 6, 12, 14\} \rightleftharpoons \{1, 6, 11, 15\}$.

**IV. CONCLUSIONS**

In this letter we have presented the results of a study of finite "dusty plasma" particle system. As a function of Debye screening length $R_D$ (for the particle charge in the plasma) we have found ground-state configurations of clusters consisting of $N \leq 40$ particles, their normal modes eigenvalues and the corresponding eigenvectors. The clusters undergo structural transitions which manifest itself as phase transitions of first or second orders with respect to parameter $R_D$. At points of first order transitions cluster coordinates experience jumps which lead either to the change in the shell distribution or to the rotation of some shells relative to each other. At points of second order transitions one of the eigenfrequencies softens and particle coordinates change continuously.

By varying $R_D$ (for example, by varying the temperature and the density of the plasma) one can modulate thermodynamic properties of the system and considerably change the temperatures of both the orientational and the total disordering. It have turned out that for some clusters, as the screening becomes sufficiently high, the disappearance of the orientational melting of different parts of the system takes place and an increase in the temperature leads straightway to the interchanges of particles between shells.

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the quantities $\psi_s$ and $g_{s_1s_2} = \psi_s \psi^*_s$ are analogous to the parameter $\psi_6$ and the correlation function $g_6(r)$ of infinite 2D systems, the softening of the correlation function $g_6(r) \to 0$, $r \to \infty$ corresponds to the relative orientational disordering of remote parts of the system (with the absence of the translational order).

Table 1.

Ground-state shell structures \{N_1, N_2, ...\} for dipole, Coulomb and logarithmical clusters of N particles confined in a harmonical potential.

| N   | Dipole cluster | Coulomb cluster | Logarithmical cluster |
|-----|----------------|-----------------|-----------------------|
| 9   | 2.7            | 2.7             | 1.8                   |
| 10  | 3.7            | 2.8             | 2.8                   |
| 11  | 3.8            | 3.8             | 3.8                   |
| ... | ...            | ...             | ...                   |
| 32  | 1.6,12,13      | 1.5,11,15       | 4.11,17               |
| 33  | 1.6,12,14      | 1.6,11,15       | 5.11,17               |
| 34  | 1.6,12,15      | 1.6,12,15       | 1.5,11,17             |
| ... | ...            | ...             | ...                   |
| 36  | 1.6,12,17      | 1.6,12,17       | 1.6,12,17             |
| 37  | 1.6,1,13,16    | 1.7,12,17       | 1.6,12,18             |
| 38  | 2.8,13,15      | 1.7,13,17       | 1.6,12,19             |

Fig. 1.

Eigenfrequencies (a) and the lowest nonzero eigenfrequency $\omega_{\text{min}}$ (b) of the ‘dusty’ cluster of 10 particles. Inset: ground state configurations in three different regions of control parameter $\gamma$.

Fig. 2.

Cluster of 33 particles. a) The first derivation of the cluster ground energy with respect to $\gamma$. In the inset the region of the first order phase transition is shown on an enlarge scale. b) Energies and configurations of the lowest local minimum (with the energy $E^{(1)}$ measured from the ground state energy $E$) of the cluster in the region of the phase transition.

Fig. 3.

Cluster of 37 particles. a) The lowest nonzero eigenfrequency $\omega_{\text{min}}(\gamma)$ and mutual orientational order parameter of different pairs of shells $g_{s_1s_2}(\gamma)$. b) The regime of strong plasma screening. Eigenfrequency $\omega_{\text{min}}$ corresponds at $\gamma > 19$ to the motion of the cluster at a whole in the confinement.

Fig. 4.

Two - shell cluster of 10 particles. a) Thermodynamical mean of the mutual orientational order parameter $< g_{21} > (\Theta)$ at different values of $\gamma$. b) radial mean - square deviations od particles vs. temperature $u^2_r(\Theta)$.

Fig. 5.

Four - shell cluster of 33 particles a) radial mean - square deviations. b) local minima distribution histogramm $\rho(E^{(\text{loc})})$ of the cluster in the ordered state (at $\Theta = 10^{-4}$) and at $\Theta = 8 \cdot 10^{-3}$, when there is an interchange of particles between the third and the fourth shells.
