Computer Simulation on Fine Particle Dynamics in a Plasma

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Abstract
Formation of Coulomb crystal structure, observed experimentally in discharge plasmas, is studied by a particle simulation in 2 and 3 dimensions. The simulation reveals the growth process of the Coulomb crystal structures in accordance with the experimental observation. The formation of structures, consisting of a finite number of fine charge dust particles, can be controlled by adjusting a confinement potential $U(r)$.

Keywords:
dust particle, Coulomb crystal, string state, 3-D Coulomb crystal

1. Introduction
Fine particles in plasmas are of current interest in plasma science and applications. The dynamics of fine particles in the presence of the external electric field has been studied using Langevin molecular dynamics simulations. The dust particles attain a negative charge $q_d$ of order of $10^4 - 10^6 e$ (electronic charge) and are a few microns in diameter. Crystallization of dust particles [1-3] has been observed to form through the interaction of Coulomb’s force acting on them. A study of Coulomb crystals is useful not only to the analysis for strong coupling plasma phenomena but also to the analysis of transition process between liquid and solid states. Liquid-solid phase transition is often expressed by a thermodynamic quantity known as the Coulomb coupling parameter $\Gamma$ which is defined as a ratio of the interparticle Coulomb potential energy to the thermal energy. A solid-liquid state phase transition is predicted by the value $\Gamma_c \approx 170$. For $\Gamma > \Gamma_c$, the phase of a system is a solid. Solid-liquid phase transition, so called 'melting of crystal', has been investigated by V.A. Schweigert for the Langevin molecular dynamics simulations [4,5]. Their analysis shows the transition governed by a parameter which characterizes friction of the particle with neutral gas. Their results agree well with experimental observations.

In the present study we analyze a growth process of the Coulomb crystal of fine particles in electrostatic field as was observed in experiments. In a system in consideration, dust particles in an ion sheath locate in a horizontal plane forming a 2D crystal structure, with only a few particles in a vertical $z$-direction. However, a three-dimensional crystal structure extending in the $z$-direction has also been observed by controlling the profile of the horizontal potential and the profile of the potential in the $z$-direction. The growth process of the crystal could be different in 2D and 3D solid states. Thus it was essential to carry out particle simulations for both 2D and 3D systems to understand the mechanism of the growth process. The present study simulates the experimental conditions for the Coulomb crystal formation and examines whether the potential model used in our simulation is suitable or not.

2. Simulation Model
We consider the growth process of crystallization of dust particles formed in a horizontal plane. In the

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experiment, a two dimensional structure was observed by introducing dust particles into a horizontal confining potential through the hole of an electrode. This situation can be reproduced by a comparatively simple model. The equation of dust particle motion in a plasma may be written as

\[
M \frac{d^2 \mathbf{r}_i}{dt^2} = F_e - \mu \frac{d\mathbf{r}_i}{dt} + \nabla U(\mathbf{r}_i),
\]  

(1)

where \( M \) is the mass of the dust particle, \( F_e \) is the electrostatic interaction force of the dust particles, \( \mu \) is the friction coefficient of the particles with neutral gas, and \( U \) is the external confining potential. The structure of the dust crystal in its equilibrium state is determined by the potential \( U \).

In our simulation model, the electrostatic Coulomb interaction force acting on a dust particle is given by

\[
F_e = \frac{q_{\text{dust}}^2}{4\pi\varepsilon_0} \sum_{j \neq i} \frac{\mathbf{r}_j - \mathbf{r}_i}{|\mathbf{r}_j - \mathbf{r}_i|^3}.
\]  

(2)

Here, we are focusing on the structure of crystal and have neglected the Yukawa potential which includes the screening effect. The external potential for the experimental system may be written as

\[
U = \alpha r_i^2
\]  

(3)

where \( r_i \) is the i-th particle radial distance and the coefficient \( \alpha = 3.0 \times 10^3 \) eV/cm\(^2\). Other parameters are chosen to satisfy the experimental conditions. The radius of a dust particle is 5.0 \( \mu \)m and the mass ratio of the dust particle to the proton is \( M_{\text{dust}}/M_{\text{proton}} \approx 3.75 \times 10^{12} \). The charge of the dust particle is \(-1.6 \times 10^{-14} \) e, the distance between the dust particles is a few hundreds \( \mu \)m, and the temperature is \( T_{\text{dust}} = 0.01 - 0.1 \) eV. The friction coefficient of the particles with neutral gas is calculated for Ar gas pressure 260 mTorr, and the \( \mu \) is estimated to be on the order of 0.02 - 0.1.

3. Coulomb Crystal Formation of Dust Particles in 2-Dimensional Systems

The simulation results are shown in Fig. 1, where locations of the individual dust particles are shown in the x-y plane. A particle is injected into the confining potential and the motion of the particle is calculated until it will stop moving. And then, we inject another particle and calculate the motion until it stops. The computation continues its process with many particles. The scale for both the x and y axis is in cm. The figures, from the top left progressing to the bottom right, show particle behavior of 4, 7, 9, and 113 dust particles, respectively. Here, it was observed that the added dust particles kept their equilibrium positions, and that they expanded to the horizontal plane forming the Coulomb crystal. As far as the growth process of the crystal is concerned, the simulation agrees well with the experimental observation. Thus, we see that our simulation recovers experimental findings well. It is confirmed that a growth process of the Coulomb crystal of a few dust particles can be controlled by the external potential as was described by eq. (3).

3.1 Growth Process of the String Structure in a 3-Dimensional System

The string state, dust particles mostly expanded to the z-direction as shown in Fig. 2 (left), was observed in the experiment. Such a string formation was achieved by controlling the potential profile not only in the horizontal direction but also in the z-direction. In order to study such a state, we carried out three-dimensional simulations taking the vertical potential into account on top of the gravitational effect. We assumed the radial potential, as was used in 2-dimensional systems, \( U(r) = \alpha r^3 \), and the z-axis direction potential as

\[
U(z) = \beta(z(i) - z(0))^2.
\]  

(4)

Here, \( z(i) \) is the position of the z-component of the i-th particle and \( z(0) \) is the equilibrium position balanced by

Fig. 1 Examples of the simulation results for two dimensional systems. In the right bottom figure, we can observe the fully formed dust particle crystal.
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Fig. 2 The left figure shows the experimental result of the three dimensional string. The right figure is the simulation result for 40 particles. Here, we observe that the formation of the Coulomb crystal in the simulation is similar to the one observed in the experiment.

the gravity and the electrostatic force. We set the coefficient \( \alpha = 6.0 \times 10^5 \text{ eV/cm}^2 \) and \( \beta = 1.5 \times 10^5 \text{ eV/cm}^2 \), to reproduce the potential profile of the experiment [6]. Figure 2 (right) shows the simulation result in 3-D. It shows that the strings have asymmetric structures in horizontal and z directions in three-dimension. The three-dimensional Coulomb crystal similar to the experimental observation is thus successfully reproduced by our simulation.

4. Conclusions

The computer simulation has successfully reproduced the formation and growth processes of the Coulomb crystal of dust particles observed in the laboratory experiment. Here, the results are summarized as follows, (i) A growth process of the Coulomb crystal in two dimensional systems is described by the potential model \( U = \alpha r^2 \). (ii) The string state in three dimensional system is described by controlling the vertical potential similar to the radial potential profile. As for the Coulomb crystal on a few fine particles, our simulation could reproduce the experimental observations in both 2D and 3D.

In the recent experiments [6], it was observed that the trapped dust particles in an ion sheath are rotating either clockwise or counterclockwise under the action of the magnetic field. Details of the rotation mechanism are still unknown and the mechanism will be investigated by the computer simulation in future.

References