Inhomogeneity of a one-dimensional Yukawa system in a trap

V S Nikolaev\(^2,1\) and A V Timofeev\(^1,2\)

\(^1\) Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
\(^2\) Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

E-mail: vladiorussia@mail.ru

Abstract. A system of like charges interacting with a weak repulsive Yukawa potential and confined in a one-dimensional parabolic electrostatic trap is under consideration. It is shown that inter-particle distance in this system grows from the center of the structure to its periphery. The same effect takes place for the mean square displacement of particles from their equilibrium positions, which corresponds to the amplitude of thermal oscillations, and for the value of Lindemann parameter. This leads to different degrees of order for particles located at different distances from the center of the structure. This result might be important for the study of phase transitions in dusty, colloidal and one-component plasmas.

1. Introduction

A model of particles interacting with the repulsive potential of Yukawa under periodic boundary conditions was used to study many physical systems (atomic nucleus [1], one-component plasmas [2], dusty plasmas [3]) during the last century. Detailed research has been carried out into the phase diagram of this system [4], wave propagation in it [5] and its thermodynamic and structural properties [6]. Results obtained for the phase transitions of an infinite Yukawa system are often applied to Yukawa systems which are finite in size and are observed in experiments [7] (e.g., colloidal plasmas, dusty plasma crystals). Transferability of the phase diagram from an infinite system to finite Yukawa clusters is based on an assumption that observed Yukawa clusters are homogeneous and that global values of thermodynamic and structural parameters (temperature, pressure, average inter-particle distance, density, amplitude of thermal oscillations of particles around equilibrium positions in the ordered state) averaged by the entire structure are equal to their local values.

However, this assumption must be verified because few studies have been conducted regarding the effect of the restriction on the properties of Yukawa clusters. Most experimentally observed Yukawa structures are confined in an electrostatic trap which is either artificial [8] (created by a conducting ring in rf discharges in dusty plasma experiments) or natural [9] (caused by ambipolar diffusion of ions and electrons to a discharge tube wall in dc discharge experiments). Close to the center of the system which is supposed to be axially symmetric, the trap is well described by the parabolic dependence of potential on the displacement of a particle from the axis.
In this work, we are considering a system of particles that interact with the Yukawa potential and are attracted to the center of the system by a one-dimensional trap. At low temperatures, this system forms an ordered linear structure arranged along one axis. Two other dimensions are excluded from consideration in order to simplify the form of Newton equations for particles and qualitatively explain the reasons for observed effects. The increase of inter-particle distance and Lindemann parameter from the center to the periphery of the structure is discovered and studied.

The article is structured as follows: the second section is devoted to the detailed description of the considered model. In the third section, an analytical solution of equilibrium equations accounting only the interaction of particles with the closest neighbor is obtained. The fourth section presents the results of molecular dynamics simulations and their comparison with the results of the analytical model. In the fifth section, the thermal oscillation amplitude and Lindemann parameter for particles in different regions of the system are discussed. The sixth section contains concluding words.

2. Considered model
We are considering a system of particles interacting with the pair Yukawa potential that is given by the following formula:

\[ U_{ij} = \frac{q^2}{r_{ij}} \exp(-kr_{ij}), \]  

(1)

where \( q \) is the electric charge of an \( i \)-th particle; \( r_{ij} \) is the distance between a pair of particles and \( k \) is the screening constant. This form of potential is often used for dusty plasma systems in gas discharges. Values of the screening constant in such systems usually lie in the range 10–1000 cm\(^{-1}\) corresponding to the values of Debye plasma radius in the range 10–1000 \( \mu \)m. The form of the trap is chosen so that a finite system, consisting of \( N \) particles, forms a structure that is ordered in one dimension:

\[ U_{\text{trap}} = \frac{1}{2} q[\alpha x_i^2 + \beta(y_i^2 + z_i^2)], \]  

(2)

where \( x_i, y_i, z_i \) are coordinates of the \( i \)-th particle; \( \alpha, \beta \) are trap parameters, and \( \beta = 0 \) SGS units for the structure to be ordered in the direction of the \( x \)-axis, \( y_i = z_i = 0 \) and \( r_i = x_i \), where \( r_i \) is the modulus of the radius vector of the particle.

Accounting both these interactions allows writing the expression for the full potential energy of a system including \( N \) particles:

\[ U_{\text{full}} = \frac{1}{2} q \sum_i \alpha x_i^2 + \frac{1}{2} \sum_i \sum_{j,j \neq i} \frac{q^2}{x_{ij}} \exp(-kr_{ij}). \]  

(3)

It is widely known that depending on the value of the screening constant \( k \), Yukawa potential can be short-range, almost hard-sphere-like when \( k \) is large and long-range like Coulomb potential in the limit \( k \to 0 \). In this work, the values of the screening constant \( k \), the particle charge \( q \) and the trap parameter \( \alpha \) are chosen to correspond to the experiments with dusty plasma at room temperatures [10, 11] because dusty plasma system is of a great interest in terms of testing the Yukawa model: \( k = 300.0 \) cm\(^{-1}\), \( q = 3000e \), where \( e \) is the elementary charge, \( \alpha = 0.01 \) SGS units. These values of parameters correspond to the short-range Yukawa potential.

3. Analytical solution of equilibrium equations for particles
For the accuracy of the first order, we are assuming that a particle interacts via the Yukawa potential only with the closest neighbor (which means that, if our system is arranged along one
axis, only one particle closer to the center with number \( i - 1 \) and only one particle further from the center with number \( i + 1 \) act on the particle with number \( i \) unless it is not on the edge of the structure. This assumption often works for weakly interacting Yukawa systems due to the exponential decline of the potential. Let us denote the instant distance to the particle located closer to the center \( a_c = x_i - x_{i-1} \) and to the particle further from the center \( -a_l = x_{i+1} - x_i \). Then the potential energy of the \( i \)-th particle looks as follows:

\[
U_{\text{rest}} = \frac{1}{2} \alpha q x_i^2 + \frac{q^2}{a_c} \exp(-ka_c) + \frac{q^2}{a_l} \exp(-ka_l).
\]

The first derivative of the potential energy of the particle with respect to its coordinate \( x_i \) gives the resulting force acting on the particle by the trap and neighboring particles:

\[
F_{\text{result}} = \alpha q x_i - \frac{q^2}{a_c} \exp(-ka_c) \left( k + \frac{1}{a_c} \right) + \frac{q^2}{a_l} \exp(-ka_l) \left( k + \frac{1}{a_l} \right).
\]

From this formula, it follows that, if particles are arranged at the same distance from each other and \( a_c = a_l \), the attractive force of the trap is not compensated, \( F_{\text{result}} \neq 0 \) and the \( i \)-th particle is in equilibrium. This means that the distance must differ between neighboring pairs of particles for the particle to stay confined around its equilibrium position. Let \( a_c = a \) and \( a_l = a + \Delta a \). Assuming that \( \Delta a/a \ll 1 \) anywhere in the system, from the condition \( F_{\text{result}} = 0 \) we get

\[
\frac{\Delta a}{a} = \frac{\alpha |x_i|}{q \exp(-ka)(a^{-2} + (a^{-1} + k)^2)}.
\]

This formula indicates that inter-particle distance increases more and more rapidly while approaching the periphery of the structure, and relative distance increase is higher for systems in a stronger trap and with a lower value of the particle charge.

The second derivative of the potential energy of the particle with respect to its coordinate \( x_i \) gives the stiffness of a potential well around its equilibrium position. This parameter defines the Einstein frequency of its oscillations [4]. Let the value of this parameter be \( B_i \), then

\[
B_i = \alpha q + \frac{2q^2}{a_c} e^{-ka_c} \left( \frac{1}{a_l^2} + \frac{k}{a_c} + k^2 \right) + \frac{2q^2}{a_c} e^{-ka_l} \left( \frac{1}{a_l^2} + \frac{k}{a_l} + k^2 \right).
\]

As it can be seen from this formula, if inter-particle spacing grows from the center to the periphery of the structure, the values of \( B_i \), on the contrary, fall, and particles are located in less deep and less stiff wells at the periphery. This might lead to an increase in the amplitude of thermal oscillations and local Lindemann parameter of particles located at the periphery of the structure.

4. Molecular dynamics simulations. Verification of analytical formulas

To verify the analytical formulas (6) and (7) and the predicted effects of growth in inter-particle distance and Lindemann parameter, molecular dynamics (MD) simulations are conducted on a system of 100 particles. The particles interact with the repulsive Yukawa potential (1) and are placed in an electrostatic trap (2) with non-periodic boundary conditions. The particle charge is \( q = 3000e \), the screening constant is 300.0 cm\(^{-1} \), the trap parameter is 0.01 SGS units. The cutoff distance after which the Yukawa potential is truncated is 0.05 cm and is verified not to affect obtained results. The Newton equations of motion are integrated with the timestep \( df = 10^{-4} \) s. At the beginning of a calculation, positions of particles are set randomly, then they move to their equilibrium positions in a Langevin thermostat [12]. Equilibrium coordinates and mean square displacements of particles are counted in a microcanonical ensemble.

Figure 1 shows the view of the structure obtained in MD simulations and the potential energy surface of the system. The spacing between particles in the central part of the structure equals...
Figure 1. Black circles—the positions of particles obtained in MD simulations; red line—the potential energy surface of the system.

Figure 2. Comparison of the relative inter-particle distance difference between neighboring pairs of particles in MD simulations and from analytical formula (6): black circles—the values of $\Delta a/a$ obtained from the analysis of particles coordinates in MD simulations; red line—the approximation of the MD values by the analytical formula (6).

$\approx 45 \mu m$, and on the periphery of the structure, it is twice as large: $\approx 90 \mu m$. It can be seen that inter-particle distance grows gradually from the center to the edge of the structure. The potential energy surface is obtained by direct calculation of potential energy of each particle in the field of the trap and other motionless particles. In this calculation, we are accounting not only the closest neighbors but all the particles in the structure. It indicates that the further a particle is from the center of the structure, the more gentle the slopes of a potential well become.

In figure 2, the relative inter-particle distance difference between neighboring pairs of particles in the structure $\Delta a/a$ is calculated by two approaches: the analytical formula (6) and MD
Figure 3. Second derivative of particles potential energies $U''(x_i)$ counted by two methods: red line—from the analytical formula (7); black line—from the approximation of the form of potential wells in figure 1 obtained from MD simulations. The second derivative is counted only in the coordinates corresponding to the positions of particles.

simulations. It can be seen in the graph that in the central part of the structure, the difference between neighboring inter-particle distances may be negligibly small. However, at the periphery of the structure which corresponds to the mentioned values of $q, \alpha, k$, the relative difference is $\approx 10\%$. This result confirms the effect predicted by the analytical model: in a finite Yukawa structure that is confined in a trap, inter-particle distance is not the same anywhere in the structure, it is higher near the edge of the structure and is lower in the central part. This effect automatically leads to different properties of potential wells in which particles “sit” at different distances from the center of the structure. Figure 3 shows the values of second derivatives of particles potential energies with respect to their positions $U''(x_i)$ counted by two different methods: by the analytical formula (7) and by an approximation of potential wells that are shown in figure 1. It is clearly seen that $U''(x_i)$ falls with the growth of distance from the center of the structure from the value $\sim 10^{-4}$ dyn/cm down to $\sim 10^{-5}$ dyn/cm. Different values obtained by the two methods for the central part of the structure can be explained by the insufficiency of accounting only two closest neighbors when deriving the formula (7). As soon as the second derivative of potential energy defines oscillation frequencies of particles around their equilibrium positions, the decrease of this parameter with distance from the center of the structure might lead to different values of thermal oscillation amplitudes for particles in different regions of the structure.

5. Amplitude of thermal oscillations and Lindemann parameter

As it was shown in the previous section, the second derivative of potential energy in the coordinates corresponding to the positions of particles falls with distance from the center of the structure and is $\sim 10$ times lower for particles at the edge. This parameter defines the oscillation properties of a particle, and as soon as particles at a different distance from the center are not equivalent, their thermal oscillation frequencies and amplitudes can be different.

In the studies of melting of Yukawa structures, the Lindemann parameter is often used as a reliable melting criterion. It says that at the melting point, the mean square displacement
of a particle from its equilibrium position $\langle \Delta x_i^2 \rangle^{1/2}$ (which is equivalent to the amplitude of thermal oscillations and is limited in a crystalline state) equals $\approx 0.15$ of the average inter-particle distance $\langle x_{ij} \rangle$. Averaging of these two values over all particles in the structure in case of an infinite Yukawa matter is based on an assumption that these properties are the same in different regions of a structure. This seems apparent because all particles, in this case, are equivalent. However, in case of a structure in a trap, particles at a different distance from the center are not equivalent as it was shown above, which might lead to different values of Lindemann parameter for different particles. We are additionally counting the local Lindemann parameter from the formula

$$\delta = \frac{2 \sqrt{\langle \Delta x_i^2 \rangle}}{a_f + a_c}$$

in order to estimate the magnitude of this effect.

In figure 4, the dependence of the amplitude of thermal oscillations on the distance from the center of the structure is shown. In the graph, there is also the same dependence obtained for a structure in the periodic boundary conditions (PBC) with no trap along the $x$-axis. The equations of motion for the structure in PBC are also integrated with the timestep $dt = 10^{-4}$ s, the values of $q, \alpha, k$ are the same. The size of the box along the $x$-axis is chosen so that the average linear density of the structure including 100 particles is the same as in the case of the structure in a trap consisting of the same number of particles. Changing the size of the box at a constant linear density (which means increasing the number of particles in the PBC structure) does not affect the results obtained in this section for the amplitude of thermal oscillations. Average inter-particle distance is the same for all pairs of particles in the structure in PBC in contrast with the case of the trap.

As can be seen from the graph, the average amplitude of thermal oscillations is approximately the same anywhere in the PBC structure. On the contrary, for the structure in a trap, this parameter gradually grows with distance from the center of the structure. The same effect takes place for the Lindemann parameter which is demonstrated in figure 5. Its change is defined by

Figure 4. Amplitude of thermal oscillations of particles at different distances from the center of the structure: black line—the structure in a trap; red line—the structure in periodic boundary conditions with the same linear density.
the competition of two factors: first, the amplitude of thermal oscillations grows with distance as shown in figure 4; second, inter-particle distance also grows with distance as shown in figure 2. The ratio of the amplitude of thermal oscillations and average inter-particle distance defines the Lindemann parameter. In the graph, it is seen that it also grows with distance from the center of the structure and at the edge of the structure is 2 times higher than in the central part.

This result is important for the theory of melting of Yukawa structures of finite size, since it indicates that the vibrational properties of particles, the amplitude of thermal oscillations, and the Lindemann parameter are local and differ in different regions of the structure. This might lead to different local temperatures of melting in different regions of two-dimensional and three-dimensional structures. The discovered effects find indirect confirmation in the works of Dubin in 1988 [13] and Schiffer in 2002 [14]. The first one showed that, in case of a three-dimensional structure, a layered cluster is observed, and particles located at outer layers have higher diffusion coefficients at different temperatures. The second one studied the temperature of melting of finite Coulomb clusters and found that it is lower than in the case of infinite matter. This indicates that the average value of the amplitude of thermal oscillations and the Lindemann parameter are higher for finite structures, which is confirmed in this work.

6. Conclusion
We have studied a one-dimensional structure of particles interacting with the Yukawa potential and confined in a parabolic one-dimensional electrostatic trap. It is shown both analytically and from MD simulations that inter-particle distance is not constant in different regions of such structure: it grows from the center of the structure to its periphery. It is shown that the second derivative of particles potential energy in the coordinates corresponding to their equilibrium positions falls with distance from the center of the system. The effect of growth from the center to the edge of the structure also takes place for the amplitude of thermal oscillations and Lindemann parameter. This might lead to different local temperatures of melting in different regions of the structure.

This result is important for the study of the phase diagram of finite Yukawa clusters.
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