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Two-dimensional density-driven segregation in vertically vibrated binary granular mixtures

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Two-dimensional segregation effect in vertically vibrated binary granular mixtures with same size is studied by molecular dynamic simulation. The results show that the lighter and mixed state, in which the lighter particles tend to rise and form a pure layer on top of the system while the heavier particles and some of the lighter ones stay at the bottom and form a mixed layer, also exists in the two-dimensional system. The validity of the scheme of the lighter and mixed state is testified by comparing the distribution profiles implied by the scheme with that of the real simulated state. We further propose to use twice the ratio of the thickness of the top layer to that of the whole system as an order parameter to describe the degree of the segregation quantitatively, and present a method that can accurately calculate the order parameter in the simulation. By use of the order parameter, we show that the order parameter is a convex monotonic function of the density ratio between the heavier and lighter particles.

Keywords: Granular matter; segregation effect; molecular dynamic simulation.

1. Introduction

Granular materials are ubiquitous and their dynamics are of central importance to many industrial processes. A remarkable property of the granular materials is the segregation phenomenon,[1–3] which shows unique mixing and separation behavior when the material is vibrated[4–9] or flowing.[10–13] The segregation effect may result from the difference in particle size, differences of density,[14,15] the angle of repose

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of the materials,[16] the temperature gradient,[17] the total amount of the particles,[18] and even the air in container.[19,20] These seriously disturb the investigation in the segregation. To understand the whole segregation phenomena, one has to study the detailed effect left by each factor on the segregation.

The segregated state is also varied. The complete segregated state is easier to describe. For example, in the size-driven segregation, the completely segregated state is that the larger particles are on top of the smaller ones. However, the segregation may be incomplete in some environment,[18,21,22] and to describe it quantitatively, one needs to know more details about the configurations of the particles. The standard method to describe this partially segregated state is to use the distribution profile of each type of particles, i.e., the probability of the filling fraction at fixed height of each type of particles.[15,23] However, the distribution profile is a function of height rather than a single quantity. It would be very helpful if a single quantity can be extracted to describe the segregation state.

Hsiau and Yu have used a segregation coefficient in the study on the size-driven segregation.[18] In their work, the segregation coefficient is defined as the relative difference between the number of the larger particles in the upper and lower half of the bed. By its use, Hsiau and Yu showed that the segregation may occur gradually or suddenly as the frequency increases and the greatest segregation effect occurs when the bed is transformed from a dense state to a loose state. It is clear that the acquirement of the conclusion is well depended on the definition of the segregation coefficient.

Similar to the size-driven segregation, the partially segregated state is also found in the binary mixture made by different materials but with the same size.[21,22] In our earlier work,[24] we made the granules from various materials to control their density, and placed two kinds of them in a glass container evacuated by a vacuum pump. Then the system was vibrated vertically by a simple harmonic vibrator. The segregation state of this system was partially segregated, and we called the states as the lighter and mixed state (LMS). According to this scheme, we have defined an order parameter to describe the segregation state quantitatively. The order parameter of LMS corresponds to a unique distribution of two kinds of particles. We have shown that the order parameter is very useful in the investigation of the density-driven segregation. By its use, some segregation properties were studied and two typical phase diagrams were given.

The experimental results are based on the intuitive observation of the segregation state. The validity of the LMS scheme is needed to be testified by comparing the distribution profile implied by the LMS scheme to that obtained by counting directly the number of particles in each height interval from the real segregation state. However, the distribution profile is hardly to be obtained in experiment researches, but is trivial in simulation researches. Because in the simulations, all information of the particles can be easily extracted, we can obtain the accurate value of the order parameter. The simulations also have many other advantages. For example, we can set up the model parameters in the simulations as we need to change the

model more smoothly. The simulation is purer, it can exclude the influences that are hardly eliminated by experiments. This allows us to study the physical phenomenon more cleanly.

In this paper, we study the two-dimensional (2D) segregation effect in vertically vibrated binary granular mixtures composed of particles with the same size by molecular dynamic (MD) simulations, and try to give some results that are hardly obtained in experiments. In Sec. 2, we describe the model and the simulation method we used in detail. In Sec. 3, we show that the LMS also exists in the 2D system, and the validity of the LMS scheme can been testified by comparing the distribution profile implied by the LMS scheme with that obtained by counting directly the number of particles in each height interval. In Sec. 4, we propose that we can define an order parameter under the LMS scheme, and it can be used to investigate some properties of the segregation. Section 5, is devoted to conclusion and discussion.

2. Models and Methods

The MD simulations are carried out in a 2D system. Totally, 1200 spheres (circles), 600 for each kind of material, in general, were placed in a container with gravity field as shown in Fig. 1. The width of the container is 50 times the size of the sphere diameter $d_0 = 2.0$ mm, which results in the spheres piling up about 24 layers. The height of the container is set to be so high that almost no spheres can reach the top of

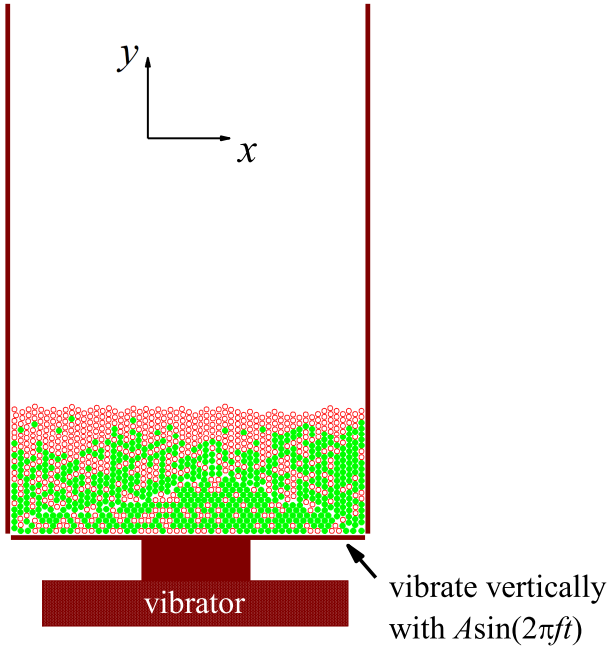

Fig. 1. The model used in simulation.

the container except at the beginning of the vibration. The bottom of the container moves vertically with a harmonic displacement function $A\sin(2\pi ft)$, where A and f are the amplitude and frequency of the vibration, respectively. As in general, frequency f and a dimensionless acceleration amplitude $\Gamma = 4\pi^2 Af^2 g^{-1}$ are used as control parameters, where $g = 9.8$ m/s^2 is the acceleration due to gravity. The other walls of the container are fixed during the vibration.

In order to treat multiple particle interactions, which seem to be the most important factor for this system, we use a soft sphere approach in our MD simulations. The Kuwabara–Kono model is used as normal interactions between granules or side wall,[25,26]

$$F_{ij}^n = -k_n \xi_{ij}^{3/2} - \eta_n \xi_{ij}^{1/2} V_{ij}^n \,, \tag{1}$$

and the tangential interactions are taken to the minor component in comparison to the viscous friction and dynamic friction,[27,28]

$$F_{ij}^\tau = \min\left(\eta_\tau V_{ij}^\tau, \mu F_{ij}^n\right), \tag{2}$$

as is generally adopted in the literature. In Eqs. (1) and (2), $\xi_{ij} = \max(0, 2d_0 - |\mathbf{r}_i - \mathbf{r}_j|)$ is the overlap of particle i and j, $\mathbf{V}_{ij} = V_{ij}^n \mathbf{e}_n + V_{ij}^\tau \mathbf{e}_\tau$ is the relative velocity between particle i and j at contact point, and the superscript (subscript) n and τ express the normal and tangential components of a vector, respectively. The detailed values of the elastic parameters are $k_n = 5.0 \times 10^9$ N/m$^{3/2}$, $\eta_n = 300.0$ Ns/m$^{3/2}$, and $\eta_\tau = 0.3$ Ns/m, and the coefficient of sliding friction is set to $\mu = 0.2$. The time step is taken as $\Delta t = 2.0 \times 10^{-6}$ s. These parameters work out the normal restitution coefficient ranging from 0.7 to 0.9 as the impact velocity varies from $1000d_0$/s to $1d_0$/s.

The simulation is firstly carried out under vibration for 40,000 vibration periods from a completely mixed initial state, in which the particles are generated randomly in the container and dropped under the gravity. During this simulation time, the segregation states always tend to their steady states for the parameters we used in this paper. Then the vibration is gradually weakened in an additional 1000 vibration periods, which results in all particles becoming still. The final configuration of the particles are defined as the static segregated states.

Our simulation shows that the convergence to a steady state strongly depends on the amplitude of the vibration. To ensure that the system finally tends to a steady state within the simulation time (40,000 vibration periods), the acceleration amplitude is set to a relatively high value $\Gamma = 24.0$ (the amplitude of the vibration $A = 0.8$ mm, about one-third of size of the diameter of the particles), and the frequency is set to $f = 85$ Hz. By the way, our results also show that above this frequency and amplitude, the segregation state does not seriously depend on the frequency or amplitude in a broad range. These vibration parameters will be used in all the simulations in this paper.

It is noticeable to point out that we used the most general interaction forms, i.e. Eqs. (1) and (2), in the soft sphere simulations, and did not consider the rolling

resistance. For an isolated rotating ball, if the rolling resistance is neglected, it will never stop its motion, including the translation and rotation. However, for a system containing multiple particles, we do not need to worry about the nonstop motion of the particles. For a multiple particle system, the translational kinetic energy and the rotational kinetic energy can be transferred into each other originating from the collisions between particles.[29] On the other hand, the collisions between particles are horizontal momentum conservation and angular momentum conservation. If there is no collision of particles with the side walls, the motion of the particles, including the translation and rotation, cannot be eliminated completely because of the horizontal momentum conservation and the angular momentum conservation. However, in our system, the horizontal momentum and angular momentum are not conserved because the particles also collide with the side walls, of which the translation and the rotation are not considered. This results in both the translation and the rotation of the particles gradually disappear when the vibration stops.

3. The Scheme of the Lighter and Mixed State

The typical static segregated states for different combinations of densities of both kinds of particles are shown in Fig. 2. In Fig. 2, we can see that the final segregated states are neither pure segregated states nor completely mixed states. They are partially segregated. These partially segregated states have characteristics similar to that we observed in experiments,[24] i.e. the lighter particles tend to go up and form a pure layer on top of the system, while the heavier ones and some of the lighter ones stay at bottom and form a mixed layer. We have called the state as the LMS in the previous work. The thickness of the pure top layer will increase as the density of the heavier particles increases, which is also consistent with that observed in experiments.

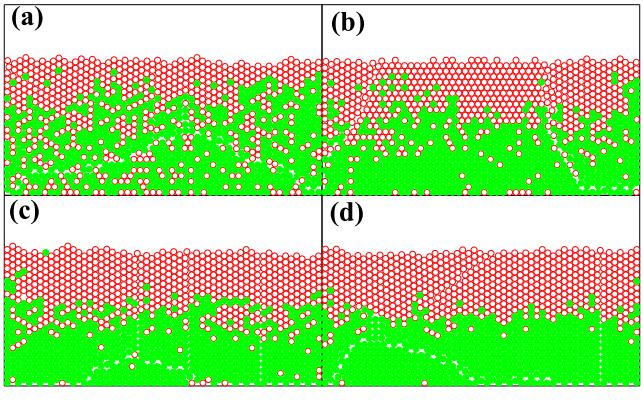

Fig. 2. Typical static segregated state of a binary granular mixture of the lighter particles with density $\rho_l = 1.0$ g/cm^3 and the heavier ones with density (a) $\rho_h = 3.0$ g/cm^3, (b) 4.0 g/cm^3, (c) 6.0 g/cm^3 and (d) 10.0 g/cm^3, respectively. The open and closed circles represent the lighter and heavier particles, respectively.

In MD simulation, the thickness of each layer can be calculated more accurately than that in experiments since every particle's position can be traced during simulations. The thicknesses of the top layer and the whole layer are calculated by

$$h_l = \frac{2N_l(y_l - y_h)}{N_l + N_h} \tag{3}$$

and

$$h = \frac{2(N_l y_l + N_h y_h)}{N_l + N_h}\,, \tag{4}$$

where y_h (y_l) and N_h (N_l) are average heights and number of the heavier (lighter) particles, respectively.

However, because finite fluctuation is an inherent property for granular system, if the average heights are calculated only from the final static state, they will have larger errors. The study of the dynamic process in segregation (to be published elsewhere) also shows that the order parameter of LMS will fluctuate over time. To reduce the effect of the fluctuations in the granular system, we calculated the average heights of the heavier and lighter particles during the vibration and take a long time average (for the final 20,000 vibration periods under vibration) to reduce the statistical error, rather than calculating them from the final static state. It is also noticeable that the average heights calculated in this way may be slightly different from that obtained from the final static state, but they will have much smaller statistical errors.

Until now, the LMS scheme (including the experimental research) is established on the basis of intuitive observation of the segregation state. Actually, the LMS scheme means a special distribution of each kind of particles. We can compare the distribution profile implied by the LMS scheme with that of the real simulated state to justify the LMS scheme. To obtain the distribution profile, we first assume that the total filling fraction of all particles for a segregated state is uniformly distributed at the lower part of the container, including a pure top layer and a mixed bottom layer, it should be equal to $N\pi(d_0/2)^2/hW$, where $N = N_l + N_h$ is the total number of both type of particles and W is the width of the container at horizontal direction. According to the LMS scheme, at the range of the pure top layer, the total filling fraction are contributed from only the lighter particles, so the filling fraction of the lighter particles equals the total filling fraction and that of the heavier particles is zero. At the range of the mixed bottom layer, the total filling fraction are contributed from both the lighter and heavier particles. However, the ratio of the filling fractions of the lighter (heavier) particles to the total filling fraction in the mixed bottom layer equal to the ratio of the number of lighter (heavier) particles to the total number of particles in the whole mixed bottom layer. The number of the lighter particles in the pure top layer can be obtained easily from the thicknesses of the pure top layer h_l and the the filling fractions of the lighter particles at the layer. Because the total numbers of both kinds of particles in the whole system are known, it is trivial to get the numbers

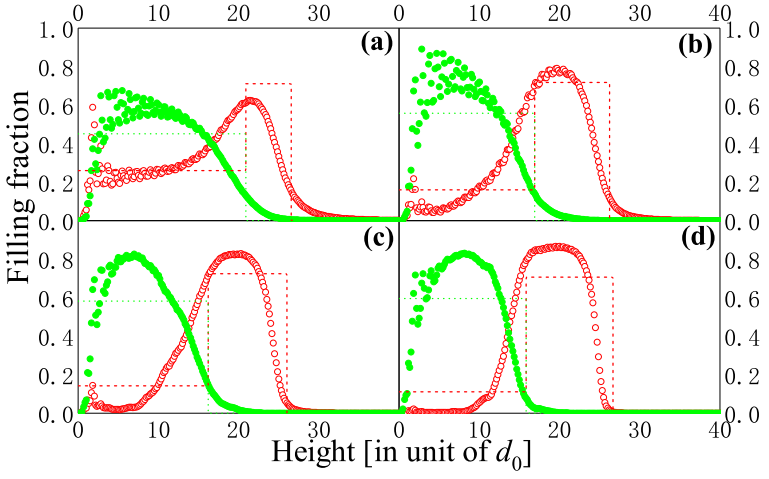

Fig. 3. Comparison between the distribution profiles obtained by counting directly the number of particles in each height interval (symbols) and by the LMS scheme (lines) for the lighter particles with density $\rho_l = 1.0$ g/cm^3 and the the heavier ones with density (a) $\rho_h = 3.0$ g/cm^3, (b) 4.0 g/cm^3, (c) 6.0 g/cm^3 and (d) 10.0 g/cm^3, respectively. The lighter and heavier particles are mixed with same ratio. The open circles and dashed lines are for the lighter particles, while the closed circles and dotted lines are for the heavier particles.

of the lighter and heavier particles, respectively, in the mixed bottom layer. We can plot both the filling fractions for lighter and heavier particles as a function of height, which are constant among both layers and change values only at the interface (see the lines in Fig. 3). The real distribution profile can be obtained by counting directly the number of particles in each height interval, which is set to $d_0/6$ in the real calculation, and taking long time average during the simulation (the final 20,000 vibration periods under vibration). Figure 3 also plot these real distribution profiles. From Fig. 3, we can see that both profiles are consistent with each other in the main characteristic, though the real distribution profile is continuous at all boundaries and that implied by the LMS scheme is discontinuous. This justify that the LMS scheme is a good approximation in describing the real configurations for this type of segregation.

It is noticeable that there is a gap between the granular bed and the bottom of the container during vibration, which is represented by the low value of the real distribution profiles as the height near to zero. This phenomenon has also been observed in the experiment on a vacuum quasi-2D granular system,[30] in which we show that the gap exists clearly at very low air pressure and disappears gradually as the air pressure increases.

From Eq. (3), one can easily find that the thickness of the pure top layer should vary with the mixing ratio seriously. However, the component of the lighter particles in the mixed bottom layer may relate to the stiffness of the mixed bottom layer and may be invariant for fixed vibration conditions. Intuitive experience tells us that the granular bed made by heavier particles is stiffer than that made by lighter

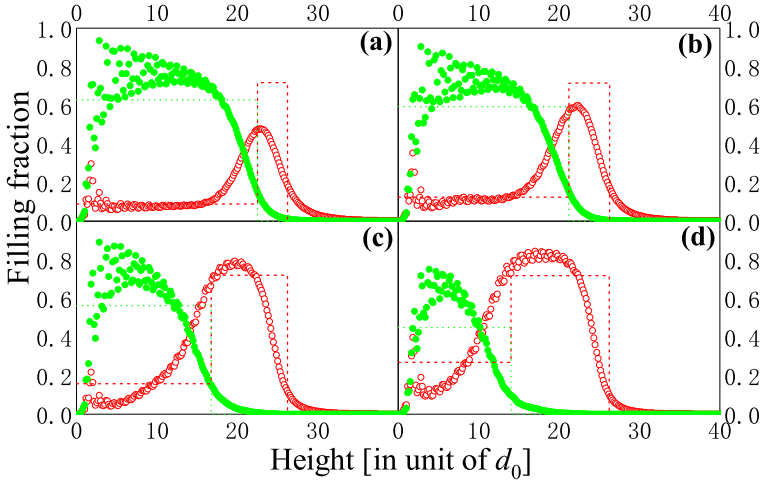

Fig. 4. Comparison between the distribution profiles obtained by counting directly the number of particles in each height interval (symbols) and by the LMS scheme (lines) for the total mixing ratio of lighter particles being (a) 25%, (b) 33%, (c) 50% and (d) 66%, respectively. The densities of lighter and heavier particles are fixed at 1.0 g/cm^3 and 4.0 g/cm^3, respectively. The symbols and lines have the same meaning as that in Fig. 3.

ones. So, the more component of the lighter particles in the mixed bottom layer may result in the bottom layer being more fragile. To check if the component of the lighter particles in the mixed bottom layer varies with the fraction of the lighter particles in the whole system, we extent the system to nonequally mixed cases. Figure 4 depicts both of the distribution profiles obtained by counting directly the number of particles and by the LMS scheme for these cases. We see that the LMS scheme also fairly describes the main characteristic of the segregation state in all the cases, and the component of the lighter particles in the mixed bottom layer slightly but systematically increases as more lighter particles are included in the system. The variation seems to not only result from the continuous change at the boundary, but also from the deeper flat region, as shown in Figs. 3(a) and 3(b).

4. The Order Parameter of the Lighter and Mixed State

In the previous experimental research,[24] we suggested using twice the ratio of the thickness of the top layer to that of the whole system as an order parameter, i.e. $2h_1/h$, for equally mixed cases. This parameter can be measured in experiment directly. In that work, we have found that the order parameter at strong vibration is only a function of density ratio between the heavier and lighter particles, which is obtained by collapsing all data from many combinations of particles into one function. The collapsed function is a convex monotonic function of the density ratio, i.e. it increases quickly at small density ratio and saturates to one at larger density ratio. This characteristic is important because it implies that there is no completely mixed phase for small density ratio except it is exactly one.

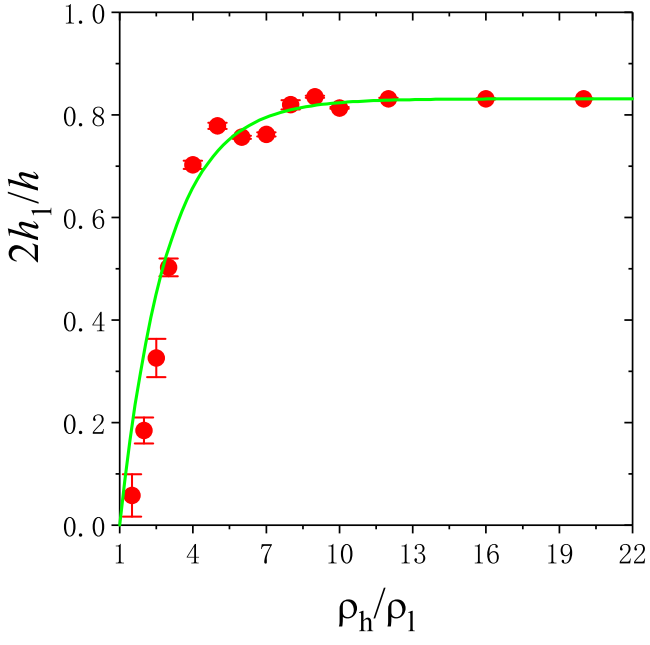

Fig. 5. The order parameter as a function of the density ratio between the heavier and lighter particles. The density of the lighter particles are fixed at $\rho_l = 1.0$ g/cm^3. The curve is fitted from a saturation curve expressed by $A(1 - e^{B(x-1)})$, where $x = \rho_h/\rho_l$.

In the simulation research, we also show that above the frequency $f > 85$ Hz and amplitude $\Gamma > 24.0$, the segregation state does not seriously depend on the frequency and amplitude in a broad range. Now, we study the characteristic of the variation with density ratio between the heavier and lighter particles. Figure 5 depicts the order parameter as a function of density ratio with fixed $\rho_l = 1.0$ g/cm^3. Figure 5 shows that the order parameters are close to a convex monotonic function of the density ratio, which increases quickly at small density ratio and saturates to a value slightly less than one at larger density ratio. These characteristics are qualitatively consistent with that shown in the experimental work. The standard error bars are also plotted in the figure. We can easily find that the errors are larger for smaller density ratio, which means that the order parameter there fluctuates strongly with time even after the steady state is reached. We have fitted the graph in Fig. 5 by a saturation curve $A(1 - e^{B(x-1)})$, where $x = \rho_h/\rho_l$. The curve fits the data well, which supports our previous conclusion, i.e. the order parameter is a convex monotonic function of the density ratio, it increases quickly at small density ratio and saturates to positive value at larger density ratio.

At the end of this paper, we point out the following noticeable facts. Firstly, the vibration amplitude used in the simulation is much higher than that used in the experiment (about $\Gamma = 7.0$) to show the LMS segregation phenomenon. In the experiment, the whole system tends to its steady state much quickly (almost

within one minute) except at very small vibration amplitude (less than $\Gamma = 1.2$). We guess that the slower convergence in the simulation results from the less freedom of the 2D system for adjusting the particle's position during vibration. Secondly, the order parameter is calculated during vibration, which results in the order parameter of a completely segregated state being a little smaller than one as we mentioned previously. This defect can be reduced by calculating the order parameter from the static segregated state. However, the static order parameter has much larger error since the average over a large number of configurations is unpractical in this case.

5. Summary and Conclusion

We have investigated the 2D segregation effect in vertically vibrated binary granular mixtures with same size by MD simulation. The results showed that the LMS also exists in the 2D system. The validity of the scheme of the LMS has been testified by comparing the distribution profile implied by the LMS scheme with that obtained by counting directly the number of particles in each height interval. It was shown that the LMS scheme fairly describes the main characteristic of the partially segregated state occurring in the system. The simulation work here together with the previous experimental work[24] have shown that the density difference can drive a special kind of segregation, in which neither size difference nor air pressure is needed. This density-driven segregation can be quantitatively described by an order parameter based on the LMS scheme. There is another kind of segregation, in which the air pressure plays very important roles, and the distribution profile is clearly different from that of the LMS scheme, though it can be described by another kind of order parameter.[30] These works conclude that there are several kinds of segregation, which result from different mechanisms and have different structures. The density difference and the gravity field are enough to cause segregation effect, which results in an LMS-type segregation. We have defined an order parameter, and presented a method that can accurately calculate it in the simulation. We have also found that the order parameter is a convex monotonic function of the density ratio, which is qualitatively consistent with that shown in experimental.

Acknowledgments

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