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Structure of spherical Yukawa clusters

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Abstract
Structure of clusters of Yukawa particles is analysed by simulations and theoretical approaches in an isotropic environment which can be realized under microgravity or by active cancellation of the effect of gravity. Yukawa particles model dust particles in dusty plasmas and such an environment is suitable to observe their inherent properties. At low temperatures, clusters are composed of spherical shells and, when scaled by the mean distance, the structure seems to depend almost only on the system size or the number of particles. The positions and populations of shells are given by simple interpolation formulae. It is shown that shells have an approximately equal spacing close to that of triangular lattice planes in the bulk close-packed structures. When the cohesive energy in each shell is properly taken into account, the shell model reproduces these structures of spherical Yukawa clusters to a good accuracy.

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1. Introduction

Systems of macroscopic dust particles in dusty plasmas provide us with an important example of strongly coupled plasma. The interaction between dust particles is approximately regarded as the Yukawa potential and they are often in the state of a finite crystal [1]. In the usual experiments, dust particles are under the influence of the gravity and their structure is characterized by almost uniformly spaced horizontal layers. Though other effects such as the ion flow and the thermophoretic force exist in dusty plasmas, these layered structures indicate that gravity plays the main role in their formation [2, 3]. It has been shown that the number of layers is determined by a competition between the mutual repulsion and the one-dimensional confining potential related to the balance of the gravity and the levitation [2, 3].

The intrinsic properties of a three-dimensional Yukawa system, however, will be observed in the isotropic environment. Recent experiments under microgravity [4, 5] and those with active cancellation of the effect of gravity [6] are expected to realize such an isotropic Yukawa system. Some results of simulations on an isotropic three-dimensional Yukawa system have been given by the authors [7]. We present here extensive analyses by numerical simulations and theoretical methods [8]. The results will become a reference when we have to take various effects such as ion flow into account.

2. Dust particles in dusty plasmas as confined Yukawa system

We start from a system in a volume V, composed of N_d dust particles of charge $-Qe$, N_e electrons of charge $-e$ and N_i ions of charge e, which satisfies the condition of charge neutrality $(-Qe)n_d + (-e)n_e + en_i = 0$, $n_d = N_d/V$, $n_e = N_e/V$ and $n_i = N_i/V$ being the densities of components. We take a statistical average over degrees of freedom except for dust particles in the adiabatic approximation and neglect the radius of dust particles and the effect of electron–electron, electron–ion or ion–ion correlation [9, 10].

We define the charge density in the system of dust particles $\rho(\mathbf{r})$ by

$$\rho(\mathbf{r}) = \sum_{i=1}^{N_d}(-Qe)\delta(\mathbf{r}-\mathbf{r}_i) + Qen_d. \tag{1}$$

Here the second term on the right-hand side is the contribution of electrons and ions which serves as the effective background charge for dust particles. Then we can rewrite the effective interaction between dust particles into the form [7, 8]

$$\frac{1}{2}\int\int_V \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'\frac{\exp(-|\mathbf{r}-\mathbf{r}'|/\lambda)}{|\mathbf{r}-\mathbf{r}'|}\rho(\mathbf{r})\rho(\mathbf{r}'), \tag{2}$$

where the subtraction of the self-interactions is implicitly assumed and λ is the screening length determined by electrons and ions. Dust particles are mutually interacting via the repulsive Yukawa potential and are confined in the potential field ϕ_{ext} exerted by the second term of $\rho(\mathbf{r})$,

$$\phi_{\mathrm{ext}}(\mathbf{r}) = -n_d(Qe)^2\int_V \mathrm{d}\mathbf{r}'\,\frac{\exp(-|\mathbf{r}-\mathbf{r}'|/\lambda)}{|\mathbf{r}-\mathbf{r}'|}. \tag{3}$$

The dusty plasma is expected to fill a space of some shape limited by the electrodes or the wall of the experimental vessel and we assume that our system occupies the inside of a sphere of radius R with the uniform density. This kind of isotropic environment may be realized in the environment of microgravity [4, 5] or by active cancellation of the effect of gravity [6].

3. Structure of spherical Yukawa clusters: molecular dynamics simulation

In our system of dust particles, we have three independent dimensionless parameters: the system size N_d, the strength of screening ξ, defined by $\xi = a/\lambda$, and the strength of coupling $\Gamma = (Qe)^2/ak_BT_d$, where the mean distance a is defined by $(4\pi/3)[N_d/(4\pi R^3/3)]a^3 = 1$ or $a = R/N_d^{1/3}$.

A snapshot of dust particle distribution is shown in figure 1(*a*). Here the positions of particles in the cylindrical coordinates (r, θ, z) are expressed by a projection onto the rz-plane. With the decrease of temperature, the boundary of distribution becomes sharper and eventually some shells are formed.

With the increase of N_d, the positions of shells move outwards and new shells appear at the centre one by one when N_d exceeds each critical value. We number the shells $1, 2, \ldots,$ from outside to inside and denote the radius of the mth shell by R_m. In figure 1(*b*), we plot

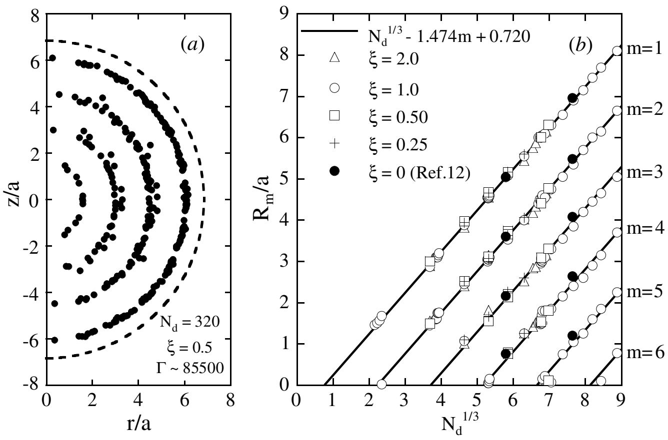

Figure 1. Results of simulations: (*a*) snapshot of particle distribution and (*b*) positions of shells (solid lines are an interpolation).

the values of R_m normalized by a, $R'_m = R_m/a$, for several values of ξ as functions of $N_d^{1/3}$. We also include the result for the pure Coulombic case of $\xi = 0$ [11, 12]. We observe that R'_m increases in proportion to $N_d^{1/3}$ and the critical values are approximately expressed as $N_{d,m}^{1/3} = a_1 m + a_2$;

$$R'_m(N_d) = N_d^{1/3} - 1.474m + 0.720 \qquad (N_d \geqslant 1.474m - 0.720), \tag{4}$$

the linear dependence of $N_{d,m}^{1/3}$ on m indicating equal spacing for the shells. The populations on shells are expressed by the formula

$$N_m = 4\pi \times 0.356\left(N_d^{1/3} - N_{d,m}^{1/3}\right)^2 = 4.48\left(N_d^{1/3} - N_{d,m}^{1/3}\right)^2. \tag{5}$$

4. Shell model

We now apply the shell model which has been successful in reproducing the ordered structures in ion traps with cylindrical symmetry [13] and in dust particles under one-dimensional confinement due to gravity [2, 3]. We start from the assumption that dust particles are organized into thin spherical shells and minimize the total energy of the system with respect to parameters determining the structure, the number of shells N_{shell}, shell radii $R_m (m = 1, 2, \ldots, N_{\text{shell}})$ and the shell populations N_m $(m = 1, 2, \ldots, N_{\text{shell}})$, under the condition $\sum_{m=1}^{N_{\text{shell}}} N_m = N_d$.

We first express the total interaction energy per particle by that of uniform spheres Ψ_{int}. When we minimize $\Psi_{\text{int}} + \Psi_{\text{ext}}$ with respect to N_{shell}, R_m, and N_m, including the energy due to confining potential Ψ_{ext}, we have the optimized structure given by an infinite number of shells or $N_{\text{shell}} \to \infty$ and $N_m \to 0$. As shown in previous analyses, it is thus essential in our shell model to take the cohesive (interaction) energy within the shell into account [2, 13].

Particles are in an ordered state on each shell and we approximate the cohesive energy per particle by that of a two-dimensional Yukawa lattice which is expressed by a dimensionless function e_{coh} as $(Qe)^2(\pi n_s)^{1/2} e_{\text{coh}}[1/\lambda(\pi n_s)^{1/2}]$. Here n_s is the surface density and e_{coh} is interpolated in [3, 14]. Including this cohesive energy Ψ_{coh}, we minimize $\Psi_{\text{int}} + \Psi_{\text{ext}} + \Psi_{\text{coh}}$ with respect to all parameters in the model, $\{R_m, N_m\}_{m=1,2,\ldots,N_{\text{shell}}}$ and N_{shell}. We observe that, with the increase of N_d, the optimum value of the total energy is realized with increasing N_{shell}. We also note that the results are almost independent of ξ for $0 < \xi < 2$.

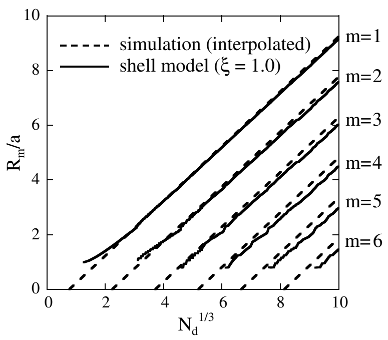

Figure 2. Positions of shells: shell model (solid lines) and simulations (dotted lines).

The overall agreement with simulation is satisfactory and our model reproduces the number, positions and populations of shells to a good accuracy as in previous cases [2, 13]. We plot the resultant positions of shells in figure 2, in comparison with those of simulations given by the interpolation (4). Our model gives somewhat smaller radii for inner shells. This may be due to our applying the cohesive energy of the planar system to spherical shells.

5. Conclusions

We have first shown that the condition of the overall charge neutrality in dusty plasmas leads to an effective external confining potential for Yukawa particles representing dust particles. Assuming isotropy of the system, we have observed the appearance of spherical shells at low temperatures. When scaled by the mean distance, the structure is almost independent of the strength of screening and shells have approximately equal spacing which corresponds to that of lattice planes in close-packed structures. Extending the shell model and including the cohesive energy within each sphere, we have shown that the structure can be reproduced to a good accuracy.

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