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Segregation of a Granular Binary Mixture in a Rotating Drum: A Critical Phenomenon

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The segregation phenomena of a 1:1 mixture of grain particles with different frictional properties in a rotating drum are studied by simulations. The surface flow is modeled by extending the rules from sandpile models while the rotation is modeled by a solid rotation. Radial segregation will occur only if the rotational transport rate w is less than some critical value ω_c. Our results show that such a segregation can be described by a non-equilibrium critical phase transition in the steady state with the particle transport rate playing the role of the temperature. Employing finite-size scaling analysis similar to standard critical phenomena, critical exponents for the order parameter and its fluctuation are also obtained numerically.

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I. Introduction

Recently, there has been much interest in granular materials both experimentally and theoretically (see Refs. [1] and [2] for a review). These granular particles are of macroscopic sizes and have been of important industrial concern in engineering. They can be thought of as an intermediate phase between solid and liquid in the sense that it can sustain shear like a solid up to a point and can also flow like liquid. Motions of granular materials are characterized by their hydrodynamic and frictional behavior. Experiments designed to probe these properties such as vibrating beds [3,4], fluidized beds [5,6] rotating drums [7,8] and cylinders [9-11] have revealed many interesting phenomena that cannot be fully understood yet. The difficulties come from the non-linear interaction between the particles which produce the observed collective behavior. One of such phenomena is the friction driven segregation of a binary mixture of granular particles in a rotating drum. Usually, segregation in a binary mixture results from the attractive interaction among like particles such as in liquid binary mixtures. Also, in hard core particle systems where attraction is absent, segregation is mainly due to size effects which are driven entropically [4,7,10-14]. On the other hand, the study of segregation driven by the difference of the frictional properties of the grains is much limited [9]. Recently, we constructed a model which can capture the essential properties of the segregation of a mixture of grains in a rotating drum

[15]. Only a difference in the frictional properties of the mixture is needed in our model to produce the segregation observed.

In the rotating drum experiments, a drum (axis of rotation through the center of the drum is horizontal) is filled to a certain fraction with a binary mixture of granular materials. Two effects are important when the drum rotates. Firstly, inclination of the originally horizontal surface formed by the grains will increase with time and grains will topple and flow down the slope when the angle of the interface is larger than the angle of repose of the particles. Secondly, the rotation transports the materials at the bottom layer upward to the surface along the drum's circumference. A steady state is reached when the increase in inclination is counter-balanced by the flow of the grains.

In this paper, we report our results on the simulation studies of such a segregation phenomenon using cellular automata rules similar to sandpile models in self-organized criticality. These rules are constructed to incorporate the difference in the frictional properties of the two types of particles. Our model can be qualitatively mapped to rotating drum experiments. We found that segregation can be produced in the radial direction only if the rotational transport rate ω is less than some critical value ω_c[15]. We present more results showing that such a segregation in the steady state can be described by a non-equilibrium critical phase transition with the particle transport rate playing the role of the temperature. Employing finite-size scaling analysis similar to standard critical phenomena, critical exponents for the order parameter and its fluctuation are also obtained numerically.

II. Rotating drum model

In our model, the grains are placed on a $L \times H$ rectangular lattice as shown in Fig.1a. The sizes of both types of grains are unity. The particles can be viewed as being arranged in L/2 shells surrounding the point 0 as shown in the figure, with the outermost shell being the $L/2$th shell. Rotation about the origin 0 is modeled by transport of particles within each shell in the clockwise direction with a rate ωr for the rth shell. The vertical portions of these shells (a total of L) are treated as sandpiles. The algorithm starts by a rotational transport in the clockwise direction about the origin 0, i.e. the left of the vertical portion of the rth shell will be raised by an amount of ωr while the right vertical portion lowered by the same amount. Note that the height of each pile is a continuous variable, but the total length of each shell is an integer. Upon rotation, the surface profile is no longer horizontal. Then a vertical pile is chosen at random and checked whether it will topple according to the modified sandpile rules to be described below. Each pile is allowed to attempt Γ trial topplings on average before the next rotational transport. Thus Γ can be interpreted as the toppling rate for the grains. All the grains can finish their topplings before the next rotation if Γ is very large. For given w and Γ, the system will eventually reach a steady state.

We extended the well-known sandpile model by Bak, Tang and Weisenfeld (BTW) [16] to our case of two-component grains. Consider two types of grains A and B in a binary mixture, A and B are different in there mutual interactions which can be thought of having different frictional properties. As in the usual sandpile model, a pile will topple if its excess height from its nearest neighbor pile exceeds some critical value A. Suppose type-A grains are rough and type-B are smooth, their difference is modeled by different critical heights

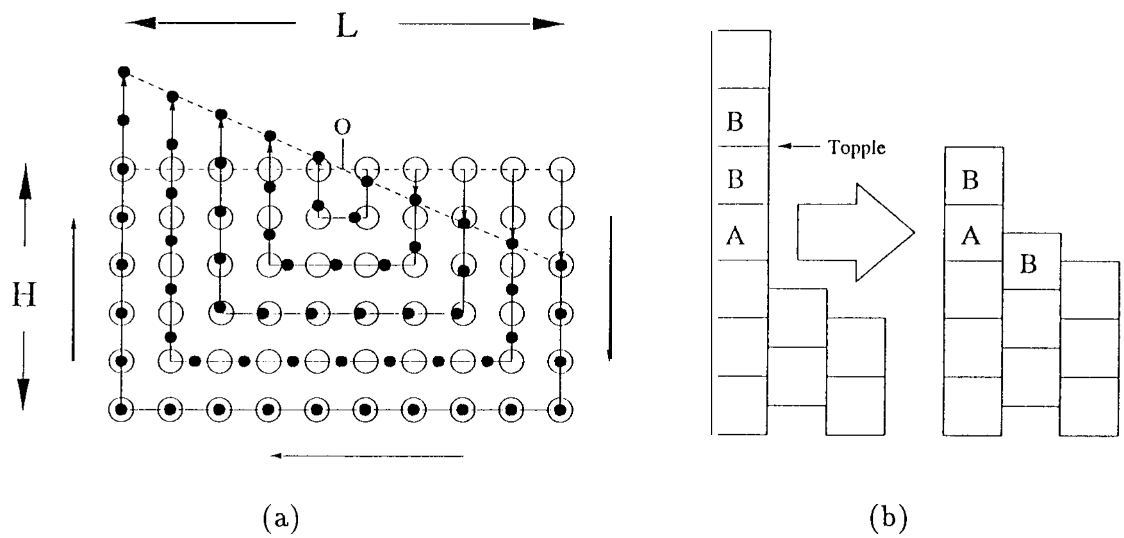

FIG. **1.** Sandpile model for a rotating drum. (a) The lattice points on each shell rotate about 0 in the clockwise sense with a rate *wr*. Open circles denote the initial grain positions and dots denote their positions after rotation. (b) An example showing the grain toppling rule.

to topple. The smooth grains B have a smaller critical angle of repose and hence a smaller critical excess height/slope. For simplicity we take Δ_{AA} = 4, Δ_{BB} = 2 and Δ_{AB} = 3 where Δ_{ij} denotes the critical excess height for the interface formed by type-i and type-j grains. The sandpile rule checks the pile upwards and noting the type of grains in the pile, topple will occur if the excess height from its neighboring pile exceed the corresponding critical height. Fig. lb shows an example, as one check the pile upwards, toppling will not occur in the first AB interface but will occur at the BB interface because Δ_{AB} = 3 and $\Delta_{BB} = 2$. In our simulation, we choose H = 2L and thus there are altogether $2L^2$ grains in the system. Here we consider a 1:1 mixture of two types of grains. Most of the data presented here are for Γ = 150. We have verified that for the case of a single component grains, our model gives an "S" shape steady state profile as observed in experiments. And indeed the early stage linear segregation dynamics in our model even agrees with experiments on size segregation [15]. Hence we believe that the essential features of the segregation should be correctly represented in our model. This extended sandpile rules can be easily generalized to study a mixture of grains of different sizes. Indeed, a somewhat similar model has been developed to explain the stratification mechanism in a mixture of grains of different sizes [17].

III. Critical phenomenon

The segregation is in the radial direction with the rough grains *(A)* at the center. Such segregation is measured by the fraction of type A grains in the rth shell (there is a total of L/2 shells in the model), $\rho(r)$, after the system has achieved a steady state. For sufficiently slow rotation rate, a complete segregation with a sharp interface in the steady state is obtained [15]. The domain size in the completely segregated state is proportional to the size of the drum. However, when the transport rate w is large, the ordered/segregated state will be destroyed and the rotating drum becomes a mixer! Thus w plays a similar role as temperature in usual critical phenomena.

In order to compare the similarity of the segregation with critical phenomena, finite-size scaling analysis is performed on our simulation results with different system sizes and w. Analogous to critical phenomena of a binary mixture, we define the quantity

$$\psi(k) \equiv \frac{1}{C(k)} \int_0^{L/2} e^{ikr}(2\rho(r)-1)dr \tag{1}$$

to characterize this segregation phenomenon where $C(k)$ is the normalization constant chosen such that $|\psi(k)| = 1$ in the completely segregated state. The order parameter, Ψ is then defined to correspond to the largest spatial structure that can possibly occur or the smallest possible wavenumber $k = 2\pi/(L/2)$

$$\Psi \equiv |\psi(4\pi/L)| \tag{2}$$

It is easy to see that $\Psi = 0$ in the complete randomly mixed state and $\Psi = 1$ in the completely segregated state. Also the fluctuation of Ψ can be described by a "susceptibility" like quantity defined as

$$\chi \equiv \frac{L^2}{\omega}(\langle\Psi^2\rangle - \langle\Psi\rangle^2). \tag{3}$$

The dependence of both (9) and X on w for different system sizes are shown in Fig. 2 and its inset respectively. It can be seen that $\langle\Psi\rangle$ becomes significant when w is below some critical value and the change becomes sharper as the system sizes increases. Also, **X** shows a prominent peak which grows as L increases; very similar to standard critical phenomenon. The critical rotational rate ω_c is obtained by extrapolating the peak position to infinite system size. If we further define $\varepsilon \equiv w - \omega_c$, finite-size scaling [18] analysis gives:

$$\langle\Psi\rangle = L^{-\beta/\nu} F(\varepsilon L^{1/\nu}) \tag{4}$$

and

$$\chi = L^{\gamma/\nu} G(\varepsilon L^{1/\nu}) \tag{5}$$

for some critical exponents β, ν, γ, and scaling functions F and G. Assuming finite-size scaling forms in Eqs. (4) and (5), the exponents extracted from our data are:

$$\frac{1}{v} \simeq 1.2 \pm 0.1; \quad \frac{\beta}{v} \simeq 0.37 \pm 0.05; \quad \frac{\gamma}{v} \simeq 1.25 \pm 0.08 \tag{6}$$

Using these values of v, β and γ, scaling plots confirming Eqs. (4) and (5) are shown in Fig. 3. Furthermore the values of these exponents are consistent with the scaling law $\nu d = \gamma + 2\beta$ with $d = 2$ within errors. Thus the segregation is very similar to a critical phenomenon

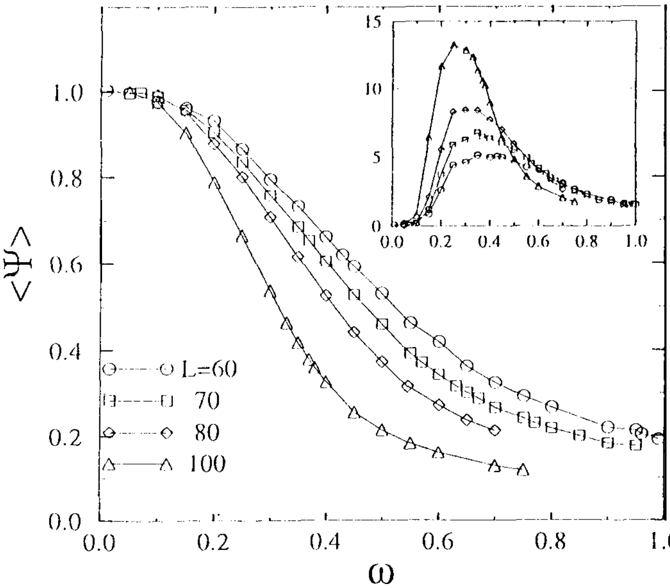

FIG. 2. $\langle\Psi\rangle$ versus ω for various system sizes. Inset: χ versus w for various L

although it is a non-equilibrium one. However, it is clear that our exponents are distinctly different from the two-dimensional Ising universality class which governs the conventional thermally driven phase transition. It would be interesting to know if these exponents are also observed in other flow driven non-equilibrium phase transitions.

In our model, the segregation is due to the different toppling critical slopes of the two types of particles and the segregation rate increases with Γ. However, the effect of transport is to mix the system, the competition between these two processes results in the phase transition. These competing effects are also reflected in the phase diagram of w vs Γ as shown Fig. 4. Here a larger Γ would result in a greater ω_c and a critical line can be obtained separating the mixed and segregated states. We have also verified that the critical exponents along the critical line are the same as given by Eq. (6) within errors.

IV. Extension to 3D rotating cylinder

In order to compare our model with the experimental results in rotating cylinders [9], we have also extended our simulation to three dimensions by the addition of an axial direction perpendicular to the rotation plane with periodic and hard wall boundary conditions imposed in the ends of the cylinder. The toppling rules are essentially the same as in 2D but toppling can also occur in the axial directions. We found that segregation occurs in the radial direction essentially the same as in the 2D drum case. No axial segregation can be produced from an initially homogeneous mixture by our toppling rules. Even an initial axially segregated state will become axially homogeneous through action of rotation. However, radial segregations are still preserved in both cases. These findings lead us to believe that in our model the radial segregation instability preempts the axial one (if there is any).

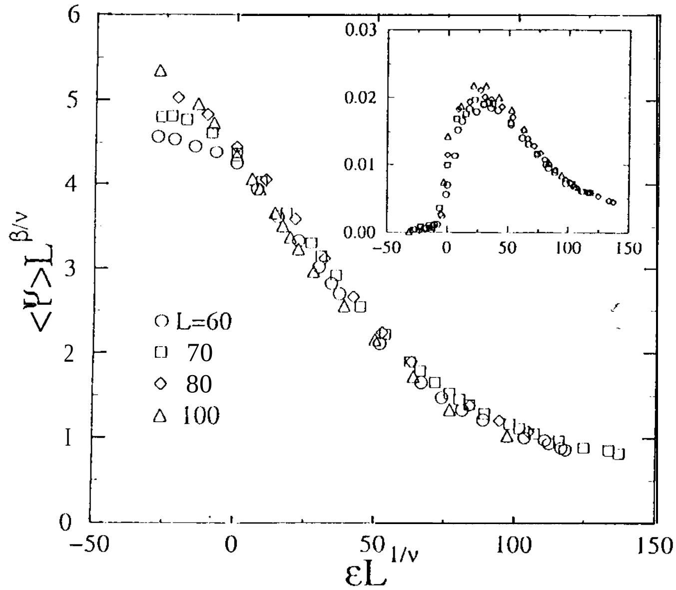

FIG. 3. Scaling plots of $\langle\Psi\rangle L^{\beta/\nu}$ versus $\varepsilon L^{1/\nu}$. Inset: $\chi L^{-\gamma/\nu}$ versus $\varepsilon L^{1/\nu}$. Values of the exponents are from Eq. (6).

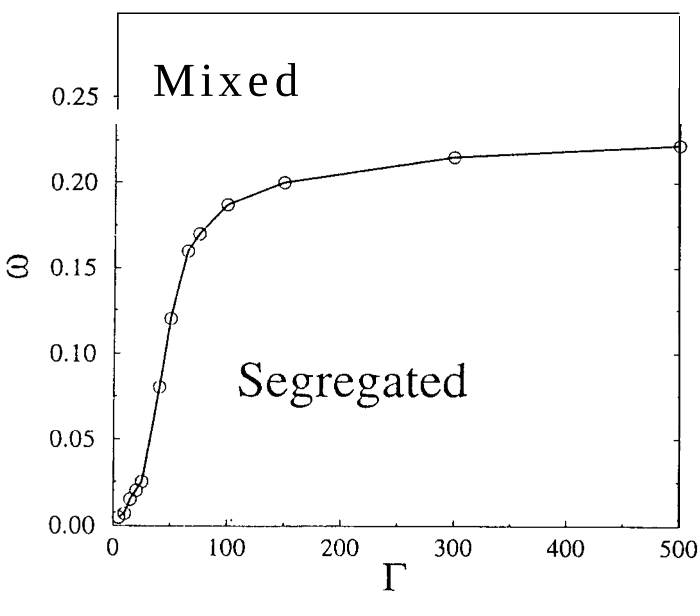

FIG. 4. Phase diagram of w versus I' .

Furthermore, MRI experiments [19] showed that radially segregation persists in parts of the cross-sections of the axially segregated state. Also, another important observation is that radial segregation occurs for rotation rate slow enough, but axial segregation is seen only when the rotation rate is fast enough with the segregation bands travelling with some slow drift velocity. Thus the experimentally observed axial segregation might be due to some other mechanisms, possibly dynamical in nature, rather than the static friction as in the case of radial segregation in drums. Notice that the local differences in frictional properties in our model do not determine the length scale of the segregated pattern. The spatial scale of the segregated domain is determined by the system size similar to Rayleigh-Benard convection rolls. Long range transport, such as rotation in our model is essential for the segregation to occur. However, there is no such long range transport of grains in the axial direction in our model and a proper inclusion of the complicated axial transport is essential in order to model the axial segregation observed in experiments [19, 20].

Finally, we note that our segregation pattern is very similar to that obtained from rotating drum experiments with particles of two different sizes [7, 8]. Although the segregation in the latter case is believed to be driven by the size effects, frictional properties may also play a dominant role in these experiments since larger grains have a smaller angle of repose and hence is effectively smoother. And indeed larger grains are observed to segregate to the outside regions of the drum as the smooth grains in our model.

However, it is important to note that our model can correctly simulate the flow in a rotating drum only when the w is small so that the flow in the bulk is more or less a solid rotation while the surface flow is close to the quasi-static condition in the sense that no bouncing off of grains in the air happens. These inertial effects of real sand grains are also neglected in the BTW sandpile model [16], which may account for the reason why real sand systems do not exhibit SOC. Therefore the scaling behavior seen in our model may not be observed in ordinary granular materials; as in the case of the BTW model. However, as SOC is observed experimentally in rice-pile [21], a special type of granular material, it is plausible that the scaling results of the present model can be seen in specially prepared systems, for example, the segregation of rice of different grain lengths. Nevertheless, the critical behavior in our model of segregation is interesting and provides plausibly a new class of segregation phenomena.

Acknowledgments

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