Segregation and Phase Inversion in a Simple Granular System

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Segregation and phase inversion are investigated through a simple granular system which consists of only two inelastic hard spheres in a square box with an energy source. With the variation of the coefficient of restitution, the mass ratio between two spheres or the box size, we show that two types of segregated states and crossover between them are realized in this small simple system.

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Granular materials exhibit various complex phenomena.^{1,2)} Examples are segregations of particle mixtures with different properties which appear upon shaking or stirring them, or confining them in a horizontally rotating drum.^{3–18)} Recently, many studies of several segregated patterns and the crossover between them have been reported.^{10–18)}

In this paper, instead of carrying out simulations with many particles, we choose a simple system consisting of inelastic hard spheres with different masses. Although the system is very simple, it will be shown to exhibit segregation of particles. This system is considered to be a simple model of local processes of highly excited granular mixtures.

Such small systems with elastic hard discs were recently investigated, and were found to exhibit a prototype of solid–liquid phase transition, glass transition, and the transition between the static and dynamic friction.^{19–21)} In the following, we show that this simple system realizes the crossover between two segregated states, similar to the change between different segregated patterns obtained in recent studies.^{10–18)}

The system under consideration consists of two inelastic hard-sphere particles with unit radius and different masses which are confined in a two-dimensional square box (Fig. 1). The left-hand wall is set at the origin of the horizontal axis and is in contact with the energy source. All walls are rigid and have a length longer than 4. The interaction between a particle and the walls without an energy source occurs only through hard-core collisions. We give the position of a light and a heavy particle in the horizontal direction, $x_{\rm L}$ and $x_{\rm H}$, as the distance from the left wall, and their masses $m_{\rm L} = 1$ and $m_{\rm H} = M > 1$, respectively. The interaction between two particles occurs through inelastic hard-core collisions with the coefficient of restitution e. A particle hitting the left-hand wall in contact with the energy source with the velocity $(v_{\rm h}, v_{\rm v})$ bounces back with the velocity $(V_{\rm h}, V_{\rm v})$ $(V_{\rm h} > 0)$. Here, subscripts h and v indicate, respectively, the horizontal and vertical directions. In this paper, we employ a heat bath at the temperature T as the energy source because of its simplicity. Then, the velocity (V_h, V_v) is chosen randomly from the probability distributions $P_h(V_h)$ and $P_v(V_v)$:²²⁾

$$P_{\rm h}(V_{\rm h}) = \frac{m_i V_{\rm h}}{T} \exp\left(-\frac{m_i V_{\rm h}^2}{2T}\right) \tag{1}$$





Fig. 1. Illustration of system with two inelastic hard spheres and energy source (left).

$$P_{\rm v}(V_{\rm v}) = \left(\frac{m_i}{2\pi T}\right)^{\frac{1}{2}} \exp\left(-\frac{m_i V_{\rm v}^2}{2T}\right),\tag{2}$$

where T is the temperature of the heat bath fixed at unity. (We give the Boltzmann constant as 1.)

In the following, we perform the simulation of the above system with the length of walls S = 4.05, 4.2, and 4.5. For this range of *S*, particles are densely packed and collisions between particles occur frequently. In order to characterize the distribution of two particles, we define the segregation parameter $\delta \equiv \langle x_L - x_H \rangle_t$, where $\langle \cdots \rangle_t$ indicates the time average. If $\delta \sim 0$, the particles are not segregated, while the sign of δ gives the average configuration of the two particles.

We draw the phase diagram of the model against $\{M, e\}$ (M > 1 and e < 1), according to the value of S. Figure 2 shows the diagrams for (a) S = 4.05, (b) S = 4.2, and (c) S = 4.5. Here, $\delta > 0$ holds in the region with $+, \delta < 0$ holds in the region with -, and $\delta \sim 0$ holds in the shaded area drawn using multiple points. (In this paper, we regard the case with $-(S-d) \times 10^{-3} < \delta < (S-d) \times 10^{-3}$ as $\delta \sim 0$, where d is the diameter of the particle.) Independently of S, each phase diagram has the following characteristics. For small M, $\delta \sim 0$ or $\delta > 0$ holds throughout the range of e < 1. When *M* increases, the system realizes two states with $\delta > 0$ and $\delta < 0$ and the crossover between them depends on *e*. In particular, the critical value e for realizing the crossover between states with $\delta < 0$ and $\delta > 0$ is independent of *M* for a large limit of M. However, the crossover points shift to larger e and larger M with the increase of S. This indicates that the change of the packing fraction of particles is also relevant to the crossover between $\delta < 0$ and $\delta > 0$ states. Moreover, the crossover points for S = 4.05 form a curve

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Fig. 2. Phase diagrams of system for each set (M, e) with (a) S = 4.05, (b) S = 4.2, and (c) S = 4.5. + and - indicate the sign of δ , and $\delta \sim 0$ in the shaded area.

with an 'N' shape, while the curve becomes smooth with the increase in S, as seen in Figs. 2(b) and 2(c).

Figure 3(a) shows δ as a function of *e* for M = 1.5, M = 2.0, M = 3.65, and M = 6.0 with S = 4.05. For large M, δ assumes a minimum value at approximately $e \sim 0.825$ and the minimum value decreases with the increase in M. In Fig. 3(b), δ is plotted as a function of M for e = 0.825, e = 0.625, and e = 0.55. Here, δ has a peak at $M \sim 1.3$. With the decrease in *e*, δ for larger M becomes larger than that for M at the peak.

To explain the existence of the two segregated states with $\delta > 0$ and $\delta < 0$, we consider two effects determining the sign of δ ; one effect contributes to the increase in δ and the other contributes to the decrease in δ with the decrease in *e*, respectively.

First, we study the former effect. The light particle's velocity immediately after the contact with the energy source on the left-hand wall tends to be higher than that of the heavy particle because the average of these velocities is a decrease function of the mass of each particle. On the other hand, by iterations of the collision between two particles,



Fig. 3. (a) δ as a function of *e* for M = 1.5, M = 2.0, M = 3.65, and M = 6.0, and (b) δ as a function of *M* for e = 0.825, e = 0.625, and e = 0.55 with S = 4.05.

their velocities approach each other because e < 1. This implies that the light particle tends to be located farther from the left-hand wall than the heavy particle. Thus, δ is expected to increase with the decrease in *e*. The contribution of this effect is expected to increase with 1 - e, and as a rough approximation, it is assumed to be proportional to 1 - e.

Second, we study the effect by which δ decreases with the decrease of e. If e is given a value close to 1, the approach of two particles' velocities by collisions between two particles is slow. Then if $M \gg 1$, the light particle moves much faster than the heavy one for most of the time and collisions between the two particles occur frequently. Then, the light particle behaves like a potential barrier against the motion of the heavy particle. In this case, the heavy particle's motion in going this potential barrier is important for determining the particle distribution. The kinetic energy of the heavy particle in the case of $x_L < x_H$ is smaller than that of $x_L > x_H$ because, in the former case, the heavy particle cannot contact the heat bath directly and the energy is supplied only by collisions with the light particle. This indicates that the mean velocity of the heavy particle in the case $x_{\rm L} < x_{\rm H}$ is smaller than that of $x_{\rm L} > x_{\rm H}$, while the ratio between the velocities is roughly estimated to be e: 1. Then, the ratio between the time required to switch from $x_{\rm L} < x_{\rm H}$ to $x_{\rm L} >$ $x_{\rm H}$ and to switch from $x_{\rm L} > x_{\rm H}$ to $x_{\rm L} < x_{\rm H}$ is given as 1 : *e*. Here, this effect on δ is prominent only for the case with the large collision frequency which is almost proportional to *e*. In addition, this collision frequency increases with the decrease in S. Then, the contribution from the above effect is approximately estimated as $\delta_1 \sim (e-1)e/C(S)$. (C is an increasing function of *S*.)

By the combination of these effects, δ for large *M* is given as

$$\delta \sim A\delta_0 + B\delta_1 = (1-e)\left(A - \frac{B}{C(S)}e\right).$$

Here, *A* and *B* are given as positive constant values. With adequate *A*, *B*, and *C* holding 0 < AC(S)/B < 1, δ takes a negative value for large e(1 > e > AC(S)/B) and a positive value for small e(0 < e < AC(S)/B). This result also indicates that the crossover value of *e* between the state with $\delta < 0$ and that with $\delta > 0$ becomes larger with the increase in *S*. If *M* is small, the contribution of δ_1 is expected to be negligible. Thus, $\delta > 0$ is realized for small *M*.

In this paper, mass segregation and phase inversion are investigated through a system which consists of only two inelastic hard spheres in a square box with a heat bath. With the variation in the coefficient of restitution, the mass ratio or the box size, two types of states with different particle distributions and crossover between them were observed for the case with a large mass ratio between two particles. The system we studied here may appear to be too small and simple. However, we expect that this system can describe the local dynamics of highly excited granular systems, and provide a basis for the understanding of particle segregations in granular systems consisting of many particles.

The effects of gravity, size difference and friction should be considered in order to investigate the generality of obtained phenomena such as the crossover between different segregated states.^{10–18)} Further analytical study of this system to clarify the presented behavior as well as the study of systems with three or more particles is necessary in the future. The author is grateful to K. Kaneko, M. Mizuguchi, H. Hayakawa, H. Nishimori and M. Otsuki for useful discussions.

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