

Molecular Dynamics of Unstable Systems

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ABSTRACT

Molecular-dynamics results for one- and two-dimensional systems of purely attractive particles are presented and are compared with a cell model.

1 Introduction

The statistical mechanics of the self-gravitating systems that occur in astrophysics and cosmology is hampered by the gravitational potential being negative, of long range, and singular in the origin. The last two difficulties disappear for a pair potential $\phi(r) = -\epsilon \exp(-r^\delta/\sigma^\delta)$, with $\epsilon, \sigma > 0$ and δ an even integer (possibly ∞). The remaining problem still is of fundamental interest: the potential disobeys the stability condition, leading to a non-extensive collapsing phase which in the microcanonical ensemble may exhibit a negative specific heat.

This has been verified theoretically for a simplified model [1,2], in which the pair-potential is replaced by a negative contribution $-\epsilon$ to the potential energy for any pair of particles in any one of the many cells in which the system is divided. The properties of this cell model fit in with canonical-ensemble results [3] obtained for more general unstable systems, and they agree remarkably well with quasi-experimental molecular-dynamics results for two-dimensional systems with $\delta = 2$ or 4 in the true pair-potential given above [2,4]. Due to the long relaxation times encountered, these earlier MD calculations were carried out for rather small systems, of about $N = 100$ particles. The question arose whether one-dimensional systems would allow large enough values of N to study the fascinating asymptotic behaviour of non-extensive collapsing systems in relation to the cell model.

2 One-Dimensional Systems

To give an impression, Fig. 1 shows the momentary configurations of 20 square-well particles ($\delta = \infty$) on a line, depicted vertically at regular intervals along the horizontal time axis. Initially, only nearest neighbours interact and only the two outermost particles, separated by the periodic boundary, are moving (to avoid identical collision times, the initial distances were not completely equal). The MD algorithm used is the same as for a hard-core system, but the simplifying feature of saturation is absent. The energy parameter $\eta \equiv 2E/\epsilon N^2 - 1/N$ was -0.2 , where E is the total energy. The final state with a single fluctuating cluster of about 10 particles was observed to be stationary.

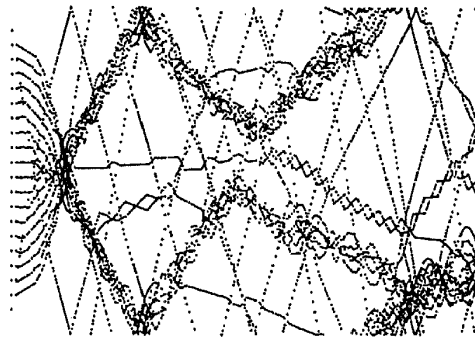


Figure 1: The trajectories of 20 purely attractive particles on a line (the time axis points to the right), at an energy for which a cluster of ≈ 10 particles is stationary.

The above form of the energy parameter is convenient for a comparison with the cell model. In the one-dimensional cell model, $\eta = 0$ corresponds to the endpoint of the homogeneous phase existing at higher energies, and in the cell model as well as in the simulated systems $\eta = -1$ corresponds to the completely collapsed state at zero kinetic energy (at temperature $T = 0$).

Simulations were carried out at many values of η for several values of N and the reduced volume V^* (measured in well-widths σ), i.e. at different reduced densities $\rho^* = N/V^*$. At each value of η , the largest cluster with N_c particles was determined by a cluster analysis, and temperature, pressure and specific heat were measured. The results support the existence of an apparently first-order transition at $\eta \approx 0$, between a homogeneous phase at higher energies and a collapsing phase with a single cluster floating in a homogeneous background at lower energies.

Two examples are given. In Fig. 2, the data points are the MD results obtained for $\nu = N_c/N$ (in the homogeneous phase, the cluster analysis overestimates the average density), and the solid line indicates the cell model results; the broken lines are drawn at the endpoints of the metastable branches of the two phases that occur in the cell model. The number of cells is taken to be $M = V^*/2$, the total width of the true pair potential being 2σ . In Fig. 3, the corresponding comparison is made for the reduced temperature $T^* = kT/2\epsilon$.

The MD results for the other quantities and at other values of ρ^* also agree with the cell model, even more so than earlier was found for two-dimensional systems (for which, however, $\delta = 2$ or 4 was used in the pair potential; the square-well with $\delta = \infty$ used for the one-dimensional system corresponds closer to the cell-model assumption). Note, that a negative specific heat is not forbidden in the microcanonical ensemble. It is found to occur when a decrease of the total energy leads to a suitable exchange between kinetic and configurational degrees of freedom due to cluster growth. The vertical tie lines of the metastable branches of the microcanonical version of the cell model (the broken lines in Fig. 3) are replaced by horizontal lines (the dotted lines in Fig. 3) in the canonical ensemble, which avoid the interesting region of negative specific heat.

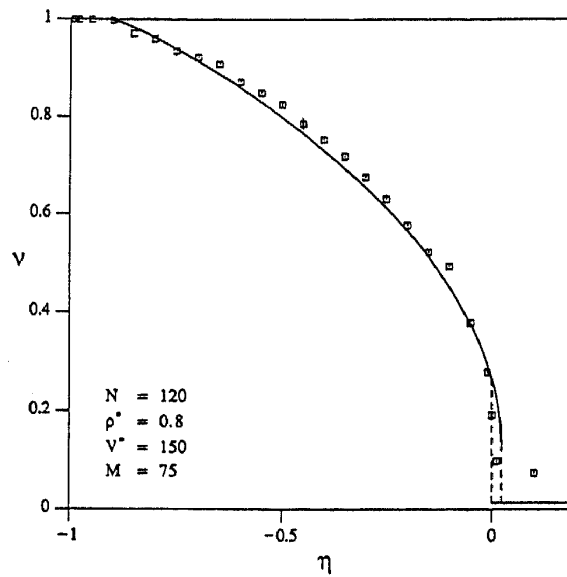


Figure 2: The relative size of the collapsing cluster versus energy. At $\eta \approx -1$ the collapse is complete.

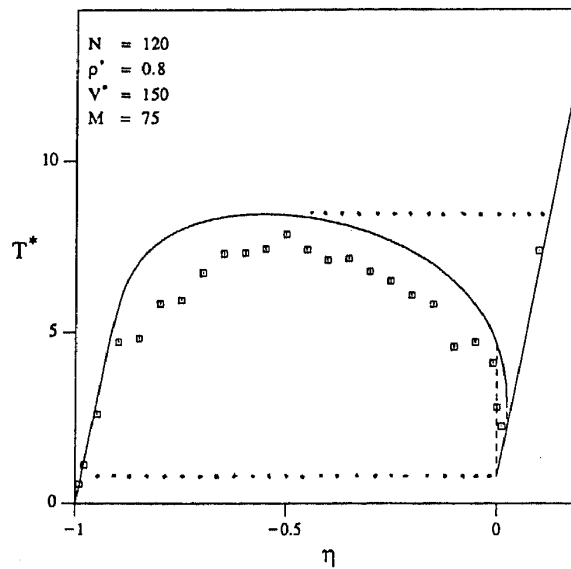


Figure 3: Temperature versus energy. Between $\eta \approx -0.5$ and $\eta \approx 1$ a negative specific heat is observed.

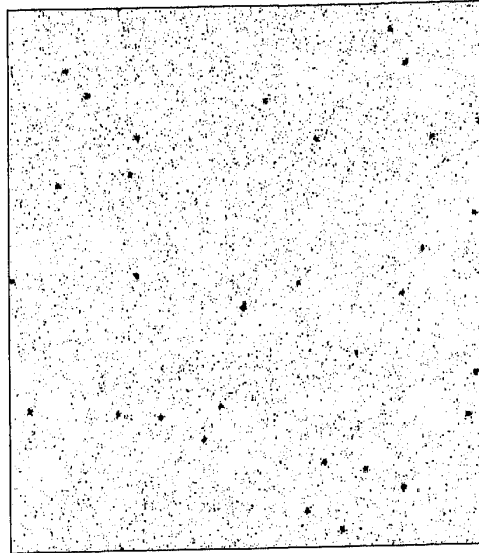


Figure 4: A transient configuration of 16000 purely attractive particles, just after entering the collapsing phase.

Unfortunately, the relaxation times observed for the one-dimensional systems were still large, preventing any study of asymptotic properties. The slow relaxation caused by the compact size and the deep collective well of the collapsing cluster is probably enhanced by the restriction of the kinetic degrees of freedom to a single dimension, and this effect is insufficiently compensated by a greater calculational efficiency for one-dimensional systems.

3 The Critical State

The transition between the homogeneous and the collapsing phase occurs at $\eta = 0$. According to the cell model, this is for finite N a first-order transition with metastable branches, which indeed are also found in the MD experiments. When N increases, the size of the metastable region decreases and relaxation times become larger: an intriguing critical state results. An impression of this state is obtained by means of the Delft Molecular-Dynamics Processor, a fast special-purpose machine for MD simulations [5] of two- and three-dimensional systems used for the earlier calculations [2]. In this machine the usual linked list of the MD algorithm is however realized in hardware, and can contain at most 256 particles. When for larger values of N the collapsing phase is entered, this list soon overflows due to the emerging cluster and correct simulations are impossible. The homogeneous phase, which resembles an ideal gas, can be studied up to $N = 16383$; it is worthwhile to look at the endpoint of this phase.

As an example, a two-dimensional system of $N = 16000$ particles, with $\delta = 4$ in the pair potential $\phi(r)$, was simulated at $\eta = 0.00056$ (just within the homo-

geneous phase) until a well-equilibrated configuration was reached. Then, in 700 elementary time steps (small enough for a correct numerical integration of Newton's equations), the system was quenched to $\eta = 0.00019$. After a further 20000 time steps the configuration of Fig. 4 was obtained. About 32 transient clusters appear, 16 of them having more than 100 (but less than 256) particles. From the same initial configuration in the homogeneous phase, another non-equilibrium state with 3 clusters (of 129, 180 and 182 particles) was found 40000 time steps after quenching less drastically to $\eta = 0.00044$ in 13600 time steps. Similar results were found for systems of 4000 particles, with varying quenching histories.

These results support the existence of a critical state similar to the one found at $\eta = 0$ in the cell model [2], which due to an entropic degeneration of the single-cluster state is characterized by a non-extensive number of transient clusters with long relaxation times.

References

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