Configurational entropy of Wigner crystals

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Abstract. We present a theoretical study of classical Wigner crystals in two- and three-dimensional isotropic parabolic traps aiming at understanding and quantifying the configurational uncertainty due to the presence of multiple stable configurations. Strongly interacting systems of classical charged particles confined in traps are known to form regular structures. The number of distinct arrangements grows very rapidly with the number of particles, many of these arrangements have quite low occurrence probabilities and often the lowest-energy structure is not the most probable one. We perform numerical simulations on systems containing up to 100 particles interacting through Coulomb and Yukawa forces, and show that the total number of metastable configurations is not a well defined and representative quantity. Instead, we propose to rely on the configurational entropy as a robust and objective measure of uncertainty. The configurational entropy can be understood as the logarithm of the effective number of states; it is insensitive to the presence of overlooked low-probability states and can be reliably determined even within a limited time of a simulation or an experiment.

PACS numbers: 61.46.Bc, 05.20.-y

Submitted to: *J. Phys.: Condens. Matter*

1. Introduction

Under the conditions of low disorder and temperature, a dilute electron gas forms an ordered structure known as the Wigner crystal [1, 2]. This term is also used to describe any other ordered system of strongly interacting particles, usually confined by an external potential. Typical experimental realizations of such structures are electrons on the surface of liquid helium [2, 3], electrons in semiconductor quantum dots [4], cooled ions in various kinds of traps [5], vortices in superfluids [6] and micrometric charged spheres in low-temperature dusty plasmas [7].

Ordered structures of two-dimensional (2D) and three-dimensional (3D) charged particle systems confined by an isotropic parabolic potential have been investigated in numerous recent studies. The configurations of stationary states have been both observed experimentally [8, 9, 10] and calculated theoretically [11, 12, 13]. It turns out that in most cases besides the unique ground-state configuration corresponding to the global energy minimum, a number of *metastable* configurations corresponding to various local energy minima are present.

Stationary configurations of small systems exhibit circular (2D) or spherical (3D) shell structure shown in figure 1 and figure 2, respectively. Two-dimensional clusters are fully characterized by the occupation numbers of each shell. In 3D systems, however, there may be several states with slightly different energies having the same shell occupation numbers. To distinguish between such states, an intra-shell structure has to be specified, for example, by using the Voronoi symmetry parameter [14]. For a larger number of particles, the nearly circular outer rings are gradually replaced by a distorted triangular lattice at the core of the cluster. As the screening increases and the inter-particle interaction range is thereby reduced, different shell configurations become stable and the size of clusters tends to shrink. For a very strong screening, the interaction becomes extremely short-ranged, and particles cluster near the centre of the system where the confinement vanishes [15]. As a result, an ordered triangular lattice is formed.

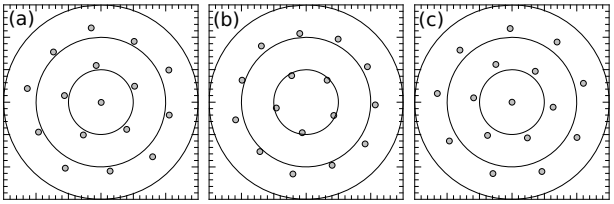

Figure 1. Ground (a) and metastable (b, c) states of a 16-particle 2D Coulomb cluster. The concentric circles mark equipotential lines of the parabolic trap. Numbers in parentheses list the numbers of particles in each shell starting with the innermost one. Note that the energy differences are quite small.

The number of stable configurations grows very rapidly with the number of particles and reaches hundreds already for the moderate systems containing only several tens of particles. In order to describe this situation in a quantitative manner it is often argued that *the number of metastable configurations grows exponentially with the system size*. However, as we demonstrate in the present paper, the total number of stationary configurations is not at all a useful concept – especially for large systems – and needs to be refined. The reason is that different stable states are typically

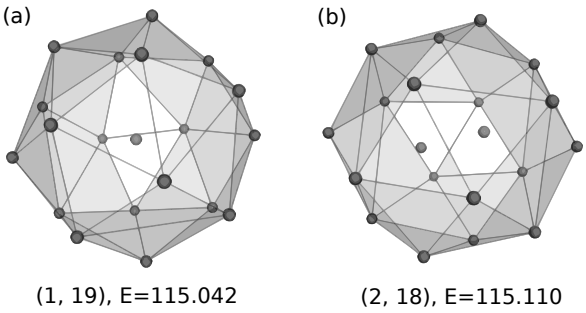

Figure 2. Ground (a) and metastable (b) states of a 20-particle 3D Coulomb cluster. The inner shell contains just one (a) or two (b) particles.

realized with very different probabilities of occurrence, and consequently, many of configurations, characterized by the smallest probabilities, remain unnoticed within the finite duration of an experiment or a simulation.

Recently, an experimental study focusing on the occurrence probabilities of the ground and metastable states in spherical clusters has been carried out [16]. The results indicate that sometimes metastable states are formed with higher probabilities than the ground state. This happens, when a metastable state controls a larger basin of attraction in the multidimensional configuration space. The effect of the temperature, screening and the cooling rate [16] on the probabilities of metastable states has been analyzed, and it was shown that stronger screening leads to higher probability of states with more particles on the inner shells. The authors also demonstrated, that the probabilities do not depend on the cooling rate when damping is strong.

The main goal of our work is to investigate the number and probabilities of metastable states in systems of up to 100 particles moving in two or three dimensions and evaluate the configurational uncertainty. We introduce the concept of *configurational entropy* as an objective measure of uncertainty, and investigate its dependence on the system size, dimensionality and screening. Thus cases of both Coulomb and Yukawa (screened Coulomb) inter-particle interactions are studied. The Coulomb forces are intended to represent the interaction between charged particles, e. g., in arrays of electrons on the surface of liquid helium or semiconductor quantum dots, while the Yukawa potential models interactions in the complex (dusty) plasma environment [7].

2. Model system and computational approach

The model system consists of $N \leq 100$ identical particles, interacting through the Yukawa potential. Particles are allowed to move in two or three spatial dimensions and are confined by a symmetric parabolic potential with the characteristic confining frequency ω_0:

$$V_{\text{ext}}(\mathbf{r}) = \frac{1}{2} m\omega_0^2 \mathbf{r}^2. \tag{1}$$

The total potential energy of the system is given by

$$U(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_{i=1}^{N} V_{\text{ext}}(\mathbf{r}_i) + \sum_{i>j}^{N} \frac{Q^2}{r_{ij}} \mathrm{e}^{-\kappa r_{ij}}. \tag{2}$$

Here, Q denotes the particle charge, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the inter-particle distance, and κ stands for the screening parameter (the inverse screening length). In the limit of $\kappa = 0$, the interaction reduces to the pure Coulomb potential. The two terms of (2) are obviously in competition: The screened Coulomb repulsion tends to increase the distance between the particles, while the confinement tries to hold them together. By introducing the units of length $r_0 = (Q^2/m\omega_0^2)^{1/3}$ and energy $E_0 = Q^2/r_0$, we can rewrite the potential energy (2) in a simple dimensionless form

$$U(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_{i=1}^{N} \frac{1}{2}\mathbf{r}_i^2 + \sum_{i>j}^{N} \frac{1}{r_{ij}} \mathrm{e}^{-\kappa r_{ij}}, \tag{3}$$

where the constant κ is now measured in the inverse r_0 units. The ground and metastable states of an interacting cluster correspond, respectively, to the global and local minima of (3).

Our goal is to find the stationary states as well as the probabilities for the system to settle in a given stationary state starting from a random initial configuration. In order to give a precise and physically motivated meaning to the above-mentioned randomness we choose to draw the starting configurations from the canonical (Boltzmann) distribution. According to this distribution, any initial configuration is in principle realizable, however, its likelihood is proportional to $\exp(-E/kT)$. Here, E stands for the energy of the configuration and kT is the simulation temperature, whose role will be explained shortly.

Thus, the numerical procedure consists of two stages: First, a random canonically distributed configuration of N particles is created. Then, the system is suddenly cooled and forced to roll down towards the closest energy minimum, or to be more precise, to the energy minimum whose basin of attraction encloses the starting configuration.

The first stage is accomplished by employing the standard Metropolis algorithm [17] that generates a Markovian sequence of configurations. Each new configuration is obtained from a previous one by a random displacement of one of the particles. If the new configuration has a lower energy it is accepted; otherwise the new state is accepted with probability $\exp(-\Delta E/kT)$, where ΔE is the energy increment. Higher values of temperature kT allow the system to overcome potential barriers between basins of attraction of different minima and thus efficiently explore the configurational phase space.

Once the thermodynamic equilibrium is reached, the second stage of the algorithm takes over. The system is suddenly cooled, that is, the closest local minimum of the potential energy is located using downhill minimization techniques. The phase space defined by all possible configurations of N particles moving in D spatial dimensions is $(D \times N)$-dimensional, the distribution of its stationary points is quite complicated. Sometimes, the desired stationary point is located in a long and narrow curved valley. Therefore, it is not an easy task for any optimization algorithm to quickly locate the stationary states. In some cases, the steepest descent optimization technique has to be combined with the Newton's method in order to increase the convergence rate and accuracy.

The whole heating and sudden cooling process is repeated a large number of times (a typical number of simulation runs is 2×10^4 – 3×10^4) to obtain accurate to one percent probabilities of occurrence of different stable and metastable states. The numerical experiment produces a list of found stable configurations and their occurrence probabilities. This information — while interesting on its own — may be further compressed into a single parameter that quantifies the uncertainty due to the availability of multiple stable states. Following the definitions accepted in information theory [18] we define the *configurational entropy* as

$$S = -\sum_{k=1}^{M} p_k \ln p_k. \tag{4}$$

Here, p_k is the probability of occurrence of k-th state, and M is the total number of found states. Performing a finite number of simulation runs it is impossible to find all stable states for a system containing a large number of interacting particles. However, as we demonstrate in section 3, the contribution of such undiscovered configurations to the entropy is negligible, since their probabilities are very low. Hence the proposed configurational entropy is an objective measure of uncertainty of the particle configurations. It could also be interpreted as the logarithm of the *effective* number of states. We note, that if there is only one available configuration, the entropy equals zero. This reflects the fact that we know the configuration that is to be found and thus there is no uncertainty.

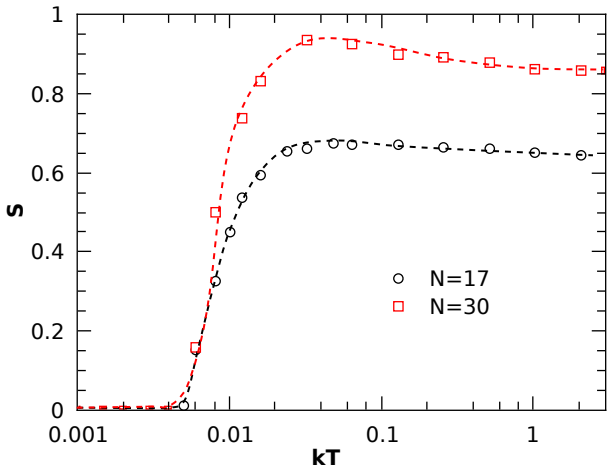

Figure 3. Configurational entropy as a function of simulation temperature kT for 2D systems with 17 and 30 particles and no screening ($\kappa = 0$).

With all that said, there remains an open question: The calculated probabilities as well as the entropy will, in general, depend on the simulation temperature. However, it is easy to see that these quantities change rapidly only at low temperatures, that is, when the simulation temperature kT is smaller than, or comparable to, the heights of the potential barriers separating basins of attraction of different minima. In the limit of high temperatures, the obtained probabilities are essentially temperature independent. Therefore, in this limit the probabilities and the configurational entropy become well-defined quantities.

These comments are illustrated in figure 3 which shows the dependence of the configurational entropy on the temperature of simulation. As long as the temperature kT does not exceed a certain threshold value (around $kT \approx 0.005$ in this case), there is only one stationary configuration that the simulation would reveal – the ground state. Naturally, in this limit there is no uncertainty and the configurational entropy remains close to zero. As the simulation temperature is increased, the potential barriers can be crossed and more states become available. Consequently, the calculated entropy rapidly increases. Eventually, in the high temperature limit, that sets in at $kT \approx 0.1$ in figure 3, the system is able to reach the areas of attraction of any available energy minimum without limitations. Thus, the calculated configurational entropy levels off and becomes essentially temperature-independent. These observations confirm that the high-temperature limit of the entropy is indeed a well defined measure of uncertainty in the model system under investigation. The value of temperature used to determine probabilities in our simulations is even higher ($kT = 2$).

3. Results

We performed numerical simulations for 2D systems containing up to $N = 100$ particles at three values of the screening parameter $\kappa = 0$ (no screening), $\kappa = 1$ and $\kappa = 5$. In three dimensions we restricted the numerically demanding calculations to two values of the screening strength $\kappa = 0$ and $\kappa = 5$ and system sizes up to $N = 80$. Let us now turn to the obtained results. We start by discussing the number of stationary states, and then proceed to the behaviour of the configurational entropy.

3.1. Number of metastable states

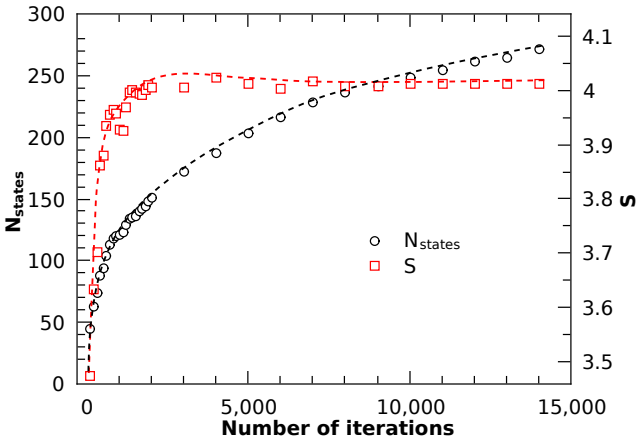

Figure 4. Number of discovered stationary configurations N_{states} and configurational entropy S, as a function of the number of performed simulation runs for the unscreened 2D Coulomb cluster with $N = 100$ particles.

The computational procedure developed in section 2 is capable of determining all existing metastable configurations only for a small number of particles N. However, when N reaches a few dozen, even a relatively large number of simulation runs does

not guarantee the discovery of all stationary states. One just keeps discovering more and more stable configurations as the iterations are performed further.

Figure 4 shows the dependence of the number of discovered stable configurations N_{states} on the number of simulation runs for a 2D unscreened Coulomb cluster in a parabolic trap with $N = 100$ particles. We see that the number of states grows steadily and fails to show any signs of convergence towards an asymptotic value as the number of simulation runs reaches 10 000. Evidently, a much larger number of iterations would be necessary to perform in order to achieve convergence. These observations confirm that, in this context, the notion of the total number of stable configurations is ill-defined, and consequently, is not that useful.

In contrast, the configurational entropy grows rapidly from the very beginning and reaches its asymptotic value already after a few thousand of simulation runs (see figure 4). There obviously exist just a few most important configurations with relatively high probabilities of occurrence and a large number of states with insignificant probabilities. The latter make only a minor contribution to the entropy, and its value does not change appreciably as the number of discovered states increases continuously. Therefore we may conclude, that the configurational entropy is, indeed, an objective parameter of uncertainty even when number of simulation runs is limited and only a fraction of all stable configurations is discovered.

As a matter of fact, the seemingly unrelenting growth of the number of discovered states is due to a heavy-tailed power-law distribution of the state probabilities. Let us investigate more closely the probabilities of the discovered stationary states for the 80-particle system. The range of probabilities is divided into the intervals of width Δp and the number of states Δn with probabilities of occurrence within the interval $(p - \Delta p,\ p)$ is calculated. Figure 5 shows that the dependence of $\Delta n/\Delta p$ on the probability p is linear on a log-log scale. That is,

$$\lg(\Delta n/\Delta p) \approx -\alpha \lg(p) + \text{const},$$

which is equivalent to

$$\Delta n/\Delta p \sim p^{-\alpha}. \tag{5}$$

Hence, there is only a tiny number of dominant configurations with significantly high chance of occurrence. The number of discovered states in a given probability interval increases rapidly as the probabilities become lower. However, the areas of attraction of those numerous stationary states account only for a very small fraction of the total phase-space volume.

The distribution (5) follows a power law which is in various contexts known as the Zipf's law or Pareto distribution. It is worth noting, that power laws appear widely in physics, economics, computer science, biology, geography, demography and social sciences [19]. Zipf's law is observed in various phenomena that have no definite characteristic scale and distribution of the relevant quantities spans many orders of magnitude. A few notable examples of Pareto-distributed items are the sizes of cities, magnitudes of earthquakes, frequencies of words in natural languages and so on.

We observe that the four lines shown in figure 5 have different slopes; this corresponds to different values of the power-law exponents α. The lowest value of the exponent α seen in figure 5 is found to be 1.25 and characterizes the two-dimensional cluster with unscreened Coulomb interaction. In general, one notes that for both 2D and 3D systems, the exponent α increases as the range of inter-particle interaction becomes shorter. Thus, we may conclude that *screening leads to the proliferation of low-probability states.*

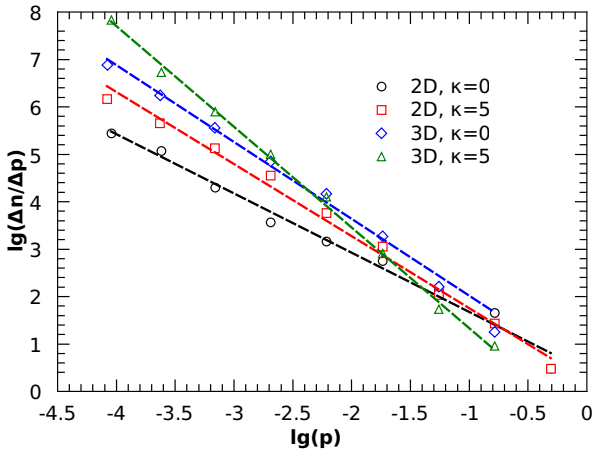

Figure 5. Power-law dependence of the normalized number of states $\Delta n/\Delta p$ whose probabilities lie in the interval $(p - \Delta p,\ p)$ on the value of $\lg(p)$ for a system with $N = 80$ particles.

The results obtained for systems with a different number of particles are similar to those pertaining to $N = 80$ shown in figure 5. Of course, we have to restrict the consideration to large systems, so that a sufficient amount of data for statistical analysis is generated. The value of the exponent α is not universal and slightly grows with the system size. Its value for a 2D system with $\kappa = 0$ reaches 1.4 for $N = 100$.

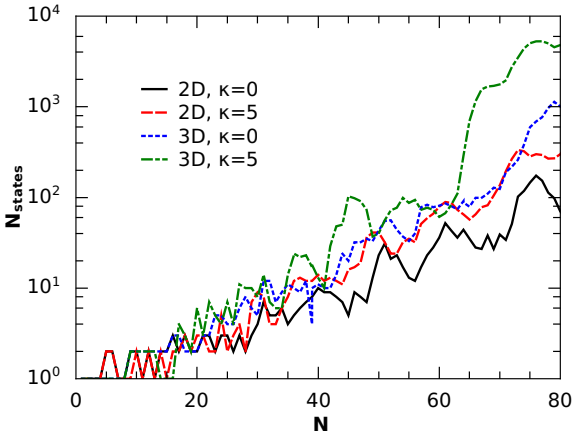

Figure 6. The number of stationary states discovered after 3×10^4 simulation runs in the two- and three-dimensional systems of N particles with screening κ.

The number of discovered stationary states of the model system grows very rapidly with the number of particles. Figure 6 shows the dependence of the number of configurations, found after 30 000 simulation runs, on the number of particles N for 2D and 3D systems without screening and with screening $\kappa = 5$. On the average, the growth is nearly exponential (note the logarithmic scale on the vertical axis) and is

Table 1. Values of the slope γ for 2D and 3D systems with different values of screening constant κ.

Dimension	$\kappa = 0$	$\kappa = 1$	$\kappa = 5$
2D	0.011	0.011	0.015
3D	0.015	—	0.021

faster for the systems with shorter range of inter-particle interaction. Just to give an example, we observe that in a 2D system with $\kappa = 0$ the number of states does not exceed three as long as $N < 16$. In contrast, in a system with the screening parameter $\kappa = 20$, three stable configurations exist already when $N = 10$.

Note, however, that here we are discussing the number of *discovered* states and not the true number of states, which is unknown. With this reservation, we may conclude that our simulations confirm (or at least, do not reject) the oft-cited conjecture of an exponential growth of the number of states.

3.2. Entropy in 2D and 3D systems

The configurational entropy, as expected, grows rapidly with the number of particles. The growth is quite erratic, with conspicuous maxima and minima.

On the average, the dependence of the entropy on the number of particles in both 2D and 3D systems with different values of screening parameter κ is clearly faster than linear. That is, the effective number of states $\Omega(N) = \exp[S(N)]$ grows faster than exponentially. In view of the combinatorial nature of the problem, it is tempting to hypothesize that the effective number of states could be proportional to the factorial of the number of particles $N!$, and the entropy behaves as

$$S = \gamma \ln(N!). \tag{6}$$

Figures 7 and 8 show the calculated dependence of the entropy on the argument $\ln(N!)$ for 2D and 3D clusters with different screening lengths. For the sake of convenience, these figures are also supplied with a nonlinear top axis that gives the corresponding values of N. We see, that the averaged trends indeed exhibit a linear growth. While it is impossible to rigorously "prove" conjectures of this sort, the results of the numerical experiment clearly do not contradict (6). Thus, taking advantage of this conjecture we may use the values of the slope γ as a convenient measure of the entropy growth. The values of γ for the 2D and 3D crystals with different values of κ are collected in table 1.

For the systems with small screening, the peak value of the entropy is close to $S = \ln 2$ as long as the number of particles is lower than $N = 20$. There are only up to 3 stable configurations discovered, and the entropy is close to $\ln 2$ when mostly two of them have comparable probabilities of occurrence. A typical example is a 2D cluster with $N = 14$, entropy $S = 0.69$ and two configurations with probabilities 0.44 and 0.56.

As the number of particles increases, the areas of attraction of many configurations become comparable in size and, as a consequence, the entropy grows. As an example, one of the peaks of the configurational entropy in a system with $\kappa = 0$ is located at $N = 40$. There are ten stable states, only three of them with high, and comparable, probabilities of occurrence (0.23, 0.23, 0.22), the remaining ones being lower by an order of magnitude or more.

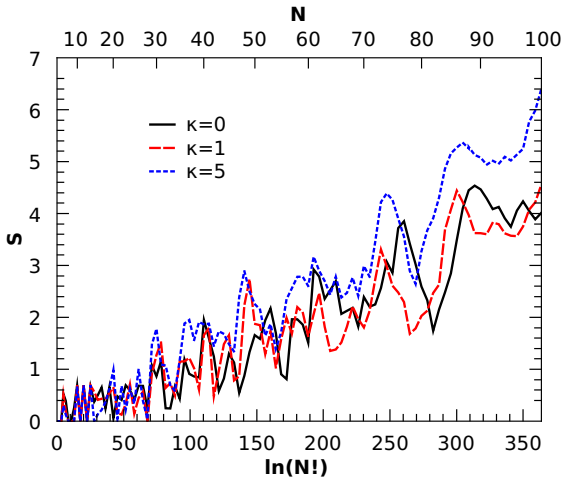

Figure 7. Configurational entropy of a 2D system with screening parameter κ as a function of parameter $\ln(N!)$.

On the other hand, the uncertainty is low when there is only one (or very few, in comparison to the total number of states) dominant configurations whose probabilities are much higher than the remaining ones. The entropy of the 3D system with $\kappa = 5$ has a sharp minimum at $N = 49$. There are 37 discovered stationary states, however, only one of them has a high chance of occurrence (0.85).

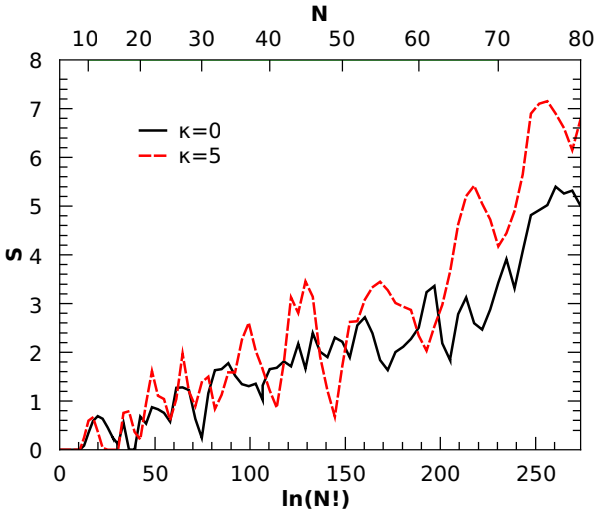

Figure 8. Configurational entropy of a 3D system with screening parameter κ as a function of parameter $\ln(N!)$.

Although the number of discovered states depends on interaction range (see figure 6), screening only weakly affects the configurational entropy of small 2D systems. Even more, the positions of major falls and growths of the entropy for different values

of screening parameter κ are close to each other. The most noticeable changes in uncertainty of the system occur near $N \approx 30,\ 40,\ 48,\ 74,\ 87$, where the addition of a few particles firstly almost doubles the value of entropy, and then suddenly decreases it to the much lower value.

Slightly different situation is observed in three dimensions (figure 8). Configurational entropy on the average grows faster ($\gamma = 0.015$ for $\kappa = 0$). Even for a small number of particles, increased screening leads to the sharper and higher peaks of the uncertainty. The most noticeable maxima of the entropy in a 3D Yukawa crystal with $\kappa = 5$ occur at $N = 27,\ 37,\ 45,\ 67,\ 76$. Growth of the entropy in a Coulomb system ($\kappa = 0$) is much smoother, the number of peaks is higher. Also, as opposed to the 2D system, no relations can be found between the positions of peaks for the different values of screening constant κ.

It is worth mentioning that although only a fraction of all possible stable configurations is found during our simulations, there exists a correlation between the number of discovered states and the effective number of configurations $\Omega = \exp(S)$. As the number of particles grows, the increasing number of discovered states parallels the growth of the entropy and vice versa. To illustrate this point, we analyze the behaviour of the logarithm of the number of states and entropy in a two-dimensional system with $\kappa = 1$. The entropy S and the logarithm of N_{states} are separated into the sums of the main linear part and the fluctuating term:

$$S = \gamma \ln(N!) + \sigma(N), \tag{7}$$

$$\ln(N_{\text{states}}) = \beta N + \nu(N). \tag{8}$$

The correlation plot between the fluctuating terms σ and ν for all values of $N \leq 100$ is shown in figure 9. We see, that nearly all points (with the exception of a single outlier) fall inside an elongated elliptic area, thus confirming the presence of correlations. Similar results are obtained for the systems with $\kappa = 0$ and $\kappa = 5$. In three dimensions, however, the correlation between the number of discovered states and the configurational entropy is weaker.

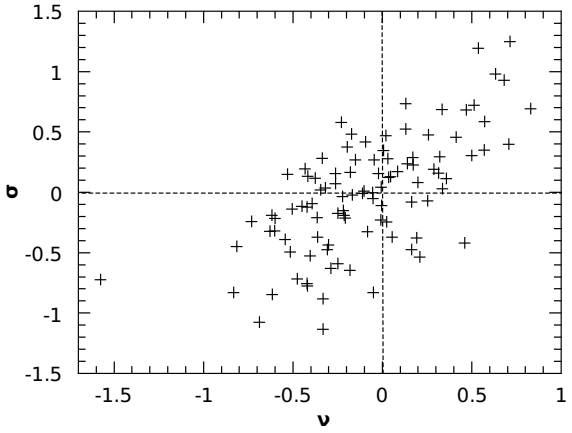

Figure 9. Correlations between fluctuations of entropy σ and the logarithm of the number of discovered stable configurations ν in a 2D system with screening constant $\kappa = 1$.

4. Conclusions

In conclusion, using the Monte Carlo and downhill minimization algorithms we have investigated the probabilities of metastable states of two- and three-dimensional classical particle clusters confined by a parabolic potential trap. It is demonstrated, that the total number of states is not a useful parameter to describe large systems due to its sensitivity to the low probabilities of the majority of stable configurations. The number of states with low chance of occurrence is further increased when the inter-particle potential is short-ranged. In order to quantitatively evaluate the uncertainty due to the presence multiple stable states, we propose to rely on the concept of the configurational entropy – a quantity that accurately describes the randomness of the final state even when the number of simulation runs is limited. It turns out that the effective number of states $\exp(S)$ grows faster than exponentially, that is, on the average $S = \gamma \ln(N!)$ for $N < 100$. Entropy grows faster in the systems with short inter-particle interaction range.

Acknowledgments

Arūnas Radzvilavičius acknowledges Student Research Fellowship Award from the Lithuanian Science Council.

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