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Irregular Oscillation of Bi-disperse Granular Gas in Cyclic Three Compartments *

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A 3-D molecular dynamics simulation of a bi-disperse vibro-fluidized granular gas in a cyclic three-compartment cell is performed. A cluster of particles is randomly found in one of the compartments. Lohse's flux model is modified to incorporate inelastic particle-boundary collisions. This model predicts that periodically there is clustering in each compartment. It is then found that if the model is further modified to incorporate Gaussian white noise, it correctly predicts the non-sequential clustering behavior confirming that there is no chaotic behavior.

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Mechanical energy is not conserved in granular gases due to inelastic interactions between colliding particles.[1] Due to inelastic collisions, granular gases have a tendency of spontaneously forming highly concentrated regions or clusters.[2−6] This clustering phenomenon is clearly apparent in a box that is divided into a number of compartments, which are interconnected through a small opening.

The granular particles are vibrofluidized by shaking the box vertically. For weak vertical shaking strength a mono-disperse granular gas in the two-compartment system spontaneously clusters into one compartment. This symmetry-breaking phenomenon in the mono-disperse granular gas called "Maxwell's demon" was observed by Schlichting and Nordmeier.[7] For a granular mixture composed of two different species, Miao *et al.*[8] found experimentally that the granular mixture clusters alternately between the two compartments and shows a cyclic oscillation with a fixed period. This oscillation phenomenon was termed to be the granular clock due to its resemblances with the classical chemical clock. To explain this oscillation phenomenon, Lambiotte *et al.*[9] simulated a system of hard disks of equal masses but different radii and suggested a simple phenomenological model by taking into account the vertical segregation (the Brazil nut effect[10]). However, Costantini *et al.*[11] simulated a system of hard disks of equal sizes but different masses and developed a mean-field theory. In a quasi-two-dimensional experimental setup, Viridi *et al.*[12] studied a horizontal oscillation of a bi-disperse granular mixture. The granular clock was also observed by using glass and steel balls of the same size and the transition from the homogeneous state to the oscillatory state was found to be via Hopf bifurcation.[13]

The study of oscillation phenomenon was also extended to more than two-compartment systems.[14,15] The oscillation behavior of the bi-disperse granular gas has been inspected experimentally in a cyclic three-compartment system, in which the clustering order is observed to be irregular, and the clustering transition interval was found to decrease with the evolution time.[16] Until now, this research is preliminary and the mechanism of the oscillatory phenomenon in three-compartment system is still unclear and needs to be explored. Hence, further experiments and simulation are needed to better understand this phenomenon.

In this Letter, by 3-D molecular dynamic simulation, we investigate the irregular oscillatory phenomenon of a bi-disperse granular gas in a cyclic three-compartment system. The modified Lohse's model, which takes into account the Gaussian white noise, is utilized to explain the simulation results.

The event-driven hard sphere molecular dynamics method is used to simulate the 3-D granular gas system. The effect of gravity field g is also taken into account. Granular particles with radius r are considered to be perfect rigid spheres. The coefficient of restitution e is fixed to be 0.9. Rotational motion and frictional forces are ignored. A bi-disperse mixture of two types of particles with the same size but different masses is used. Heavy particles are 8 times heavier than the light ones, i.e. $m_h/m_l = 8$, where m_h is mass of heavy and m_l is the mass of light particles. The particles are placed in the container consisting of three cyclic compartments with ground area $\Omega = 60\times 60r^2$. The lateral boundaries of the container are infinitely high. Two adjacent compartments are connected through a window in width $H = 6r$ and located at $h = 65r$ above the base of the compartments.

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The Bottom plate moves in a saw-tooth manner with a fixed normalized vertical velocity $v' = v/\sqrt{4gr}$. The vibration amplitude is quite small in comparison with the mean free path of this granular gas system. In the simulation we assume that the bottom plate is fixed at its position. Particles colliding with the bottom plate will bounce back gaining a velocity $2v'$. The length unit is taken in terms of r and time unit in $\sqrt{r/g}$. Particles are initially placed in one compartment and vibrated vertically. N_0 is the total number of the two types of particles and is fixed to be 1600 throughout the simulation. $N_{i\sigma}$ represents the number of type-i particles in compartment σ. Whereas $i = l, h$ for light and heavy particles and σ may be 1, 2 or 3 for the three compartments. For example, N_{l2} represents the number of light particles in the compartment 2.

In the simulation, at different driving velocities, three steady states are observed: asymmetric distribution state (ASY), homogenous state (HOM) and oscillatory state (OSC). The time evolutions of the number of particles for these three states are shown in Figs. 1(a)–1(c). When driving velocity is moderate, the majority of the particles cluster in one of the three compartments, we call this the ASY state (Fig. 1(a)). When driving velocity is very high, the light and heavy particles are able to populate homogeneously in all three compartments; the HOM state is observed (Fig. 1(b)). In an intermediate driving velocity, particles alternatively cluster in an irregular order in one of the compartments as shown in Fig. 1(c) (snapshots shown in Figs. 2(a)–2(e)).

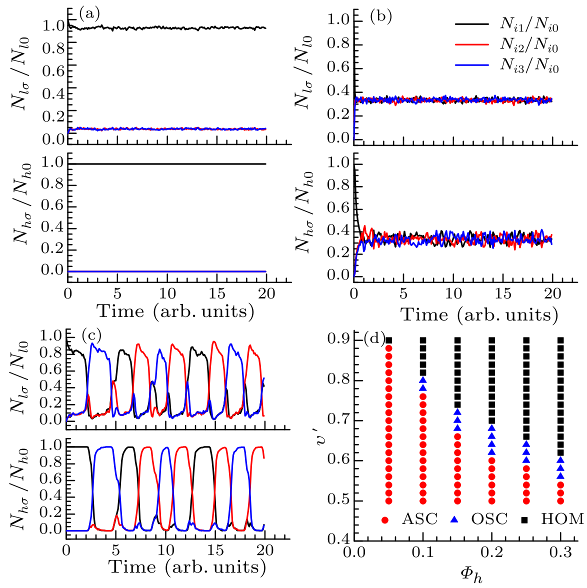

Fig. 1. (Color online) (a)–(c) Time evolution of number of particles in the simulation of bi-disperse granular gas in three-compartment system: (a) an asymmetrical state, (b) a homogenous state, and (c) a disordered oscillatory state. (d) A phase diagram drawn between base velocity v' and heavy particle ratio Φ_h.

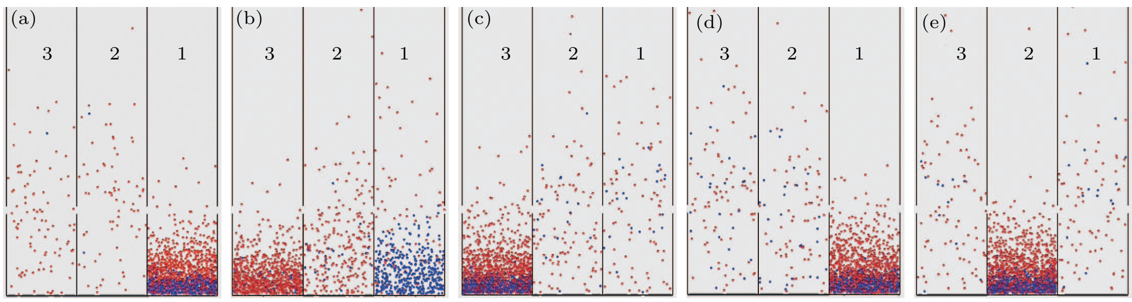

Fig. 2. (Color online) Snapshots of the oscillatory state of bi-disperse granular gas showing an irregular clustering phenomenon in the cyclic three-compartment system. Red ones are light particles and blue are heavy particles. (a) An initial state of the system, with most of the particles in compartment 1; (b) transition of particles from compartment 1 to compartment 3; (c) all the particles then cluster in the compartment 3; (d) particles back from 3 to 1, and (e) particles cluster transition to compartment 2.

The oscillatory clustering has also been observed in two-compartment bi-disperse granular gas systems, in which particles cluster back and forth in the two compartments. In the three-compartment system the oscillatory state becomes more interesting because there is a choice in which compartment the clustering will form next. Will the cluster oscillate in an orderly manner or will it be irregular?

In Fig. 2, snapshots of the oscillatory states are presented to show what have been observed from the simulation of the process. During the vertical vibrations, light particles are pushed upwards by the heavy particles. This is because the light particles gain velocity, due to momentum conservation, when colliding with heavy particles. Hence, the light particles leave the compartment preceding the heavy ones and are easier to distribute among the rest of the two compartments. For example, initially starting from compartment 1, the light particles leave the compartment 1 prior to heavy particles and are distributed between compartment 2 and compartment 3, as shown in Figs. 2(a) and 2(b). The light particles fluctuate between these two compartments. The fluctuations are obvious in Fig. 1(c). Due to the presence of the heavy particles in compartment 1, there will be no net flux of light particles into this compartment. When the majority of the light particles have left compartment 1, the heavy particles get sufficient energy from the base and proceed to compartment 2 or 3. For the compartment having instantly more particles, due to frequent collisions a rapid decrease in the kinetic energy would occur and it will become an attractor of particles compared to the other two compartments. Thus, there will be a net flow of particles towards this compartment. As soon as most of the light and heavy particles cluster in one of the two compartments, i.e. compartment 2 or 3, the same cycle repeats. Since the chance for the particles to cluster in compartment 2 or 3 seems to be equal, the clusters are formed irregularly among the three compartments, for example, as shown in Figs. 2(a)–2(d) (also shown in Fig. 1(c)), in such an order 1-3-1, or 2-3-2 $\cdots$.

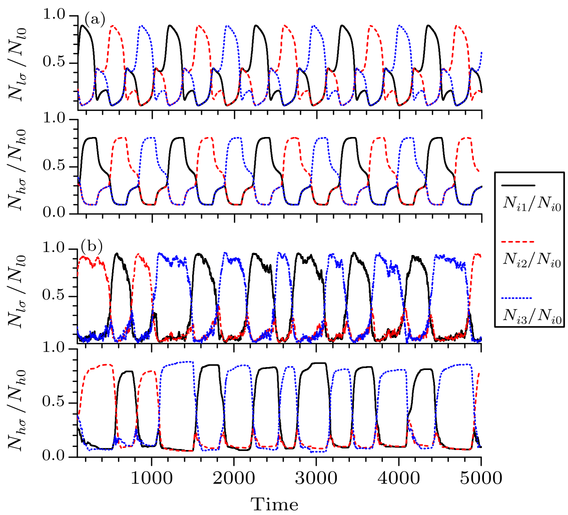

Fig. 3. (Color online) Time evolution of the particles number obtained from the numerical solution of the flux model: (a) without noise term and (b) including white noise term. The upper half is for the light particles and the lower part shows the heavy particles. Black, red and blue shows the numbers of particles in compartments 1, 2 and 3, respectively.

A phase diagram, which shows these three states at different shaking strength v' and the percentage of the heavy particles among the total number $\varPhi_h = N_{h0}/N_0$, is obtained, as shown in Fig. 1(d). The phase diagram shows that the threshold driving velocity for the oscillatory state drops with increasing $\varPhi_h$. This is because light particles gain velocity, while heavy particles lose velocity, when colliding with each other due to conservation of momentum. When the driving velocity is low, all particles are trapped in the original compartment. As the driving velocity increases, light particles with the help of heavy particles start to jump out of the compartment. When remaining light particles are few enough, heavy particles are able to follow the light ones to flow out. When most of the particles are clustered in the other compartment, the same cycle will occur and oscillation phenomenon emerges. Increasing (decreasing) the total number of heavy (light) particles will help the light particles to gain velocity to flow out of the compartment, therefore the threshold of driving velocity becomes lower as the fraction of heavy particles increases. This is what is seen in Fig. 1(d) when $\varPhi_h$ is in the range of 0.1–0.3. As $\varPhi_h$ is increased to the range of 0.3–0.5 only part of the heavy particles will be needed in the cycle, the OSC state will decay to degenerate oscillatory state (d-OSC)[17] (not shown in Fig. 1(d)). When $\varPhi_h$ is even greater than 0.5, the oscillation phenomenon disappears. There are only ASC and HOM states as in the case of the mono-disperse granular system.

In order to explain the irregular clustering phenomenon in the three-compartment system we use Lohse's flux model[18] for bi-disperse granular gas in the two-compartment system and generalize it to the three-compartment system. The development of a number of the particles in one compartment is considered to be the net balance between the outgoing flux from this compartment and the incoming flux to this compartment. Hence the evolution of a number of light and heavy particles in compartment 1 can be written as

$$\begin{aligned}\frac{\partial N_{i1}}{\partial t} =& -2F_i(N_{l1}, N_{h1}) + F_i(N_{l2}, N_{h2})\\ &+F_i(N_{l0}-N_{l1}-N_{l2}, N_{h0}-N_{h1}-N_{h2}),\end{aligned} \tag{1}$$

where $i = l, h$ for light and heavy particles, and $F_i(N_{l1}, N_{h1})$ is the flux function. The equations for compartments 2 and 3 can be written in the similar form.

For simplicity, three main assumptions are taken,[18] while the flux function is derived for the bi-disperse granular system: (1) the temperature of both species is considered to be the same; (2) the temperature of each of the two species is independent of height z; (3) velocity distributions of particles are Maxwellian and isotropic. At the height of the windows, it is found that the assumptions hold approximately right.[18−20] In our case the flux function, keeping in view of these assumptions,[18] is given as

$$\begin{aligned}F_i(N_l, N_h) =& \frac{bN_i}{\varOmega}\sqrt{\frac{k_{\rm B}T}{2\pi m_i}}\exp^{-m_i gh/k_{\rm B}T}\\ &\cdot(1-\exp^{-m_i gH/k_{\rm B}T}),\end{aligned} \tag{2}$$

where b is the width of the wall, $\varOmega$ is the ground area of compartment, m_i is the mass, $n_i(z)$ is the number density of the type-i particles, $k_{\rm B}$ is Boltzmann's constant, H is the window width, and T is the granular temperature.

We modify Lohse's flux model,[18,20] which considers particle-boundary collisions to be elastic, to incorporate inelasticity of such collisions. The rate of energy loss due to particle-particle and particle-boundary collisions is balanced by the input energy rate and the modified temperature is found as follows:[21]

$$(k_{\mathrm{B}}T)^{1/2} = -\frac{\beta_1+\beta_2}{\delta_1} + \frac{\delta_1}{3\alpha_1}, \tag{3}$$

where β_1, β_2, α_1 and δ_1 depend on the system parameters.

Now solving Eq. (1) numerically, using the 4^{th}-order Runge–Kutta method, with the initial condition that all the particles initially lay in the compartment 1, the corresponding time evolution of the particles distribution is shown in Fig. 3(a). It is found that the initial condition does not affect the final results. The oscillatory clusters predicted by theory show that the clustering of particles is in a certain order but the direction may be random, i.e. (1–2–3, 1–2–3$\cdots$ or 3–2–1, 3–2–1$\cdots$). This deterministic flux model can not envisage the irregular oscillatory phenomenon as observed in simulation of a cyclic three-compartment system.

Adding an additional white noise term into the flux model, we have

$$\frac{\partial N_{i1}}{\partial t} = -2F_i(N_{l1},N_{h1})+F_i(N_{l2},N_{h2})+F_i(N_{l0}-N_{l1} - N_{l2}, N_{h0}-N_{h1}-N_{h2}) + \xi_{i1}(t), \tag{4}$$

where $\xi_{i1}(t)$ is the Gaussian white noise, which obeys the auto correlation $\langle\xi_{i1}(t)\xi_{i1}(t')\rangle = \sigma^2[\xi_{i1}(t)]\delta(t-t')$ with σ^2 being the variance.

According to Mikkelsen *et al.*,[20] the variances of the noise terms read

$$\sigma^2[\xi_{i1}(t)] = K_i^2[2F_l(N_{l1},N_{h1}) + F_i(N_{l2},N_{h2}) + F_i(N_{l0} - N_{l1} - N_{l2}, N_{h0} - N_{h1} - N_{h2})],$$

and $K_i = 2.8$.

Now solving Eq. (4) numerically, with the same initial condition that all the particles lie in the compartment 1, the corresponding time evolution of the particle distribution is shown in Fig. 3(b). The modified flux model, with the white noise term, shows irregular ordering (2–1–2, 3–1–3$\cdots$) of clustering behavior in the three compartments. Therefore, this disordered clustering phenomenon observed in the compartmentalized granular system can be described by noise fluctuations rather than a deterministic chaotic behavior.

As discussed above, the two ordered oscillatory behaviors predicted by the deterministic flux model correspond to two stable limit cycles. At some parts of the system trajectories, both the limit cycles are so close to each other that even a small system fluctuation caused by Gaussian white noise can root the system to jump from one limit cycle to the other. The observed random ordered oscillatory behavior is generated due to the random hopping behavior, which is induced by system noise between the two attractors.

In the 3-D molecular dynamics simulation, the clustering behavior of the bi-disperse granular gas in the cyclic three-compartment system is studied. For the different shaking strengths, asymmetric, homogenous and oscillatory states are observed. In the oscillatory state, the cluster formation in the three compartments is found to be arbitrarily ordered. A modified Lohse's flux model is utilized to explain our simulation results. However, even considering the particle-boundary collisions to be inelastic, the modified model is just able to figure out the ordered clustering behavior. The irregular oscillatory cluster formation observed in the simulation of the cyclic three-compartment system can be reproduced in our modified model when a Gaussian white noise term is considered. It shows that the observed random ordered oscillatory behavior is provoked by the system noise which induces the hopping between the two attractors, rather than a deterministic chaotic behavior as it looks to be.

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