

Urn model of separation of sand

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We introduce an urn model that describes spatial separation of sand. In this dynamical model, in a certain range of parameters spontaneous symmetry breaking takes place and equipartitioning of sand into two compartments is broken. The steady-state equation for an order parameter, a critical line, and the tricritical point on the phase diagram are found exactly. The master equation and the first-passage problem for the model are solved numerically and the results are used to locate first-order transitions. Exponential divergence of a certain characteristic time shows that the model can also exhibit very strong metastability. In certain cases characteristic time diverges as N^z , where N is the number of balls and $z = \frac{1}{2}$ (critical line), $\frac{2}{3}$ (tricritical point), or $\frac{1}{3}$ (limits of stability).

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I. INTRODUCTION

Recently, granular systems have been intensively studied using methods of statistical physics. The main motivation of this research is to get a basic understanding of these technologically important materials whose behavior, however, very often appears elusive and mysterious [1,2].

One of the classical experiments in this field concerns the spatial separation of shaken sand [3]. In this experiment one uses a box that is divided into two equal compartments by a wall that has a narrow horizontal slit at a certain height. When the box is filled with a sand and shaken, one observes that under certain conditions (e.g., frequency and amplitude of shaking) one compartment of a box is preferentially filled with sand. Theoretical arguments to understand how the symmetry breaking arises in this experiment were given by Eggers [4]. In his approach, Eggers studied a continuous model based on partial differential equations that takes into account certain particular characteristics of shaken granular systems [5]; namely, the fact that effective temperature of a granular system decreases when the density of particles increases. This, at first counterintuitive, feature of granular systems is now understood as a result of inelastic collisions between particles that effectively cool the system [7]. This feature is also responsible for the symmetry breaking in the experiment with shaken sand. Indeed, with nonequal distribution of sand the temperature in the compartment with the majority of particles is substantially reduced. Consequently, particles from this compartment are less likely to cross the slit. Eggers has shown that a continuous phase transition accompanies the symmetry breaking. The approach used by Eggers was generalized for a larger number of compartments separating the box. It was shown that in such a case the phase transition becomes discontinuous [8].

Eggers's model is, however, quite complicated and its analysis must be supplemented with some simplifying assumptions. The analysis of fluctuations or dynamical properties seems to be particularly difficult for this model. A possible alternative might be to examine a different, presumably simpler model, which would nevertheless grasp the essence of the phenomena.

The main goal of the present paper is to define and analyze such a model. Our model is a certain generalization of the urn model introduced by Ehrenfest [9]. In the Ehrenfest model one has balls that are distributed between two urns and certain dynamical rules according to which balls can change their location. The Ehrenfest model greatly contributed to the understanding of some basic notions of statistical mechanics such as the equilibrium or approach to the equilibrium. Various modifications of this model were examined [10].

At first sight it seems natural that the Ehrenfest model could provide an approximate description of experiments with shaken sand. However, none of its generalizations described in the literature exhibits a spontaneous symmetry breaking [11]. The modification that we propose does exhibit a spontaneous symmetry breaking. Although the model is rather simple it exhibits a rich behavior. In addition to having a line of continuous transitions, the model has a tricritical point and a line of discontinuous transitions. The discontinuous transitions are screened by very strong metastability. The existence of this, in fact unobservable (due to metastability) transition in our dynamical model requires, however, some comments. In equilibrium systems it is the free energy that unambiguously determines the phase, which is stable for a given set of parameters. For our dynamical model we do not know how to calculate the free energy. Nevertheless, certain features enabled us to locate the discontinuous transitions in our model. Namely, probability distribution of the order parameter exhibits characteristics that are typical to equilibrium systems with discontinuous transitions. Additional evidence of such a transition in our model comes from the analysis of characteristic times, which we determine solving numerically the first-passage problem.

Our paper is organized as follows. In Sec. II, we introduce the model and examine its steady-state properties. In Sec. III, from the solution of the master equation we analyze the steady-state probability distribution and fluctuations in the model. Section IV is devoted to the metastable properties and characteristic times obtained from the solution of the first-passage problem. Conclusions and possible extensions of our work are discussed in Sec. V.

II. MODEL AND ITS STEADY STATE

Our model is defined as follows: N particles are distributed between two urns A and B and the number of particles in each urn is denoted as N_A and N_B , respectively ($N_A + N_B = N$). Particles in a given urn are subject to thermal fluctuations and the temperature T of the urn depends on the number of particles in it. To mimic the effect that a larger number of particles leads to a smaller temperature, we use the following rule:

$$T(n_{A,B}) = T_0 + \Delta(1 - n_{A,B}), \quad (1)$$

where $n_{A,B} = N_{A,B}/N$ is a fraction of a total number of particles in a given urn and T_0 and Δ are positive constants. With such a choice, temperatures of urns changes linearly with $n_{A,B}$ from the value T_0 to $T_0 + \Delta$. For granular systems the relation between temperature and the number of particles is very complicated and depends on certain parameters such as density of particles or the type of driving [5]. For the experiment with separation of sand certain arguments suggest that $T \sim n_{A,B}^{-2}$ would be more suitable [4], however, indications of the linear dependence like Eq. (1) can also be found in the literature [6]. With a choice $T \sim n_{A,B}^{-2}$ the location of the critical point changes with N . As expected on general grounds, the observed behavior for finite N is only a crossover and a well-defined phase transition exists only in the limit $N \rightarrow \infty$. Our choice (1), leads to results that are well defined in the thermodynamic limit $N \rightarrow \infty$. However, it would be interesting to examine other choices too.

Next, we assume that particles within a given urn obey the standard Maxwell-Boltzmann distribution. It means that their distribution changes with the height z (above the bottom of an urn) as

$$p_{A,B}(z) = \frac{mgN_{A,B}}{T(n_{A,B})} \exp\left[\frac{-mgz}{T(n_{A,B})}\right], \quad (2)$$

where m is the mass of a particle and g is the gravitational acceleration. One can easily calculate that the fraction of particles obeying distribution (2), which are above a certain height h is given as $\exp[-mgh/T(n_{A,B})]$. Next, we define dynamics of our model as follows: (i) One of the N particles is selected randomly. (ii) With probability $\exp[-mgh/T(n_{A,B})]$ the selected particle changes urns. ($n_{A,B}$ is the fraction of particles present in the urn of the selected particle). In the following, we assume that temperature is measured in units such that $mgh = 1$. It means that our model is parametrized only by T_0 and Δ . The Ehrenfest model is recovered in the limit of infinite temperature where every selected particle changes urns.

We define ϵ as a measure of the difference in the occupancy of the urns,

$$\epsilon = \frac{N_A - N_B}{2N}. \quad (3)$$

For our model, one can find a simple, but exact equation that determines the time average $\langle \epsilon \rangle$ in the steady state. Indeed, in the steady state the flux of particles changing their posi-

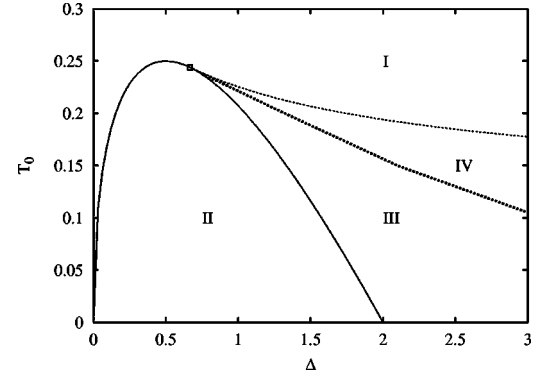


FIG. 1. Phase diagram of the urn model. Regions I and II are symmetric ($\langle \epsilon \rangle = 0$) and asymmetric ($\langle \epsilon \rangle \neq 0$) phases, respectively. In region III (IV) the symmetric (asymmetric) phase is metastable (see text). The solid line is the critical line (6). The thick dotted line is the line of first-order phase transitions. The tricritical point $(\frac{2}{3}, (\sqrt{3}-1)/3)$ is denoted as \square .

tions from A to B equals to the flux from B to A . It is easy to realize that since the selected particles are uncorrelated, the above requirement can be written as

$$\langle N_A \rangle \exp\left[\frac{-1}{T(\langle N_A/N \rangle)}\right] = \langle N_B \rangle \exp\left[\frac{-1}{T(\langle N_B/N \rangle)}\right]. \quad (4)$$

Using the parameter $\langle \epsilon \rangle$ and the relation $N_A + N_B = N$, Eq. (4) can be written as

$$\left(\frac{1}{2} + \langle \epsilon \rangle\right) \exp\left[\frac{-1}{T\left(\frac{1}{2} + \langle \epsilon \rangle\right)}\right] = \left(\frac{1}{2} - \langle \epsilon \rangle\right) \exp\left[\frac{-1}{T\left(\frac{1}{2} - \langle \epsilon \rangle\right)}\right]. \quad (5)$$

Of course, Eq. (5) admits symmetric solution $\langle \epsilon \rangle = 0$ for any T_0 and Δ . However, a physically satisfactory solution must be stable with respect to fluctuations. To make the stability analysis of $\epsilon = 0$ solution of Eq. (5), we have to expand it in powers of ϵ . Equating linear terms we obtain that the critical line that separates stable and unstable regions for symmetric solution is given as

$$T_0^c = \sqrt{\Delta/2} - \Delta/2. \quad (6)$$

This line is plotted as a solid line in Fig. 1.

What is more interesting, however, Eq. (5) has also asymmetric solutions with $\langle \epsilon \rangle \neq 0$. Although such solutions cannot be written in a closed form, they can be easily determined numerically. An example of such a solution is shown in Fig. 2. In addition, expanding Eq. (5) in powers of $\langle \epsilon \rangle$, one can easily check that in the vicinity of the critical point $|\langle \epsilon \rangle| \sim (T_0 - T_0^c)^{1/2}$, which recovers an equilibrium mean-field exponent $\beta = 1/2$ (we assume that Δ is kept constant).

It turns out, however, that in a certain region of phase diagram both symmetric and asymmetric solutions are stable (see Fig. 1). It suggests that in this region a line of discontinuous transition should exist. This line would meet a critical line at a certain point which, by analogy with equilibrium

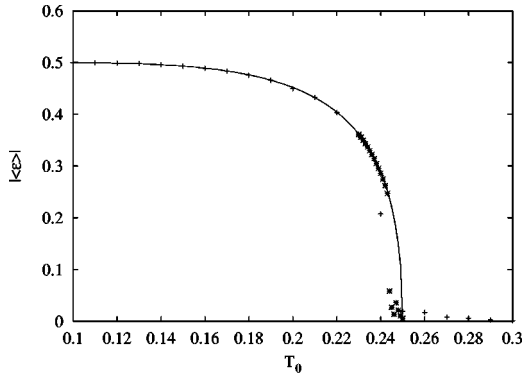


FIG. 2. Absolute value of the order parameter $|\langle \epsilon \rangle|$ as a function of T_0 for $\Delta = 0.5$. The solid line corresponds to the numerical solution of Eq. (3). Monte Carlo simulations were made for $N = 500$ (+) and 5000 (*).

systems [12], can be called a tricritical point. Location of this point can be easily determined from Eq. (5). Indeed, required that the third-order (in ϵ) coefficients are the same [13] and taking in account Eq. (6), we obtain the tricritical point is located at $\Delta = \frac{2}{3}$, $T_0 = (\sqrt{3} - 1)/3$. However, it is by no means obvious how to determine the line of discontinuous transitions in our model. In equilibrium systems, one can calculate the free energy of each phase and this line is determined from the condition that the free energy of both phases are equal. Our model is not an equilibrium system and this procedure cannot be used. Nevertheless, as we will show below, behavior of certain quantities show striking similarity to equilibrium counterparts. With this observation we will be able to locate discontinuous transitions in our model. To address this problem, we have to go beyond the steady-state Eq. (5), which is the subject of the following section.

III. MASTER EQUATION

For our urn model one can write evolution equations for the probability distribution $p(M, t)$ that in a given urn (say A) at the time t there are M particles. These equations easily follow from the dynamical rules,

$$\begin{aligned}
 p(M, t+1) &= \frac{N-M+1}{N} p(M-1, t) \omega(N-M+1) \\
 &\quad + \frac{M+1}{N} p(M+1, t) \omega(M+1) + p(M, t) \\
 &\quad \times \left\{ \frac{M}{N} [1 - \omega(M)] + \frac{N-M}{N} [1 - \omega(N-M)] \right\} \\
 &\quad \text{for } M = 1, 2, \dots, N-1, \\
 p(0, t+1) &= \frac{1}{N} p(1, t) \omega(1) + p(0, t) [1 - \omega(N)], \\
 p(N, t+1) &= \frac{1}{N} p(N-1, t) \omega(1) + p(N, t) [1 - \omega(N)],
 \end{aligned} \tag{7}$$

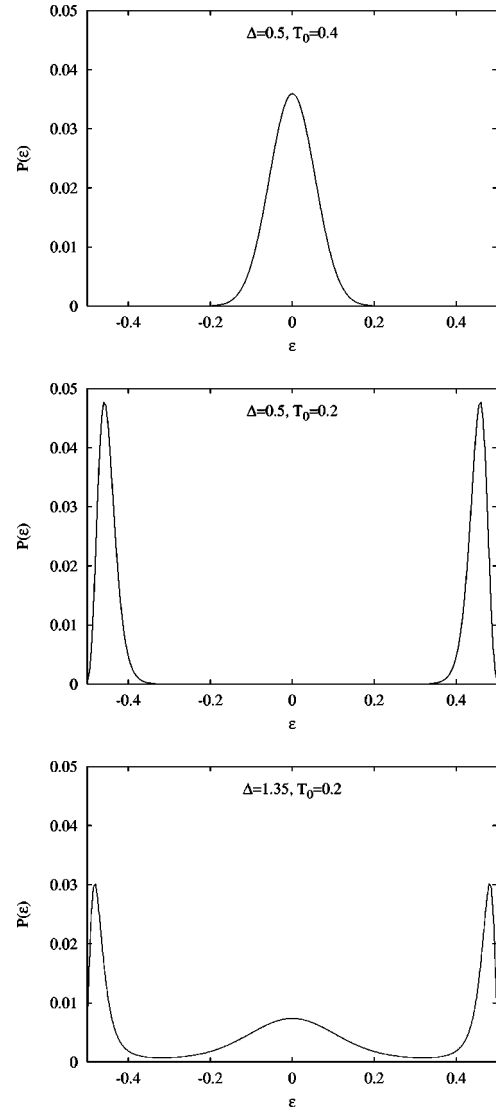


FIG. 3. Probability distribution $p[N(\epsilon + \frac{1}{2}), t]$ obtained as a numerical solution of Eq. (7) in the long-time limit ($N = 200$).

where $\omega(M) = \exp[-1/T(M/N)]$. For $\omega(M) \equiv 1$ the above equation are equivalent to the ones of the Ehrenfest model [9]. Supplementing the above equations with initial conditions one can solve them numerically [14]. Examples of such solutions in a long-time limit are shown in Fig. 3.

As expected, one finds a single- and double-peak distribution in regions I and II, respectively. The width of these peaks decreases with the number of particles N . The behavior of the probability distribution in regions III and IV is however more complicated. Although for small N it has three-peak structure, the shape changes in the limit $N \rightarrow \infty$. The final distribution depends whether the parameters Δ and T_0 are in region III or IV. In region III, for increasing N , the central peak diminishes and in the limit $N \rightarrow \infty$ we obtain a two-peak distribution. On the other hand, in region IV only the central peak survives in the thermodynamic limit. As we will show, a line that separates these two regions can be interpreted as a line of discontinuous transitions. Before we approximately locate this line, let us study fluctuations of the

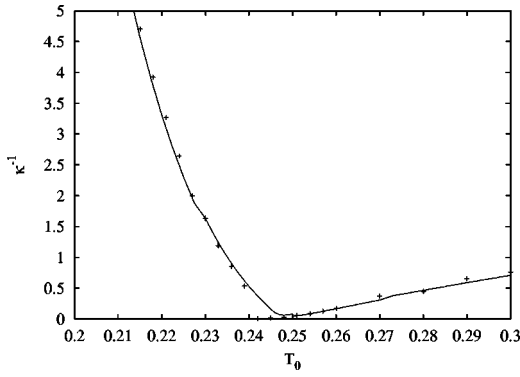


FIG. 4. Inverse of the susceptibility κ^{-1} as a function of T_0 for $\Delta = 0.5$. The solid line corresponds to the numerical solution of Eq. (3) for $N = 5000$. Monte Carlo simulations were made for $N = 5000$

(+). In the asymmetric phase ($T_0 < 0.25$) to calculate κ we used only a half of the probability distribution.

order parameter. Since we know the probability distribution, these fluctuations can be calculated numerically, without making additional assumptions [4]. Using the variance of the order parameter we define the susceptibility κ as

$$\kappa = N \langle (\epsilon - \langle \epsilon \rangle)^2 \rangle = \frac{1}{N} \left\{ \sum_{i=0}^N i^2 p(i, \infty) - \left[\sum_{i=0}^N i p(i, \infty) \right]^2 \right\}, \quad (8)$$

where $p(\dots, \infty)$ denotes the steady-state probabilities obtained from Eqs. (7). Susceptibility is known to diverge at the continuous phase transition. Our calculations for $\Delta = 0.5$ confirm such a behavior (Fig. 4). For $T_0 > 0.25$ the inverse susceptibility κ^{-1} decays linearly that implies $\gamma = 1$ (mean-field value). For $T_0 < 0.25$ (asymmetric phase) the behavior is less clear but we also expect a linear decay of κ^{-1} .

To check our steady-state and master-equation calculations we performed Monte Carlo simulations that are also presented in some cases. The implementation of this method for the present model is rather straightforward.

Let us notice that the behavior of the probability distribution as seen in Fig. 3 bears some similarity to equilibrium systems. In particular, it is known that the simultaneous existence of peaks of both phases is an indicator of the first-order phase transitions [15]. Although our model is defined only using dynamical rules and thus has no free energy (at least as defined for equilibrium systems) it does exhibit some other features typical to equilibrium systems. To precisely locate the transition point we calculated the scaled susceptibility κ/N . We expect that when only a single peak survives κ/N vanishes, while it remains positive in the double-peak region. For $T_0 = 0.2$ the obtained results (Fig. 5) locate the transition around $\Delta = 1.31$. As we will see in the following section there is also a dynamical indicator of this transition.

IV. METASTABILITY AND THE CHARACTERISTIC TIME

Analysis of the probability distribution for our dynamical model, which was done in the preceding section shows some

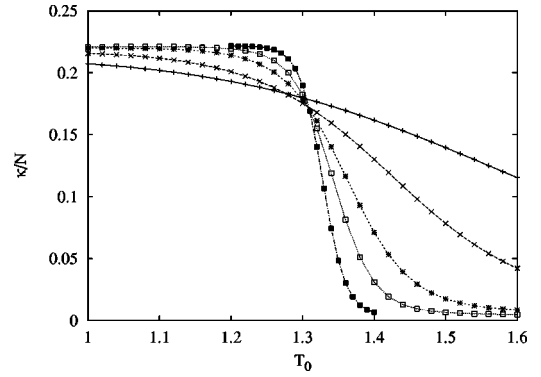


FIG. 5. Scaled susceptibility κ/N as a function of Δ for $T_0 = 0.2$ obtained from the numerical solution of Eq. (7) for $N = 50, 100, 200, 300,$ and 500 .

similarity to equilibrium discontinuous transitions. It is known that such transitions are usually accompanied by metastability. In the present section, we examine such effects in our model.

The most transparent indication of metastability is hysteresis. That our model exhibits such a behavior is clearly seen in Fig. 6. One can see, that upon increasing Δ , the system prepared in the asymmetric state remains in this state up to $\Delta \sim 1.7$ that is close to the limits of stability of this state (see Fig. 1). On the other hand, when Δ decreases the symmetric state persists up to $\Delta \sim 1.1$ that is again close to the limits of stability of symmetric phase. Simulations show that the range of the hysteresis only slightly depends on the system size and the simulation time. For large system sizes the model will persist in the initial state until the limits of stability of this state are reached, as calculated from the steady-state equation (5). Such a behavior indicates a very strong metastability. As we will show below, in regions III and IV of the phase diagram certain characteristic times diverge exponentially with the system size that corresponds to the broken ergodicity (i.e., dynamical phase space of the model is decomposed into disconnected sectors). Let us notice that in (short-ranged) equilibrium systems metastability has always

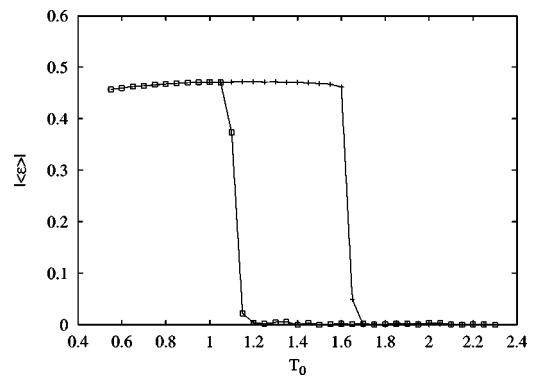


FIG. 6. Absolute value of the order parameter $|\langle \epsilon \rangle|$ as a function of Δ for $T_0 = 0.2$ calculated using Monte Carlo simulations for $N = 2000$. Two runs were made with Δ increasing (+) and decreasing (\square), respectively. Due to strong metastability no sign of the transition exists for $\Delta = 1.31$.

a finite lifetime and longer simulations or larger system size shrink the hysteresis.

To examine the metastable properties of our model further we will calculate certain characteristic times. It is known that for urn models some of these quantities can be calculated as the so-called first-passage problem. We will use a similar approach. More specifically, let us consider a configuration where there are M and $N-M$ balls in urn A and B , respectively (N even). Now, we define an average time $\tau(M, N-M)$ needed for such a configuration to reach a symmetric configuration ($M=N/2$). From the dynamical rules of our model one finds that $\tau(M, N-M)$'s obey the following $N/2$ linear equations (to simplify notation we omit the second argument in τ 's):

$$\tau(N) = \omega(N)[\tau(N-1) + 1] + [1 - \omega(N)][\tau(N) + 1],$$

$$\begin{aligned} \tau(N-1) &= \frac{N-1}{N} \omega(N-1)[\tau(N-2) + 1] + \frac{1}{N} \omega(1) \\ &\quad \times [\tau(N) + 1] + \left[1 - \frac{N-1}{N} \omega(N-1) - \frac{1}{N} \omega(1) \right] \\ &\quad \times [\tau(N-1) + 1], \\ &\dots \\ \tau(M) &= \frac{M}{N} \omega(M)[\tau(M-1) + 1] + \frac{N-M}{N} \omega(N-M) \\ &\quad \times [\tau(M+1) + 1] + \left[1 - \frac{M}{N} \omega(M) - \frac{N-M}{N} \right. \\ &\quad \left. \times \omega(N-M) \right] [\tau(M+1) + 1], \\ &\dots \\ \tau(0.5N+1) &= \left(0.5 + \frac{1}{N} \right) \omega(0.5N+1) + \left(0.5 - \frac{1}{N} \right) \\ &\quad \times \omega(0.5N-1) [\tau(0.5N+2) + 1] \\ &\quad + \left[1 - \left(0.5 + \frac{1}{N} \right) \omega(0.5N+1) \right. \\ &\quad \left. - \left(0.5 - \frac{1}{N} \right) \omega(0.5N-1) \right] \\ &\quad \times [\tau(0.5N+1) + 1]. \end{aligned} \quad (9)$$

Similar equations can be written for the Ehrenfest model [16].

We were unable to write an explicit solution of the above set of equations. However, its tridiagonal structure greatly simplifies its numerical solution. In particular, the so-called Gaussian elimination can be used to calculate τ 's recursively [17]. Since implementation of this algorithm is straightforward we present only final results. Our unit of time corresponds to a single on average update per ball, i.e., we divide the time τ calculated from Eqs. (9) by N .

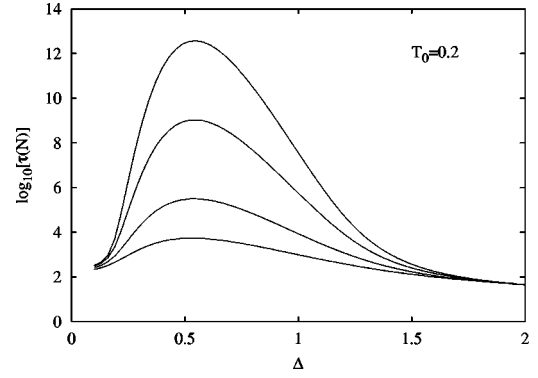


FIG. 7. Characteristic time $\tau(N)$ as a function of Δ for (from the bottom) $N=50, 100, 200$, and 300 .

In Fig. 7, we present the Δ dependence for $\tau(N)$. This is the lifetime of totally asymmetric solution. Its rapid increase (as a function of N) in certain range of Δ indicates the stability of the asymmetric solution.

To provide more details on the stability of this solution we have to look at the size dependence of the characteristic time and the results are shown in Figs. 8 and 9. One can see (Fig. 8) that the limits of stability of asymmetric solution, which for $T_0=0.2$ equals $\Delta = \Delta_c(0.2) = 1.7440675\dots$, separates two regimes. For $\Delta > \Delta_c(0.2)$ $\tau(N)$ approaches a finite value for increasing N , while it diverges for $\Delta < \Delta_c(0.2)$. From Fig. 9 one can conclude that for $\Delta < \Delta_c(0.2)$, $\tau(N)$ diverges exponentially fast with N . It confirms our previous observations, based on Monte Carlo simulations, that a given phase persists up to the limits of its stability.

From Fig. 10 it follows that at the limits of stability $\tau(N)$ increases but as a power of N . From the slope of these data we estimate that both for $T_0=0.2$ and 0.15 $\tau \sim N^{1/3}$. A different exponent governs the increase of $\tau(N)$ along the critical line (6) [18]. In this case we find $\tau(N) \sim N^{1/2}$, while at the tricritical point $N^{2/3}$ increase is observed (see Fig. 10). It would be desirable to explain such simple power laws using analytical arguments.

The above results concern the behavior of $\tau(N)$. We have shown that this quantity can be used to locate the critical line or the limits of stability of the asymmetric solution. How-

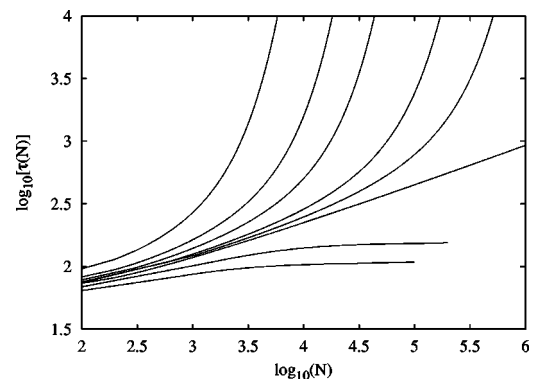


FIG. 8. Characteristic time $\tau(N)$ as a function of N for $T_0=0.2$ and (from the left) $\Delta = 1.65, 1.7, 1.72, 1.735$, and 1.74 , $\Delta_c(0.2) = 1.7440675\dots, 1.77$, and 1.8 .

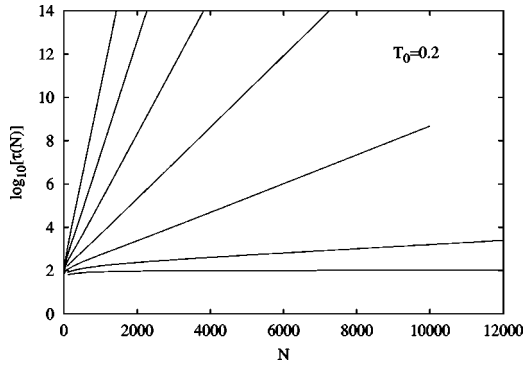


FIG. 9. Characteristic time $\tau(N)$ as a function of N for $T_0=0.2$ and (from the left) $\Delta=1.2, 1.3, 1.4, 1.5, 1.6, 1.7,$ and 1.8 .

ever, this quantity does not provide any indication of the discontinuous phase transition that we located between regions III and IV on Fig. 1. To have a dynamical indication of this transition we have to look for other characteristic times. First, let us notice (Fig. 11) that in region II the distribution of τ 's as function of M is rather flat that means that there is basically a single time scale in the model. In regions III and IV, however, one can see a more pronounced variability of $\tau(M)$. In Fig. 12, we show that $\tau(0.5N+1)$ (which is the shortest of our τ 's) can be used to locate a discontinuous phase transition. Indeed, this quantity increases exponentially fast with N for $\Delta < 1.31$ and remains bounded for larger values of Δ . The change of behavior of $\tau(0.5N+1)$ coincides, within our numerical accuracy, with the change of the probability distribution as shown in Fig. 5.

Let us also notice that the time scale reached in the numerical solution of Eq. (9) ($\sim 10^{14}$) is much larger than what is accessible using Monte Carlo simulations. The main limitation in our calculations is finite accuracy of the computations. Using longer representations of real numbers (we used the FORTRAN real*8 type) one can study much larger time scales.

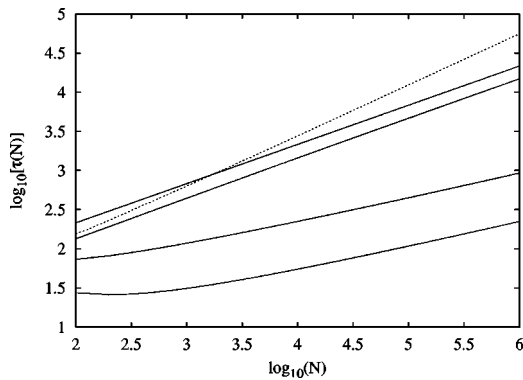


FIG. 10. Characteristic time $\tau(N)$ as a function of N calculated (Δ, T_0) equal to (solid lines, from the top): $(0.25, \sqrt{0.25/2} - 0.25/2)$, $(0.5, 0.25)$, $(1.744\ 067\ 5, 0.2)$, and $(6.775\ 493\ \dots, 0.15)$. For two upper lines the points (Δ, T_0) are on the critical line (6), while for bottom ones, they are on the lines of the limits of stability of the asymmetric solution. The dotted line corresponds to the tricritical point.

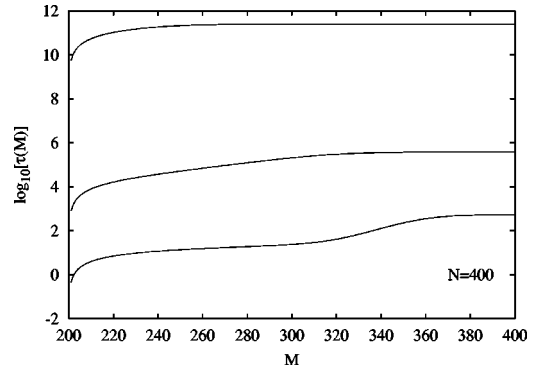


FIG. 11. Distribution of characteristic times $\tau(M)$ as a function of M calculated $T_0=0.2$ and (from the top) $\Delta=0.9, 1.2, 1.5$.

V. CONCLUSIONS

In the present paper, we examined an urn model that undergoes a symmetry-breaking transition. Our work was motivated by recent experiments on the separation of shaken sand. The proposed model exhibits a rich behavior (continuous/discontinuous transitions, a tricritical point, metastability) and its properties could be reliably determined. There are experimental indications that in the three-compartment case the separation of shaken sand is a discontinuous transition [8]. However, due to strong metastability only the hysteretic behavior is observed, similarly as in our simulations in Fig. 6. Our work suggests, that there are some indicators (probability distributions, characteristic times) which could be used to locate a discontinuous transition in such systems. It would be interesting to look for such indicators in experimental systems.

As an extension of our work, one can examine models with a different relation between the effective temperature and the number of particles or models with larger number of compartments. Even further extensions are related with a much different interpretation of our model. One can imagine that two compartments A and B are two groups of people (e.g., supporters of certain presidential candidates). It seems reasonable to assume that under certain conditions a larger number of people in a given group will increase attractive

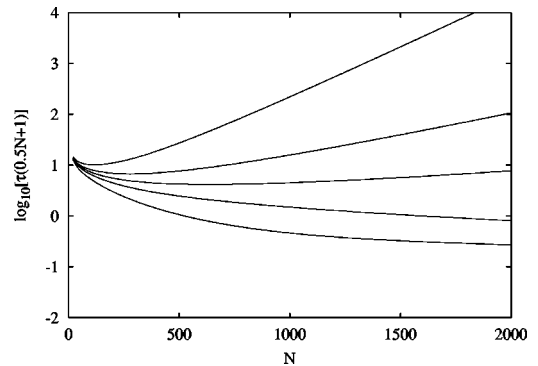


FIG. 12. Characteristic time $\tau(0.5N+1)$ as a function of N calculated $T_0=0.2$ and (from the top) $\Delta=1.27, 1.29, 1.30, 1.31,$ and 1.33 .

bonds within this group (energy). On the other hand, it will also increase the probability that a certain member will leave the group (entropy). Competition of these two effects is likely to produce a similar symmetry-breaking transition to the one described in the present paper. However, since people are known to create various local connections (e.g., within a group) it would be desirable to take such effects into account

too. In our model particles are chosen randomly and such correlations are omitted.

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