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Phase transitions in mesoscopic dust crystals.

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Abstract

Phase transitions of an externally confined one-component Yukawa plasma are studied using a standard metropolis alogrithm Monte Carlo technique. The structure of Yukawa balls is analyzed to measure potential barriers in the cluster and compare those results with the solid-liquid transitions determined by distance fluctuations over the whole cluster.

Introduction

Coulomb crystal formation is among the most exciting cooperative phenomena in charged particle systems and has been observed in a variety of fields, including ultracold ions [1, 2] and dusty plasmas [3, 4]. Furthermore, computer simulations predict electron crystallization in quantum dots, e.g. [5, 6], crystallization of holes [7] and excitons [8, 9] in semiconductors and ion crystallization in expanding neutral plasmas [10] showing the universality of this phenomenon.

Particular recent attention has been devoted to three-dimensional spherical crystals (so-called “Yukawa balls”) after their experimental observation in dusty plasmas [11]. These clusters consist of tens to thousands of micrometer sized plastic particles in an rf-discharge. Due to the higher mobility of electrons the dust particles are charged with $q \approx 10^3 e$. The confinement in experiments is realized by thermoforetic force, electric field force of the rf-discharge, gravity and ion winds. A closer analysis of such an confinement can be found in [12] which concludes that the confinement potential is nearly parabolic and spherically symmetric. The simplest theoretical model of these finite systems, containing between a few and a few thousand particles, is given by the hamiltonian

$$H = \sum_{i}^{N} \frac{p_i^2}{2m} + \sum_{i}^{N} \frac{\alpha}{2} r_i^2 + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{q^2}{r_{ij}} e^{-\kappa r_{ij}}. \tag{1}$$

It consists of kinetic energy, a confinement potential and the interaction potential, all particles here are considered to have the same mass m and charge q. The Hamiltonian, with $r_{ij} = |r_i - r_j|$ as the interparticle distance and α as the confinement strength, will get dimensionless with the length scale $r_0 = (2q^2/\alpha)^{1/3}$ and the energy scale $E_0 = (\alpha q^4/2)^{1/3}$, the two particle equilibrium distance and energy for Coulomb interaction. The particles interact via a Yukawa potential, the screening parameter κ reflects the influence of the surrounding plasma, electrons and ions.

In Ref. [4] it was shown that ground state configurations computed from this model reproduce the structure of the experimentally observed Yukawa balls very well, including their radius and shell populations. A comparsion between the Kiel experiment of the group of A. Piel [11] and simulations showed that a screening parameter of $\kappa r_0 = 0.62 \pm 0.23$ (r_0 is defined below) is able to accurately reproduce the experimental shell configurations.
However, these comparisons have neglected effects of finite temperature of the dust particles on the shell configuration. These effects will be discussed here. Further, the comparison was performed for Yukawa balls with $100 \leq N \leq 500$. Here we present new theory-experiment comparisons with an independent experiment which involves small clusters with $N \leq 54$.

Monte Carlo simulation technique

We performed extensive Monte Carlo (MC) simulation with a standard metropolis algorithm [13] and adaptive steps so that 50% of the MC steps are accepted in average. The transition probability between two states in the Markov chain is given by the energy difference of these two states,

$$W(\vec{r}_i \rightarrow \vec{r}_j) = \begin{cases} e^{-\beta \Delta V} & \text{if } \Delta V > 0 \\ 1 & \text{otherwise} \end{cases} \tag{2}$$

We used 10^7 MC steps to generate a Markov chain of 10^6 configurations of the system for a set finite temperature. The metropolis transition probability allows to compute thermodynamic averages by a simple arithmetic average over the sample configurations.

Results and discussion

As an example we look at the phase transitions of the cluster with $N = 31$ particles. The ground state configuration with Coulomb interaction is $(4;27)$, 4 particles on the inner shell and 27 particles on the outer shell. This ground state configuration will change with increased screening to $(5;26)$ at $\kappa \approx 1.5$. Nevertheless there are also other metastable states, namely $(3;28)$ and $(6;25)$, of the system available at finite temperatures. We first measured the radial potential barriers by performing a MC simulation where we moved one particle from one shell to another while all other particles were allowed to relaxate. This will calculate the minimum energy barrier of the system between these two states since in every step in radial direction the system is allowed to get into thermal equilibrium. The results for two different screening parameters are shown in figures 1. One clearly sees that with increased screening the potential barrier between the ground state $(4;27)$ and the first excited state $(5;26)$ decreases in height. Also the energy difference between the two states decreases which is not surprising since at $\kappa \approx 1.5$ the ground state will change to $(5;26)$.

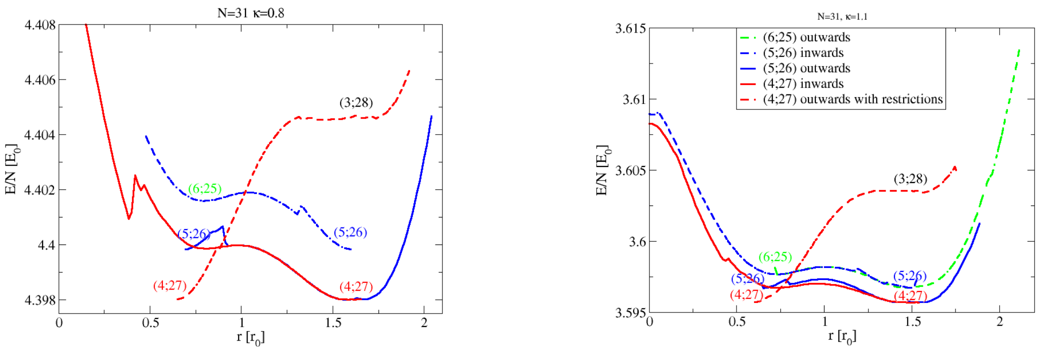

Figure 1: Potential barriers in a Yukawa ball with $N = 31$ particles. The dotted lines are the outward barriers, moving an inner shell particle to the outer shell and the solid lines are the inward barriers.

Performing a Monte Carlo simulation for $N = 31$, $\kappa = 0.8$, starting from the ground state and

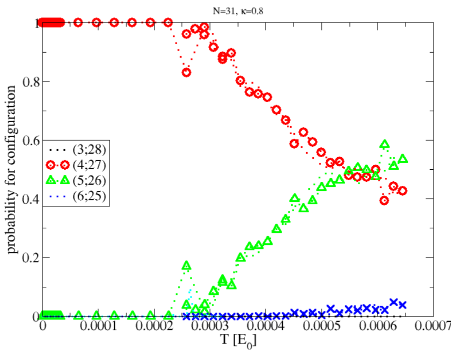

Figure 2: Occurance probabilities for the possible configurations of a dust cluster with $N = 31$ particles and a screening parameter $\kappa = 0.8$.

increasing the temperature, figure 2 shows the probability of occurances of metastable states. Even at low temperatures or $\Gamma_C < 1600$, the first excited state has a higher probability of occurance than the ground state. This is very surprising but can be understood when takeing into account that one has more possibilities to choose 5 particles out of 31 then choosing 4.

We have presented the potential barriers and occurance probabilities of an exmaple cluster with $N = 31$ particles. There we could show that finite temperatures have influence on the occurance probability of the configurations in the experiment.

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