

## Phase transitions in systems with $1/r^\alpha$ attractive interactions

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Collapse, or a gravitational-like phase transition is studied in a microcanonical ensemble of particles with an attractive  $1/r^\alpha$  potential. A mean-field continuous integral equation is used to determine a saddle-point density profile that extremizes the entropy functional. For all  $0 < \alpha < 3$ , a critical energy is determined below which the entropy of the system exhibits a discontinuous jump. If an effective short-range cutoff is applied, the entropy jump is finite; if not, the entropy diverges to  $+\infty$ . A stable integral equation solution represents a state with maximal entropy; the reverse is always true only for a modified integral equation introduced here.

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### I. INTRODUCTION

The behavior of systems with long-range interactions is often different from those considered in traditional thermodynamics. As an example we take self-gravitating systems, i.e., particle ensembles with purely attractive  $1/r$  interactions. It is known that such systems exhibit collapse, sometimes called a zero-order phase transition, when the energy in the microcanonical ensemble (ME) or the temperature in the canonical ensemble (CE) drop below a certain critical value  $e_c$  or  $T_c$ , respectively [1–3]. During such a transition, the corresponding thermodynamic potentials (entropy in the ME or free energy in the CE) exhibit a discontinuous jump. If the interaction between the particles is purely attractive and no short-range cutoff is introduced, then the discontinuous jump is infinite and the entropy and free energy go to  $+\infty$  and  $-\infty$ , respectively. This makes all normal (noncollapsed) states of the self-attractive system metastable with respect to such a collapse; the collapse energy  $e_c$  is in fact an energy below which the metastable state ceases to exist. If, on the other hand, some form of short-range cutoff is introduced, the entropy and free energy jumps are finite. In this case as a result of the collapse, the system goes into a nonsingular state with a dense core, the precise nature of which depends on the details of the short-range behavior of the potential. Then only the normal states that are in some interval of energies above the collapse point are metastable with respect to such a transition (see Fig. 1).

There is an energy  $e^*$  for which both collapsed and normal system have the same entropy (cf.  $e_1^*$  and  $e_2^*$  in Fig. 1); above this energy the collapsed state becomes metastable and at some higher energy it ceases to exist [4,5]. It is possible to regard the energy  $e^*$  as that where a true phase transition occurs. When the effective cutoff vanishes, such phase transition energy  $e^*$  increases to infinity, so that without a cutoff all the finite energy states are metastable [6]. However, the value of  $e^*$  is highly sensitive to the details of the short-range cutoff. On the contrary, the collapse energy  $e_c$  depends on the long-range part of the interparticle interactions and is almost unaffected by a cutoff, provided that it is sufficiently short range. Therefore, in studies of the phase behavior of the long-range interacting systems, the collapse phenomena usually gain the most attention, considering then

a phase transition at  $e^*$  as a mere artifact of an often auxiliary cutoff.

While these rather elaborate studies of gravitational collapse have usually been motivated by cosmological applications and were performed solely for an  $1/r$  potential, a natural question is, what happens if the particles interact via an attractive  $1/r^\alpha$  potential with arbitrary  $\alpha$ . Apart from pure theoretical interest and possible astrophysical applications, systems with  $1/r^\alpha$  potentials are often found in condensed-matter physics. It has been noticed before that in systems with nonintegrable interactions, i.e., when  $\alpha$  is less than the dimensionality of the space, first-order phase transitions occur differently in the ME than in the CE, even for  $N \rightarrow \infty$  [7]. However, in the examples considered in the literature, the potential energy was always bounded from below (usually by putting the system on a lattice), allowing only for normal first-order phase transitions and excluding any singular collapse.

In this work we consider a possibility of collapse in systems, similar to the gravitational self-attracting Hamiltonian particle systems, but with a general  $1/r^\alpha$  potential. The paper is organized as follows: after this brief introduction we for-

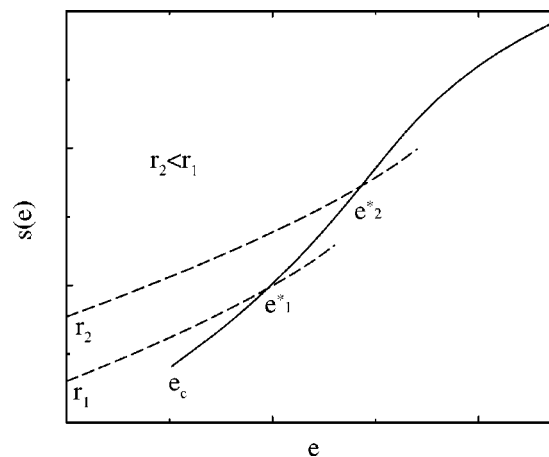


FIG. 1. Sketch of an entropy vs energy plot for a system with gravitational-like collapse. The entropy of the normal (noncollapsed) state is shown by a solid line, the entropies of the two collapsed states for different cutoff radii  $r_1$  and  $r_2$ ,  $r_2 < r_1$ , are shown by dashed lines. The entropies of the two collapsed states intersect the entropy of the normal state at energies  $e_1^*$  and  $e_2^*$ .

mally define the model and derive an integral equation to solve for a saddle-point density profile. Then we describe the results obtained by a numerical iterative solution of this equation for various  $0 < \alpha < 3$ . After this, we look at the local stability of the solutions of the integral equation and link their stability to the stability (metastability) of the corresponding states of the self-attracting system. Finally, we discuss the results and directions for further investigation.

While the collapse is shown to be a generic property of self-gravitating systems occurring in both the ME and the CE, the ME allows to obtain more information about the system than the CE. For example, negative heat-capacity states, that precede the collapse in the ME, are not accessible in the CE, as it is in the much better studied case of normal first-order phase transitions [8,7,9]. In the rest of our paper we consider systems only in the ME. In our studies we strongly rely on the large body of existing results derived for  $\alpha = 1$ , often rigorously [2,3,10].

## II. THE MODEL

Let us consider a three-dimensional ME of  $N$  particles each having mass  $m$ , interacting with an attractive pair potential  $V_{ij} = -G/|\vec{r}_i - \vec{r}_j|^\alpha$ . These particles are confined to a spherical container with radius  $R$ ; the total energy of the particles is  $E$ . The microcanonical entropy (equal to the logarithm of the density of states; here and in the following we put  $k_B = 1$ ) can be expressed as

$$S(E) = \ln \left\{ \frac{1}{N!} \int \dots \int \prod_{k=1}^N \frac{d\vec{p}_k d\vec{r}_k}{(2\pi\hbar)^3} \delta \left[ E - \sum_{l=1}^N \frac{p_l^2}{2m} - \sum_{i=1}^N \sum_{j=1+1}^N V_{ij} \right] \right\}, \quad (1)$$

After integrating over the momenta and introducing a dimensionless energy  $\epsilon = ER^\alpha/GN^2$  and radial coordinates  $x_i \equiv r_i/R$ , Eq. (1) can be reduced to

$$S(\epsilon) = S_0 + \ln \left[ \int \dots \int \prod_{k=1}^N d\vec{x}_k \Theta(\epsilon_{kin}) \epsilon_{kin}^{3N/2-1} \right], \quad (2)$$

where  $\epsilon_{kin}$  is a dimensionless kinetic energy

$$\epsilon_{kin} = \epsilon + \frac{1}{N^2} \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|^\alpha}, \quad (3)$$

and  $S_0$  is an energy-independent term

$$S_0 = \ln \left[ 2m \left( \frac{m}{2\pi\hbar^2} \right)^{3N/2} \left( \frac{GN^2}{R^\alpha} \right)^{3N/2-1} \frac{R^{3N}}{\Gamma(3N/2)N!} \right]. \quad (4)$$

Here  $\Gamma(x)$  is a Gamma function,  $\Theta(x)$  is a unit step function that guarantees positiveness of the kinetic energy, and the integration for each  $d\vec{x}_i$  runs over a three-dimensional unit sphere. It follows from Eq. (2) that the entire thermodynamic behavior of our system depends on the single variable  $\epsilon$ ; and for a system to remain in the same state when the num-

ber of particles is varied but the energy per particle is fixed, the system size  $R$  should scale as  $R \sim N^{1/\alpha}$ . This indicates that  $\alpha = 3$  is the largest value of  $\alpha$  for which no thermodynamic scaling is observed and hence some nontraditional phase transitions may exist.

We assume that the number of particles  $N$  is large and go to a continuum limit, replacing a  $3N$ -dimensional configurational integral in Eq. (2) by a functional integral over possible density profiles  $\rho(\vec{x})$  (see, for example, [2,3]),

$$S(\epsilon) \approx S_0 + \ln \left\{ \int \mathcal{D}\rho \int_{-i\infty}^{+i\infty} \frac{d\gamma}{2\pi i} \int_{-i\infty}^{+i\infty} \frac{d\beta}{2\pi i} \times \exp\{N\tilde{s}[\rho(\cdot), \epsilon, \gamma, \beta]\} \right\}, \quad (5)$$

where the ‘‘effective action’’ functional  $\tilde{s}$  is defined

$$\begin{aligned} \tilde{s}[\rho(\cdot), \epsilon, \gamma, \beta] = & \beta \left( \epsilon + \frac{1}{2} \int \int \frac{\rho(\vec{x}_1)\rho(\vec{x}_2)}{|\vec{x}_1 - \vec{x}_2|^\alpha} d\vec{x}_1 d\vec{x}_2 \right) \\ & + \gamma \left( \int \rho(\vec{x}) d\vec{x} - 1 \right) - \frac{3}{2} \ln \beta \\ & - \int \rho(\vec{x}) \ln \frac{\rho(\vec{x})}{e} d\vec{x}. \end{aligned} \quad (6)$$

Here we introduced two auxiliary Fourier integrations: one over  $d\beta$  to replace the  $\Theta$  function in Eq. (4) (see e.g. [2]),

$$x^\sigma \Theta(x) = \frac{\Gamma(\sigma+1)}{2\pi} \int_{-\infty}^{+\infty} e^{i\omega x} \frac{d\omega}{(i\omega)^{\sigma+1}}, \quad (7)$$

and similarly one over  $d\gamma$  to express the  $\delta$  function  $\delta[\int \rho(\vec{x}) d\vec{x} - 1]$ . Equation (5) is applicable only for  $0 < \alpha < 3$  when the integrals on  $d\vec{x}_1$  and  $d\vec{x}_2$  are convergent at the lower limit.

Using that  $N$  is large, the integral in Eq. (5) can be evaluated by the saddle-point (mean field) method. To determine the dominant contributions to the integral, we differentiate Eq. (6) with respect to  $\gamma, \beta$ , and  $\rho(\vec{x})$  and look for  $\{\gamma_s, \beta_s, \rho_s(\vec{x})\}$ , which give the extrema to the effective action (6). As a result, unique solutions are obtained for  $\{\gamma_s, \beta_s\}$ ; while for  $\rho_s(\vec{x})$  a nonlinear integral equation is obtained for which the number and the nature of solutions is generally unknown,

$$\begin{aligned} \gamma_s = & -\ln \left\{ \int \exp \left[ \frac{\beta_s \rho_s(\vec{x}_1)}{|\vec{x}_1 - \vec{x}_2|^\alpha} d\vec{x}_1 \right] d\vec{x}_2 \right\}, \\ \beta_s = & \frac{3}{2} \left[ \epsilon + \frac{1}{2} \int \int \frac{\rho_s(\vec{x}_1)\rho_s(\vec{x}_2)}{|\vec{x}_1 - \vec{x}_2|^\alpha} d\vec{x}_1 d\vec{x}_2 \right]^{-1}, \\ \rho_s(\vec{x}) = & \exp \left[ \gamma_s + \beta_s \int \frac{\rho_s(\vec{x}_1)}{|\vec{x}_1 - \vec{x}|^\alpha} d\vec{x}_1 \right]. \end{aligned} \quad (8)$$

It follows from Eq. (8) that  $\beta_s$  is equal to 3/2 of the inverse kinetic energy, hence it is equal to the entropy derivative with respect to the energy, i.e., to the inverse temperature,  $\beta_s = [\partial s(\epsilon)/\partial \epsilon]_R \equiv 1/T$ .

Using Eqs. (6) and (8) and ignoring terms independent of  $\epsilon$ , we obtain for the entropy per particle  $s(\epsilon) = S(\epsilon)/N$  in the saddle-point approximation

$$s(\epsilon) = \frac{3}{2} \ln \left[ \epsilon + \frac{1}{2} \int \int \frac{\rho(\vec{x}_1)\rho(\vec{x}_2)}{|\vec{x}_1 - \vec{x}_2|^\alpha} d\vec{x}_1 d\vec{x}_2 \right] - \int \rho(\vec{x}) \ln[\rho(\vec{x})] d\vec{x} + \mathcal{O}\left(\frac{1}{N}\right). \quad (9)$$

The mean-field saddle-point approximation works only if the second derivatives of the effective action functional  $\tilde{s}$  are not too small; we will return to the question of its validity in Sec. IV.

The above equations look similar to those for the gravitational ( $\alpha=1$ ) cases that are derived, for example, in Refs. [2,3], to where the reader is referred for a more detailed description of the derivation. However, we cannot proceed further along the lines developed in the references mentioned above, all of which deal with the gravitational case. For, unlike the gravitational case, when the  $\Delta(1/r) = -4\pi\delta(r)$  property of a Coulomb interaction  $1/r$  allows one to reduce Eq. (8) to a second-order differential equation, no such property exists for a general  $\alpha$ , and we have to deal with the integral equation for  $\rho_s(\vec{x})$  in Eq. (8) directly.

In what follows a further simplification is made by disregarding the angular dependence for the saddle-point density profile, i.e.,  $\rho(\vec{x}) = \rho(x)$ ; for the gravitational case this is justified in Refs. [2,3]. After performing a straightforward angular integration in the exponential of Eq. (8), we obtain for  $\alpha \neq 2$ ,

$$\rho(x) = \rho_0 \exp \left\{ \frac{2\pi\beta_s}{(2-\alpha)x} \int_0^1 \rho(x_1)x_1[(x+x_1)^{(2-\alpha)} - |x-x_1|^{(2-\alpha)}] dx_1 \right\},$$

$$\rho_0 = \left\{ \int_0^1 \exp \left[ \frac{2\pi\beta_s}{(2-\alpha)x'} \int_0^1 \rho(x_1)x_1((x'+x_1)^{(2-\alpha)} - |x'-x_1|^{(2-\alpha)}) dx_1 \right] dx' \right\}^{-1}, \quad (10)$$

$$\beta_s = \frac{3}{2} \left\{ \epsilon + \frac{4\pi^2}{(2-\alpha)} \int_0^1 \int_0^1 \rho(x_1)\rho(x_2)x_1x_2[(x_1+x_2)^{(2-\alpha)} - |x_1-x_2|^{(2-\alpha)}] dx_1 dx_2 \right\}^{-1};$$

and for  $\alpha=2$ ,

$$\rho(x) = \rho_0 \exp \left\{ \frac{2\pi\beta_s}{x} \int_0^1 \rho(x_1)x_1[\ln(x+x_1) - \ln|x-x_1|] dx_1 \right\},$$

$$\rho_0 = \left\{ \int_0^1 \exp \left[ \frac{2\pi\beta_s}{x+x'} \int_0^1 \rho(x_1)x_1[\ln(x'+x_1) - \ln|x'-x_1|] dx_1 \right] dx' \right\}^{-1}, \quad (11)$$

$$\beta_s = \frac{3}{2} \left\{ \epsilon + 4\pi^2 \int_0^1 \int_0^1 \rho(x_1)\rho(x_2)x_1x_2[\ln(x_1+x_2) - \ln|x_1-x_2|] dx_1 dx_2 \right\}^{-1}.$$

Once the Eqs. (10) and (11) have been solved and the entropy (9) has been calculated, the nature of the phase behavior of the system can be deduced from an entropy-energy plot. In the next section we analyze the Eqs. (10) and (11) numerically.

### III. NUMERICAL SOLUTION

If  $\beta_s$  is considered an independent parameter rather than a factor depending on  $\epsilon$  and  $\rho_s$ , the Eq. (8) is often called a generalized Poisson-Boltzmann-Emden equation [10]. Very little is known about this equation even in the gravitational  $\alpha=1$  case. The only exactly known, so called ‘‘singular,’’ solution is for  $\beta_s=2$  [10] and has the form  $\rho_{sing}(x) = (4\pi x^2)^{-1}$ , which leads to  $\epsilon = -1/4$  and  $s = \ln(\sqrt{2}\pi) - 2$ . However, we are interested here in general  $\alpha$  and  $\epsilon$ ; and  $\beta_s$  in the ME is not an independent variable but a function of  $\epsilon_s$ . As we will discuss below, this has a crucial effect on the numerical accessibility of solutions in a certain interval of  $\epsilon$ .

To solve the Eqs. (10) and (11) numerically for general  $\alpha$  and  $\epsilon$ , we use a simple iterative method. For a fixed  $\alpha$  we start at a relatively high value of  $\epsilon$  with a flat density profile,  $\rho_0 = 3/4\pi$ , which is the solution of Eqs. (10) and (11) for  $\epsilon \rightarrow +\infty$ . Putting  $\rho_0$  into Eqs. (10) and (11), we calculate  $\beta_s$  and obtain a new density profile  $\rho_1(x)$ . In other words, an iterative map

$$\rho_{i+1}(x) = F_\epsilon[\rho_i(\cdot), x], \quad (12)$$

is introduced, with a nonlinear functional  $F_\epsilon[\rho_i(\cdot), x]$  defined by Eqs. (10) and (11).

After a sufficient convergence of the iterations Eq. (12) is achieved, i.e., when

$$4\pi \int_0^1 |\rho_{i+1}(x) - \rho_i(x)| x^2 dx < \delta \ll 1, \quad (13)$$

the entropy is calculated with Eq. (9). We then move to a lower-energy point, use the previous energy point density profile as  $\rho_0$ , and repeat the procedure again. Caution in

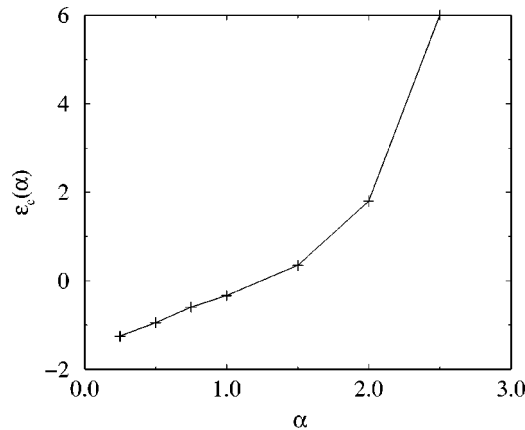


FIG. 2. Plot of collapse energy  $\epsilon_c(\alpha)$  vs potential exponent  $\alpha$ .

selecting the initial energy as well as the energy step has to be exercised to maintain the positiveness of the kinetic energy. In fact the initial energy has to be larger than  $-[3^2 2^{2-\alpha}/(6-\alpha)(4-\alpha)(3-\alpha)]$ , which is the potential energy for the flat density profile. As we progress towards lower energies, the density profiles get more and more peaked near the origin, and the absolute value of the potential energy increases. To allow for improper integrals in the numerical integration of Eqs. (10) and (11), we use a simple midpoint trapezoid rule. Uniform meshes of 1000–2000 points were usually sufficient. However, in order to determine the position of a phase transition point with a sufficiently high precision in order to compare our results to the existing ones for  $\alpha=1$ , and to achieve also a discontinuous phase transition for smaller  $\alpha$ , we had to use finer meshes with up to 5000 points. The convergence parameter  $\delta$  was usually set to be  $10^{-6}$ .

The main conclusion that can be derived from the numerical results obtained is the following: for all  $0 < \alpha < 3$ , as for  $\alpha=1$ , there is a certain energy  $\epsilon_c(\alpha)$  below which the system collapses and the entropy exhibits a discontinuous jump. The results for  $\epsilon_c(\alpha)$  are presented in Fig. 2. To verify our calculations of  $\epsilon_c(\alpha)$ , we compare our result for  $\epsilon_c(\alpha=1)$  with the existing data obtained by other methods. Our number,  $\epsilon_c(\alpha=1) = -0.3346$ , is consistent with  $\epsilon_c(\alpha=1) = -0.335$ , quoted in Refs. [3,4].

Since the behavior of self-attractive systems is quantitatively similar for all  $0 < \alpha < 3$ , let us consider in more detail, for example, a system with  $\alpha=1/2$ . Plots of entropy  $s(\epsilon)$  and inverse temperature  $\beta_s(\epsilon) = ds(\epsilon)/d\epsilon$  are presented in Fig. 3.

As we go down along the energy axis  $\epsilon$ , the entropy decreases as well, passing through an inflection point  $\epsilon_i$  where  $\beta$  reaches its maximum  $\beta_m$ . For energies below this inflection point, the system has a negative specific heat [ $d^2s(\epsilon)/d\epsilon^2 > 0$ ] and is, therefore, unstable in the CE. As we pass through the  $\epsilon_i$  point and continue decreasing the energy, the convergence of Eq. (12) becomes slower and slower, and at the point  $\epsilon_c$  the iterations start to diverge. It is straightforward to show for all  $0 < \alpha < 3$  (see, e.g., [10] for  $\alpha=1$ ) that the entropy is unbounded from above with respect to uniform squeezing of all the matter into a sphere with a radius going

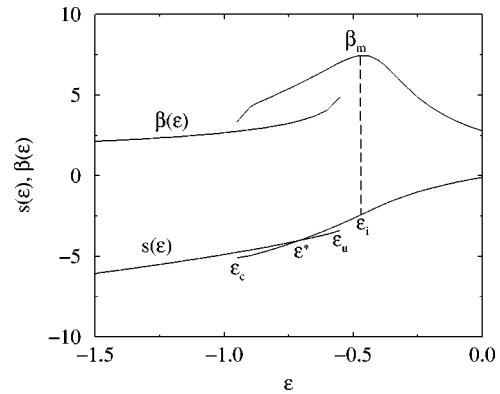


FIG. 3. Plots of entropy  $s(\epsilon)$  and entropy derivative  $\beta(\epsilon)$  for  $\alpha=1/2$ . The radius of excluded central volume  $r_0=5 \times 10^{-4}$ . The points  $\epsilon_c, \epsilon^*, \epsilon_u$ , and  $\epsilon_i$  are defined in the text.

to zero. Hence, if no short-range cutoff is present, it is reasonable to assume that the entropy discontinuity at  $\epsilon_c(\alpha)$  is infinite.

If some form of a short-range cutoff is introduced, the entropy discontinuity may become finite. To investigate this we tried two approaches. One, suggested in Ref. [4], is to place a small spherical excluded volume with a radius  $r_0$  in the center of the system, or, in other words, to replace a spherical container with a spherical shell container. The other approach is to replace the original ‘‘bare’’ potential  $1/r^\alpha$  with a ‘‘soft’’ potential of the form  $1/(r^2 + r_0^2)^{2\alpha}$ . For a reasonably small short-range cutoff ( $r_0 \sim 10^{-3}$  for small  $\alpha$ ,  $r_0 \sim 10^{-2}$  for  $\alpha \approx 3$  for both approaches) the behavior of the precollapsed system is virtually unaffected. A finiteness of the integration mesh can also play the role of an effective central excluded volume; for our method of integration the size of such an effective excluded volume is roughly of the order of the mesh step. Our numerical studies indicate that both the central core and the soft potential short-range cutoff approaches lead to qualitatively similar phase behavior.

Introduction of a short-range cutoff makes the existence of a nonsingular collapsed phase possible. However, being applied directly, the iterative method (12) still diverges when  $\epsilon < \epsilon_c$ . To make it convergent, we introduced a map with a variable ‘‘step’’

$$\rho_{i+1}(x) = \sigma F[\rho_i(\cdot), \epsilon] + (1 - \sigma)\rho_i(x), \quad (14)$$

where  $0 < \sigma \leq 1$  is the step size parameter. Choosing  $\sigma$  sufficiently small (as small as  $\sim 10^{-2} - 10^{-3}$ ), we were able to make the algorithm convergent for  $\epsilon < \epsilon_c$ . The connection between the numerical stability of the iterative algorithm and the thermodynamic stability of the corresponding phase is analyzed in the next section. A typical density profile in the collapsed phase exhibits a much higher concentration around the origin than to the normal (uncollapsed) phase; plots of density profiles for  $\alpha=1/2$  are presented in Fig. 4.

A collapsed phase exists not only for  $\epsilon < \epsilon_c$ , but for  $\epsilon > \epsilon_c$  as well. In fact, this phase is globally stable in the range of energies where its entropy is higher than that of the normal phase, i.e., when  $\epsilon < \epsilon^*$ . For  $\epsilon > \epsilon^*$ , the collapsed phase is metastable and above some energy  $\epsilon_u$  becomes unstable



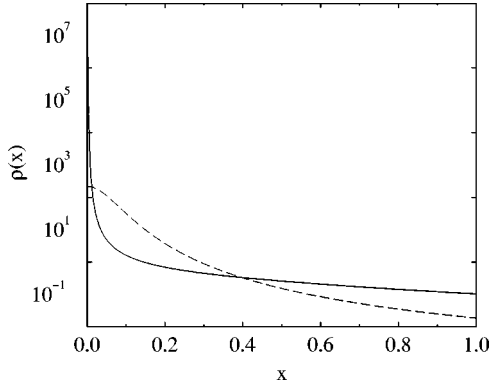


FIG. 4. Density profiles  $\rho(x)$  for  $\alpha=1/2$  for normal (dashed line) and collapsed (solid line) phases for the energy  $\epsilon^* = -0.708$ , when entropies of both phases are the same. The radius of the excluded central volume is  $r_0 = 5 \times 10^{-4}$ .

even locally (see Fig. 3). However, being cutoff dependent,  $\epsilon^*$  and  $\epsilon_u$  are not directly related to the fundamental properties of the original  $1/r^\alpha$  self-attracting system.

Finally we return to the exact  $\rho_{sing}(x) = (4\pi x^2)^{-1}$  solution that exists for  $\epsilon = -1/4$  and  $\alpha = 1$ . Our attempts to approach this solution by the numerical iterative methods (12) and (14) failed. In fact, even after substituting the  $\rho_{sing}(x)$  into Eq. (14) as an initial approximation  $\rho_0(x)$ , the iterative solution of Eq. (14) evolved either to a normal or to a collapsed solution depending on the value of the step  $\sigma$ . We calculated the entropies for the three solutions, that exist at  $\epsilon = -1/4$ : a normal  $s_n$ , a collapsed  $s_c$  (with a sufficiently small central core, so that it still exists at this energy), and a  $s_{sing}$  for  $\rho_{sing}$ . It turns out that  $s_{sing} < \min\{s_n, s_c\}$ , which, together with the evidence obtained from the iterative procedures mentioned above, strongly suggests that in the space of solutions (or fixed points) of Eq. (14), both normal and collapsed  $\rho(x)$  are at least locally stable (attractive), while  $\rho_{sing}$  is unstable (repulsive).

#### IV. STABILITY OF THE THERMODYNAMIC STATE AND THE ITERATIVE MAP

The iterative solutions of the integral equations (10) and (12) for the saddle point density profile  $\rho_s(x)$  of the self-attracting system correspond to thermodynamically stable or unstable states. In this section we will give the necessary and the sufficient conditions for the thermodynamic stability of the  $\rho_s(x)$  in terms of the stability of the iterative solutions of the integral equation (10). To that end we will look at the stability of Eq. (12) for a certain trial function  $\rho_i(x)$ . Let us assume that  $\rho_s(x)$  is a solution (fixed point) of (12), and  $\delta\rho_i(x) = \rho_i(x) - \rho_s(x)$  is a small deviation of the  $i$ th iteration from the solution  $\rho_s(x)$ . After one iteration we obtain for  $\delta\rho_{i+1}(x) = \rho_{i+1}(x) - \rho_s(x)$ ,

$$\delta\rho_{i+1}(x) = \int_0^1 \frac{\delta F_\epsilon[\rho(\cdot), x]}{\delta\rho(x')} \Bigg|_{\rho=\rho_s} \delta\rho_i(x') dx' + O(\delta\rho^2). \quad (15)$$

For the iterations to converge,  $|\delta\rho_{i+1}(x)| < |\delta\rho_i(x)|$  for all  $x$ . This condition is equivalent to a requirement that the absolute values of all the eigenvalues  $\lambda_i$  of the first variation operator defined below are less than one,

$$\lambda_i \phi_i(x) = \int_0^1 \frac{\delta F_\epsilon[\rho(\cdot), x]}{\delta\rho(x')} \Bigg|_{\rho=\rho_s} \phi_i(x') dx', \quad (16)$$

where the  $\phi_i$  are the eigenfunctions corresponding to  $\lambda_i$ . Recalling the definition of  $F_\epsilon[\rho(\cdot), x]$  (8),(10),(11) we note that it can be expressed through a first variation of the effective action functional  $\tilde{s}[\rho(\cdot), \epsilon, \gamma, \beta]$ ,

$$F_\epsilon[\rho(\cdot), x] = \exp \left[ \frac{\delta \tilde{s}[\rho(\cdot), \epsilon, \gamma, \beta]}{\delta\rho(x)} \Bigg|_{\gamma=\gamma_s, \beta=\beta_s} + \ln\rho(x) \right]. \quad (17)$$

Then one obtains for the first variation of  $F_\epsilon[\rho(\cdot), x]$ ,

$$\frac{\delta F_\epsilon[\rho(\cdot), x]}{\delta\rho(x')} \Bigg|_{\rho=\rho_s} = \rho_s(x) \frac{\delta^2 \tilde{s}[\rho(\cdot), \epsilon, \gamma, \beta]}{\delta\rho(x) \delta\rho(x')} \Bigg|_{\gamma=\gamma_s, \beta=\beta_s, \rho=\rho_s} + \delta(x-x'). \quad (18)$$

Now for a state  $\rho_s(x)$  to be thermodynamically stable and for the saddle-point approximation to be applicable at all, the second variation of the effective action  $\tilde{s}$  on the right-hand side of Eq. (18) must be negative for all  $x$  and  $x'$ . This is equivalent to the requirement that all the eigenvalues of the operator on the right-hand side of Eq. (18) are less than one. For, the only eigenvalue of the delta function  $\delta(x-x')$  is one with any function being its eigenfunction and the density  $\rho_s(x)$  is strictly positive for all  $0 \leq x \leq 1$ . Hence, the convergence of the map (12) to the function  $\rho_s(x)$  is a sufficient condition for the thermodynamic stability of  $\rho_s(x)$  and the validity of the saddle-point approximation. However, the reverse is not true, i.e., stable thermodynamic states do not necessarily correspond to stable iterative solutions. For, the operator on the left-hand side of Eq. (18) may have eigenvalues that are less than  $-1$ , which will make the map (12) unstable. Therefore, let us instead of Eq. (12) consider the variable step map (14) with eigenvalues of its first variation  $\lambda_i^*(\sigma) = \sigma\lambda_i + (1-\sigma)$ . Then for any negative  $\lambda_i$  we can choose an appropriate  $\sigma$  so that  $|\lambda_i^*(\sigma)| < 1$ . Evidently, this is what happened in the case of the collapsed phase, which possessing the highest entropy, is definitely stable, but can be accessed numerically only by using Eq. (14) with a sufficiently small  $\sigma$ . On the other hand, for thermodynamically unstable states, such as  $\rho_{sing}$ , some of the eigenvalues of the operator in the right-hand side of Eq. (18) are larger than 1, which make the iterative maps (12) and (14) unstable, so that such solutions cannot be found iteratively. This completes the demonstration of the equivalence of the two stabilities.

## V. DISCUSSION

(1) In the previous sections we revealed the existence of collapse and associated with it a discontinuity in the entropy in the microcanonical ensemble of particles with  $1/r^\alpha$  attraction for  $0 < \alpha < 3$ . This discontinuity was an infinite jump if no short-range cutoff was present. A carefully introduced short-range cutoff leaves the properties of precollapsed system virtually unaffected, but makes the entropy jump finite and allows to observe the collapsed phase. We proved that the stability of the iterative method of solution of the integral equation for a saddle-point density profile is a sufficient condition for the profile to make the entropy a maximum and, therefore, be either stable or metastable. We modified the iterative method to make the reverse also true.

(2) In the range of  $\alpha$  we have been working with,  $0 < \alpha < 3$ , the potential is often called “nonintegrable,” since the integral  $\int d^3r/r^\alpha$  diverges at its upper limit. As the potential becomes integrable ( $\alpha > 3$ ), the continuum approach used here becomes inapplicable because the short-range density fluctuations, which the continuous approach cannot account for, become dominant over the long-range effects. Formally, the short-range nature of the behavior of the systems for  $\alpha > 3$  manifests itself as the divergence of the integral  $\int d^3r/r^\alpha$  at its lower limit.

(3) A very important question which remains is that of the order of the gravitation-like phase transition. Here we have to distinguish between the collapse itself, that happens at  $\epsilon_c$ , and the phase transition which happens at the energy  $\epsilon^*$  where the entropies of noncollapsed and collapsed states are equal (see Fig. 3). Since the entropy at the collapse point  $\epsilon_c$  exhibits a discontinuous jump, the collapse is often called a zero-order phase transition [2]. However, the collapse is not a normal phase transition since it converts a metastable state into a stable one, which can be singular or finite, depending on the presence of the short-range cutoff.

On the other hand, the “true” phase transition between stable phases, which happens at  $\epsilon^*$ , is sometimes referred to as a “gravitational first-order phase transition” [5]. Its distinct features include an inability of the two phases (noncollapsed and collapsed) to coexist and a discontinuous  $\beta(\epsilon)$ , i.e., temperature [5]. Yet in the “normal” ME first-order phase transition in a long-range interacting system (such as a mean-field Potts model),  $\beta(\epsilon)$  remains continuous and smooth, but exhibits non monotonous behavior: the interval of energies where phases coexist includes an interval where  $d\beta(\epsilon)/d\epsilon$  is positive and the specific heat is negative (see

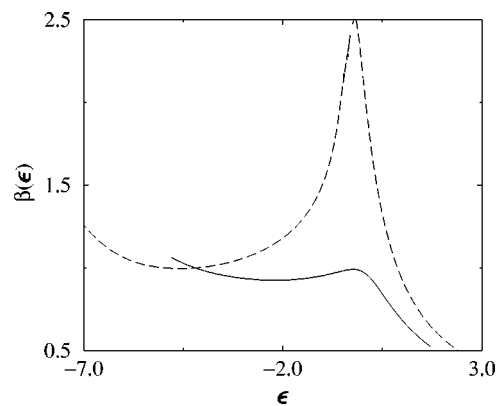


FIG. 5. Entropy derivative  $\beta(\epsilon) = ds(\epsilon)/d\epsilon$  vs energy  $\epsilon$  plot for  $\alpha=2$  and central core radius 0.5 (solid line), and  $\alpha=1$  and soft potential radius 0.05 (dashed line).

Fig. 5) [7–9]. Hence there is an intrinsic difference between the normal and the gravitational first-order phase transitions.

Even more, normal first-order phase transitions are found to replace gravitational first-order phase transitions that occur in the self-attracting systems that we consider here, if the short-range cutoff is sufficiently increased. As was noted in Ref. [5] for  $\alpha=1$ , there is a critical excluded volume radius  $r_c$  above which there is no discontinuity in the entropy vs energy plot. We observed that this trend is generic for all  $0 < \alpha < 3$  and holds for both excluded volume and soft potential cutoffs. Now the critical cutoff radius  $r_c(\alpha)$  increases with increasing  $\alpha$ , roughly varying in value from below  $10^{-3}$  for  $\alpha=1/4$ , to above  $10^{-1}$  for  $\alpha=5/2$ , respectively. For a system with a cutoff radius larger than  $r_c(\alpha)$ , the entropy vs energy plot is continuous and exhibits all characteristics of a normal first-order phase transition [7,9]: the convex dip and associated with it an interval of energies, where  $d^2s(\epsilon)/d\epsilon^2$  is positive and the heat capacity is negative (Fig. 5). We leave the more detailed study of the difference between the gravitational-like and the normal first order phase transitions and the nature of crossover between them for a future paper.

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