Phase Transition in a Model Gravitating System

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We present recent developments in the study of an interacting gravitational system of concentric, spherical, mass shells. The existence of two distinct phases is demonstrated. The nature of the transition in the microcanonical, canonical, and grand canonical ensembles is studied both theoretically in terms of mean field theory and via dynamical simulation. Striking differences are found in each environment, especially the last. [S0031-9007(98)07737-0]

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One-dimensional models have provided a testing ground for astrophysical theories of gravitational evolution for several decades. The systems studied fall into two classes, parallel mass sheets of infinite spatial extent and concentric, spherical mass shells. It has been conjectured that these idealized systems can be identified with processes occurring in nature: The parallel sheet system with the motion of stars perpendicular to the plane of a highly flattened galaxy [1], and the shell system with the dynamics of a spherical globular cluster [2]. However strained these connections may appear, the central motivation for studying these systems is the ease and accuracy with which their dynamical evolution may be simulated with the computer. In contrast with the evolution of three-dimensional point masses, for these systems numerical integration of the orbits can be replaced by the direct computation of successive sheet (or shell) crossings, permitting accurate orbit computations over many dynamical time scales. Since these are the simplest N body gravitational systems available, they are worthy of consideration in their own right.

Thermodynamics of systems of particles interacting via gravitational forces differs strongly from typical "chemical" systems, where the interactions have finite range and are repulsive at short distances [3]. Antonov originally noted that, due to the singularity in the two body interaction potential, in the mean field (Vlasov) approximation a confined spherical system of gravitating point masses lacks a global, and for sufficiently low energy a local, entropy maximum [4]. Thus it is not subject to the usual thermodynamic analysis and may undergo a spontaneous collapse, presently referred to as the gravothermal catastrophe following Lynden-Bell and Wood who also conjectured that, if the singularity is screened by a hard sphere interaction, the collapse may be replaced by a phase transition to a more centrally condensed state [5]. (Such a system was first investigated theoretically by Aronsen and Hansen [6] and, more recently, by both Stahl and Kiessling [7] and Podmanabhan [8] by introducing a local pressure due to the short range repulsion.) Later Hertel and Thirring showed that the thermodynamics of a model system interacting via purely attractive forces of finite range and potential depth could undergo a phase transition to a more condensed state [9]. Lyndem-Bell may be the first to have demonstrated a phase transition in a particular model *gravitating* system in which all of the particles are restricted to lie on the same spherical surface [10]. More recently, Keissling has rigorously proven that (1) a truly isothermal, three-dimensional, Newtonian, gravitating system will condense to a droplet of zero size and that (2) a phase transition is possible in the three-dimensional gravitating gas of fixed energy restricted to a spherical box with a *regularized* two body interaction potential [11]. However, regardless of all of these predictions, until now the occurrence of a gravitational phase transition has not been demonstrated either experimentally (granted this would be a challenge) or by dynamical simulation.

Here we consider a model system of uniform, concentric, mass shells. The shells undergo radial motion, i.e., they expand and contract, under the influence of their mutual gravitational forces. Other investigators have used concentric mass shells to model the evolution of globular clusters [2,12,13]. In contrast with these studies, our shells have no angular momentum or rotational energy and, in addition, are confined between two reflecting barriers with inner and outer radii (a, b). In contrast with the system of planar sheets, our shells appear to have strong ergodic properties and spread out rapidly in their μ(position, velocity) space [14,15]. We have studied the system both theoretically and via dynamical simulation under three different conditions: microcanonical (constant energy), canonical (constant temperature), and grand canonical (constant temperature and chemical potential). Below we show that mean field theory predicts the existence of two possible phases when the inner barrier radius is less than a critical value, a_c. Each phase has a smooth density profile in (a, b), but one of them has a higher central concentration of mass. For each $a < a_c$ mean field theory predicts that the more concentrated phase is favored thermodynamically for sufficiently low energy (temperature) in the constant energy (temperature) ensemble. Dynamical simulations support the predictions of mean field theory in all cases. As far as we are aware, this is the first reported dynamical demonstration of a phase transition in a gravitational system.

(I) Mean field theory.—Consider a system of N concentric, uniform, irrotational, Newtonian, shells of mass

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m $(= M/N)$. Each shell has a single coordinate, its radius r, and acceleration $-G[M(r) + m/2]/r^2$ where G is the gravitational constant and $M(r)$ is the mass of the interior shells. To both prevent escape and shield the singularity at the system center, the shells are confined to move between two likewise spherical reflecting barriers located at $r = (a, b)$. Without loss of generality, we define units of distance, time, and mass for which $b = G = M = 1$.

In the Vlasov limit, i.e., letting $N \rightarrow \infty$ while both the total mass and energy are held constant, the system is represented by a fluid in the $\mu(r, v)$ space with mass density $f(r, v, t)$. Intuitively, it seems natural to assume that our system obeys the identical Vlasov (collisionless Boltzmann equation, or CBE) for $f(r, v, t)$ as for a spherically symmetric three-dimensional system [3,16]. However, since here the dynamical system is one dimensional, this is not the case. The stationary, maximum entropy, solution of the CBE is still of the form $f(r, v) = MC \exp[-\beta(v^2/2 + \varphi(r)]$ where C is a normalization constant and $\varphi(r)$ is the gravitational potential [3], but here v is the radial velocity of a shell, and the system density, $\rho(r)$, is the mass per unit length. Thus $g(r)$, the normalized, *linear*, mass density, obeys

$$\frac{d}{dr} r^2 \frac{d}{dr} \ln g(r) = \beta MG g(r)$$

$$\text{subject to } \frac{d}{dr} g(r)|_{r=a} = 0 \quad \text{and} \quad \int_a^b g(r)\, dr = 1\,. \tag{1}$$

The solutions of Eq. (1) depend on the single parameter βMG $(= \beta$ in our units). By direct numerical integration we find that for sufficiently large $a < b = 1$ there is only one solution of (1). However, as the value of a is reduced we reach a critical value, say, a_c, such that for $a < a_c$, it is possible to construct three distinct solutions of (1) for $\beta \in \Delta\beta(a)$, a particular interval of $(0, \infty)$. Outside this interval the solution is unique. The solutions for large β, i.e., to the right of $\Delta\beta(a)$, are more centrally concentrated than those to the left.

It is possible to construct a complete formulation of the equilibrium thermodynamics of this system in the mean field (Vlasov) limit. All macroscopic quantities of interest can be expressed in terms of the solutions of (1). It is natural to regard a, the inner barrier radius, as the generalized thermodynamic coordinate of the system and $\theta \equiv 1/\beta$ as the generalized temperature [17]. In order to track the phase transitions which occur in the microcanonical and canonical ensemble, it is convenient to choose the virial ratio, i.e., the ratio of kinetic to potential energy, as the system order parameter. With a little work it can be shown that the energy, entropy, Helmholtz free energy, and grand potential depend explicitly on $g(r)$. Thus they are single valued functions of β except when $a < a_c$ and $\beta \in \Delta\beta(a)$, where they can take on multiple values. This is the parameter region where phase transitions can occur.

(II) Dynamical simulations.—Numerical simulation of the shell dynamics is facilitated by the fact that, between events (shell crossings, turning points, and barrier collisions), the equations of motion can be integrated analytically to yield the time as a function of position. In two earlier studies we showed that the shell system has stronger ergodic properties than the parallel sheets [14] and relaxes on a much shorter time scale [15]. This can be clearly seen in the following example of a system of 3200 shells prepared by uniformly distributing them in position and alternately assigning velocities of equal size and opposite sign. After about only fourteen characteristic infall times, we see that the system is well mixed in the μ space (see Fig. 1).

(a) Microcanonical ensemble: The system is isolated and the energy is conserved. The thermodynamic state is determined by the total energy, E, and inner barrier radius, a. Equilibrium states are states of maximum entropy $S = \mathrm{S}(E, a)$. To explore the system properties in the context of mean field theory we need to determine the solution of (1) corresponding to a given (E, a) which, in turn, requires finding $\beta = \beta(E, a)$. When $a < a_c$ and $\beta \in \Delta\beta(a)$, multiple phases are possible; the stable phase corresponds to the branch with maximum entropy. From Fig. 2 we see that, corresponding to $\beta \in \Delta\beta(a)$, there is an energy interval in which both phases can exist, but one is more stable. As usual, the third solution tying the stable phases together is thermodynamically unstable [17]. As the energy is lowered, there is a sharp transition to the more centrally concentrated phase.

At the transition point (the intersection in Fig. 2) each phase is equally stable. Thus we can construct a "coexistence" curve in the (E, a) plane along which the transition occurs. Here, however, we must use the term coexistence guardedly. In contrast with chemical systems, our phases are associated with a particular density profile in (a, b) and cannot simultaneously exist in the same volume.

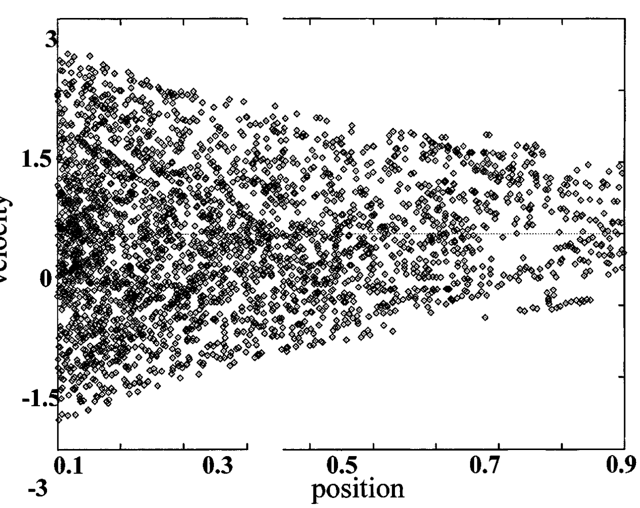

FIG. 1. Final condition in μ space for 3200 shell system after 14 infall times.

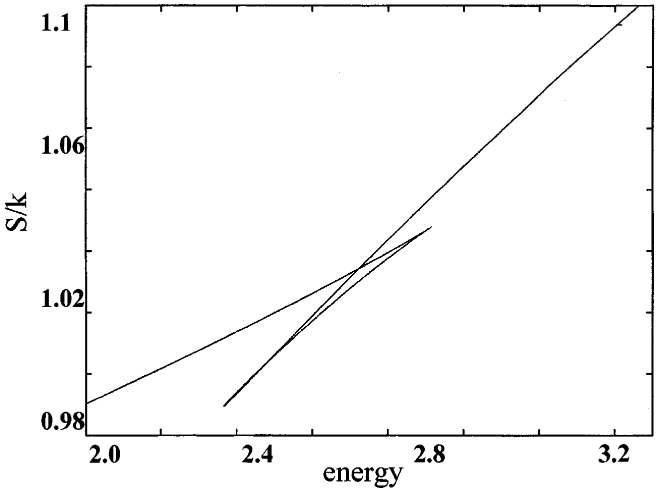

FIG. 2. Entropy vs energy for isolated system in two phase region.

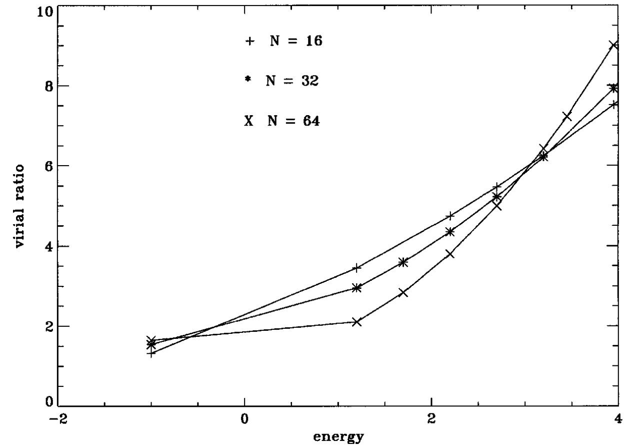

FIG. 3. Virial ratio vs energy for $N = 16$, 32, and 64 shells.

Note the sharp temperature decrease as the system becomes less concentrated. This occurs because above the transition ($a > a_c$) the isolated gravitational system can support a negative heat capacity [7].

In earlier work we compared dynamical simulations of systems with $N = 16$, 32, and 64 shells with the Vlasov equilibrium predictions for $a > a_c$ [15]. We found good agreement with increasing N. At the largest value, the time averaged density profile agreed within a few percent with the mean field predictions obtained from the numerical solution of (1) over the complete interval (a, b). Here we have extended the simulations into the transition region. For given inner barrier radius, away from the transition energy we also find close agreement with the mean field density profile. However, as the transition is approached, differences occur. This is expected: Finite size scaling theory [18] predicts that the transition is sharp only in the limit $N \to \infty$. For finite N the transition energy is shifted as $N^{-\lambda}$ and broadened as $N^{-\gamma}$. By comparing the time averaged virial ratio from simulations with the predicted mean field values, we found that the results accurately conformed to the scaling predictions with shifting and rounding exponents of 0.97 and 0.74 (see Fig. 3).

(b) Canonical ensemble: The system is no longer isolated and may now exchange energy with a reservoir at constant temperature $\theta \equiv 1/\beta$. For a given population the thermodynamic state is determined by a and θ. Equilibrium states are states of minimum Helmholtz free energy [17]. In common with the entropy, for $a < a_c$, it too is a multivalued function of θ for $1/\theta \in \Delta\beta(a)$. As before, mean field theory predicts a sharp transition where the free energies of the two phases intersect. However, here there is a jump in the value of E while β remains constant, showing that the thermodynamic behavior of a gravitational system depends on the specific ensemble. In the canonical ensemble negative heat capacities cannot be supported in equilibrium [7]. The coexistence curve now bisects a portion of the (a, θ) plane.

Dynamical simulation of the canonical ensemble was accomplished by converting the reflecting barrier at $r = b$ into an isothermal wall for every hundredth collision. In such an event, detailed balance is respected by returning the shell to the system with kinetic energy determined by randomly sampling the exponential distribution with mean θ. Again good agreement was found between the time averaged density profile and that predicted by mean field theory away from the transition temperature. Near the transition the results were again consistent with finite size scaling, but with shifting and rounding exponents of 1.1 and 1.4.

An interesting feature of the simulations was the robustness of the concentrated phase *above* the transition temperature, where it is thermodynamically less stable than the more uniform phase. For $N > 16$, if the system was prepared in the former, we were never able to observe a dynamical phase transition to the more stable phase during the typical run times of the numerical experiments. Another interesting feature was the lack of critical slowing down. The point on the coexistence curve where $a = a_c$ is a thermodynamic critical point of the system. In our dynamical simulations, measurements of both temporal and positional correlation functions were carried out for the thermostated system. While differences were found in each phase, no hint of divergence of the relaxation time or length was indicated near the critical point. However, strong positional correlation occurred across the entire system when $a \geq a_c$, i.e., in the "fluid" phase.

(c) Grand canonical ensemble: The system can now exchange both energy and particles (shells) with a reservoir. An equilibrium thermodynamic state is defined by θ and μ, the temperature and chemical potential of the reservoir, as well as the inner barrier radius a. For the sake of comparison, for each a and θ the value of μ was fixed by requiring that the average system mass is unity, i.e., the same as for each of the ensembles described above. In equilibrium, the grand potential has a global minimum for the stable state [17]. Plots of Φ vs θ do not exhibit the kink structure found for the other thermodynamic potentials, even for $a < a_c$. In contradistinction with both the microcanonical and canonical ensembles, here mean field theory predicts that the more uniform phase is more stable over the complete (a, θ) plane. Thus a transition to a more centrally concentrated density profile is not predicted.

Dynamical simulation of the open system (grand canonical ensemble) was accomplished by randomly introducing new shells at the outer barrier with a carefully chosen mean creation rate. This was selected by imitating the effect of a reservoir surrounding the system with the desired temperature and chemical potential. To weaken the interaction between the system and reservoir, the boundary was assumed to be only "semipermeable" [17]. The creation rate was chosen to be only one hundredth of the virtual external particle flux striking the outer barrier. The kinetic energy of a new shell was chosen by employing the same thermostat described above for the canonical ensemble. To balance the flux, every hundredth system shell striking the outer barrier from within was removed from the system.

As above, the results of the dynamical simulations were in complete accord with the mean field predictions. The system was initiated with a variety of initial conditions. In each case the time averaged density profile agreed with that predicted for the more uniform phase. No sign of a transition was every observed, even when the initial state was highly concentrated near the inner barrier.

(III) Conclusions.—The one-dimensional systems described above are the simplest gravitating systems we can construct, lacking the complicating features associated with escape and binary formation. Because simulating their evolution is similar to iterating a multidimensional map, they are ideal testing grounds for dynamical theories. After a rocky start, it has been recently shown that the dynamics of both one [19] and two [20] component systems of parallel mass sheets conform to the predictions of mean field (Vlasov) theory. Here we have demonstrated via dynamical simulation that the shell system also follows this pattern.

Although relaxation in the shell system proceeds at a much higher rate than the parallel mass sheets, the reason for this is not known. The presence of the reflecting barriers may play an important role. Relaxation in either system is still not understood. A diffusion model of relaxation based on a maximal stochastic assumption has been introduced [21] which may explain the gross features but, to date, it has been only marginally tested for the sheet system [22]. It predicts a relaxation time scale proportional to the population, and has yet to be applied to the shell system.

A final issue is whether the shell system behavior has relevance for astrophysics. Certainly the observations of galactic nuclei and globular clusters reveal a wide variety of structures. Is there a connection between the observed core-halo structures and the centrally concentrated phase described in the preceding pages? Both globular clusters and galactic nuclei may be closest in essence to a grand canonical ensemble since each can exchange both energy and mass with its surroundings. We have shown that the thermodynamic properties of the open system are very different from the constant temperature and constant energy ensembles and, for our simple model, a transition to a condensed state will not take place. In the earliest paper which considers a mean field approach to a gravitating system, Aronson and Hansen raise the question of whether the introduction of a semipermeable membrane will alter the structural stability of a gravitating system [6]. Here we have provided an answer for this specific model.

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