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Non-Gaussian and Clustering Behavior in One-Dimensional Polydisperse Granular Gas System*

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Abstract *We present a one-dimensional dynamic model of polydisperse granular mixture with the fractal characteristic of the particle size distribution, in which the particles are subject to inelastic mutual collisions and are driven by Gaussian white noise. The inhomogeneity of the particle size distribution is described by a fractal dimension D. The stationary state that the mixture reaches is the result of the balance between energy dissipation and energy injection. By molecular dynamics simulations, we have mainly studied how the inhomogeneity of the particle size distribution and the inelasticity of collisions influence the velocity distribution and distribution of interparticle spacing in the steady-state. The simulation results indicate that, in the inelasticity case, the velocity distribution strongly deviates from the Gaussian one and the system has a strong spatial clustering. Thus the inhomogeneity and the inelasticity have great effects on the velocity distribution and distribution of interparticle spacing. The quantitative information of the non-Gaussian velocity distribution and that of clustering are respectively represented.*

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Key words: inelasticity, restitution coefficient e, inhomogeneity, fractal dimension D, polydisperse granular gases

1 Introduction

Granular gases,[1,2] i.e., a large number of macroscopic particles colliding with one another and losing a little energy at each collision, exhibit a fascinating phenomenology, such as non-Maxwellian velocity distributions, clustering, and so on. Generally speaking, granular gases cannot be described as equilibrium systems either from the configurational point of view or from the dynamical point of view, because of the intrinsic inelasticity of the collisions among the grains. It is known in fact that these systems remain easily trapped in some metastable configurations, which can last for long time intervals unless they are shaken or perturbed.[2] Therefore, in order to maintain the dynamics of granular gases in a long run, external driving forces are inevitable.

Both experiments and computer simulations show that the dynamics of granular gases stems from the inelastic nature of their collisions, which leads to the non-Gaussian velocity distribution[3–6] and clustering.[3,4,7,8] Non-Gaussian velocity distributions display low-velocity and high-velocity overpopulated regions. But, the present consensus emerging from various studies tends to reach the conclusion of the absence of universality in the velocity distribution:[9] various experimental conditions and various energy injection modes lead to different distributions. For example, a uniform heating mechanism, namely Gaussian white noise acting on each particle, was first introduced by Williams and Mackintosh.[8] Based on the model, Barrat *et al.*[6] considered the systematic force due to inelastic collisions, and studied the velocity distributions of one-dimensional inelastic driven monodisperse granular gases. In the heated steady state, they found that, depending on the inelasticity, the distribution function may display two different stretched exponential tails at large velocities. Later, on the basis of the model of Williams and Mackintosh, Puglisi *et al.*[3] added a second ingredient, consisting of a friction term that prevents the kinetic energy from diverging. With such a modification, the system reaches a steady state and time averages can be safely computed. In the case far from equilibrium, they investigated the non-Gaussian velocity distribution and clustering behavior of the monodisperse granular gases in the stationary state, which are the result of the energy loss by the dissipative interactions. These phenomena are more and more obvious as the value of the restitution coefficient e decreases. Thereafter, Cecconi *et al.*[4] also studied the one-dimensional driven granular gases with a single component. They discussed the effect of the restitution coefficient e on the velocity distribution and distribution of distances between nearest neighbors. However, these works were only about a uniform granular system.

In actual granular systems, the sizes of particles are different, namely the dispersion of the granularity is non-

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uniform. Zhang *et al.*[10] presented a fractal model of a non-uniform granular system with an example. Since the experimental study of the dynamics in a real granular system is a great challenge, the increasing power of computers awakens an interest in "actual granular gases" simulations. By numerical simulations, Zhang *et al.*[11−13] studied that the fractal dimension D of the granularity distribution, which can be considered to be a measure of the inhomogeneity in the particle size distribution, influences the dynamic behavior of the non-uniform granular system in the steady-state. The simulation results indicate that the fractal dimension D and the restitution coefficient e have great influences on the dynamic actions of the system. However, in Refs. [11] ∼ [13], although the phenomena of the non-Gaussian velocity distribution and the clustering were described, no quantitative analysis is given about the deviations from the Gaussian and clustering. Moreover, in order to solve problems in an easier way, the particle sizes were neglected and the particles were assumed as mass points.

In the present paper, we present a one-dimensional dynamical model, in the spirit of the one introduced by Puglisi *et al.*,[3] containing an important difference regarding the particle size following the fractal distribution. We consider, by analogy, "heat bath" as the external driving mechanism to maintain the system in a statistically steady state. By molecular dynamics simulations, it is further studied how the inhomogeneity of the particle size distribution and the inelasticity of collisions influence the velocity distribution and distribution of interparticle spacing in the steady-state. Also, the quantitative information of the non-Gaussian velocity distribution and that of clustering are given, such as kurtosis of the non-Gaussian velocity distribution, behavior of the tail of the distribution and degree of clustering.

2 Model

We consider a polydisperse granular mixture with the fractal characteristic of the particle size distribution, in which the size distribution of N particles is continuous ($r_{\min} \le r \le r_{\max}$, $r_{\min}$ is the minimal size of particles, and $r_{\max}$ is the maximal size of particles). Fortunately, experimental results showed that the particle size distributions of many granular materials exhibit the fractal characteristic.[14,15] Moreover, there is a fractal dimension D as a measurement of the inhomogeneity in the particle size distribution, and higher D implies greater dispersion of the finer particles, which leads to more pronounced inhomogeneity of the system.[15]

So, it is reasonable that we consider the polydisperse granular mixture with the fractal characteristic of the particle size distribution, and use the fractal dimension D to describe the inhomogeneity of the particle size distribution. When $n_0/N \ll 1$, where n_0 is the number of particles with the maximum size $r_{\max}$, the particle size distribution of the granular system satisfies the size-frequency character by fractal theory,[10]

$$Y_{n_r}(r) = 1 - N^{-1} n_0 \Big(\frac{r}{r_{\max}}\Big)^{-D} , \tag{1}$$

where Y_{n_r} is the ratio of n_r to N, n_r is the number of particles whose size is smaller than r, N is the total number of particles, and D is the fractal dimension of particle size distribution, $2 < D < 3$.

For simplicity, we assume that the surface of particles is smooth and the material of every particle is identical, but the size distribution of particles is different. From Eq. (1), the radius and the mass of any particle in the mixture can be respectively expressed as

$$r = r_{\max} \Big[\frac{N}{n_0}(1 - Y_{n_r})\Big]^{-1/D} , \tag{2}$$

$$m = m_{\max} \Big[\frac{N}{n_0}(1 - Y_{n_r})\Big]^{-3/D} . \tag{3}$$

If the values of N, $m_{\max}$, $r_{\max}$, n_0, and D are given, according to Eqs. (2) and (3), we can randomly evaluate the radius and the mass of every particle in the non-uniform granular system.

To study the non-uniform granular gases, we present the following model. First, an ensemble of N polydisperse inelastic hard sphere particles is constrained to move along a circle of length L, and subject to a volumetric Gaussian white noise forcing, which describes the energy exchange of particles with an external heat bath; Secondly, the radius and the mass distribution of particles satisfy Eqs. (2) and (3), respectively; Thirdly, the initial positions of particles are assigned corresponding to an initial uniform spatial density, the initial velocities of particles are generated using a Gaussian random generator, and the particles are subject to inelastic mutual collisions. Thus, the particles obtain the kinetic energy from the white noise forcing, display Brownian motion between collisions, and dissipate the kinetic energy through inelastic collisions and dump. The statistically stationary state of the system is the result of the equilibrium of the dissipating energy and the injected energy.

Consequently, the movement of each particle obeys the Kramers' equations between two consecutive collisions:

$$m_i \frac{d\nu_i}{\mathrm{d}t} = -m_i \gamma \nu_i + \xi_i(t) , \tag{4}$$

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \nu_i(t) . \tag{5}$$

where $1 \le i \le N$, m_i is the mass of i-th particle, $x_i(t)$ is the centroid position coordinates of i-th particle, γ is the viscous friction coefficient, and $\xi_i(t)$ is a Gaussian white noise. The stochastic forcing term satisfies $\langle \xi_i(t) \rangle = 0$ and $\langle \xi_i(t)\xi_j(s) \rangle = 2\gamma m_i T_b \delta_{ij} \delta(t - s)$, where T_b is the "heat-bath" temperature, δ_{ij} is the Kronecker delta, and $\delta(t)$ is the delta function. Via the random force, the opportunity of every particle obtaining energy will be equipotent.

The inelastic collisions, in contrast, are considered at the kinetic level. Because of the hard-core character of the repulsive forces among particles, we reduce the interactions to single binary, instantaneous, and centric impact events occurring whenever two consecutive particles reach a distance $d_{ij}(t) = x_i(t) - x_j(t)$ equal to the center-to-center length $(r_i + r_j)$ at contact of nearest-neighbor particles. When two inelastic hard particles collide, their postcollisional velocities (primed symbols) are related to precollisional velocities (unprimed symbols) through the following collision rules:

$$\nu_i' = \nu_i - \frac{m_j}{m_i + m_j}[(1+e)(\nu_i - \nu_j)]\,, \tag{6}$$

$$\nu_j' = \nu_j + \frac{m_i}{m_i + m_j}[(1+e)(\nu_i - \nu_j)]\,, \tag{7}$$

where e is the coefficient of restitution, $(\nu_i' - \nu_j') = -e(\nu_i - \nu_j)$. It has to be noted that, because of the "hard" nature of collisions, the particles never deform (this effect is taken into account in the restitution coefficient picture).

When collisions are considered, a characteristic time emerges, that is the average collision time τ_c between two successive encounters. The average collision time τ_c is estimated by assuming a mean free path $\lambda = (L - \sum_{i=1}^{N} 2r_i)/N$, where $(L - \sum_{i=1}^{N} 2r_i)$ is the free volume. As a function of average free path and typical velocity, τ_c can be expressed by

$$\tau_c = \frac{\lambda}{\sqrt{\langle \nu^2 \rangle}} = \frac{L - \sum_{i=1}^{N} 2r_i}{N\sqrt{\langle \nu^2 \rangle}} \tag{8}$$

It is usually assumed that $\langle \nu^2 \rangle$ reaches a stationary value with statistical fluctuations (of order $\sim 1/N$), as it is observed in simulations.

Starting from any initial configuration, the system with dissipation $(0 < e < 1)$ reaches a steady state with certain properties after a long transient, as the result of the balance between the energy dissipation due to inelastic collisions and friction with the surroundings, and the energy injection due to the external thermal bath.

3 Simulations and Results

First, in order to demonstrate that the polydisperse granular mixture has the fractal characteristic of the particle size distribution in our simulations, we randomly sample the radii distribution of the particles. Figure 1 gives the granular radii randomly chosen by Eq. (2) under the given parameters $N = 200$, $r_{\max} = 0.5$, $n_0 = 1$, and $D = 2.5$ respectively for the actual granular system. From Fig. 1 it is seen that the number of larger granular is much less than that of smaller granular, this is qualitatively consistent with fractal theory. It is also found from Fig. 1 that the minimum granular radius is about 10^{-3}, which implies that $r_{\max}/r_{\min} > 10^2$ ($r_{\max}$ and $r_{\min}$ are the maximal radius and the minimal radius of particles, respectively) in our simulations satisfies the fractal criterion introduced by Yu *et al.*[16] According to the analysis above, the system has the fractal characteristic of the particle size distribution. Therefore, our simulations are valid.

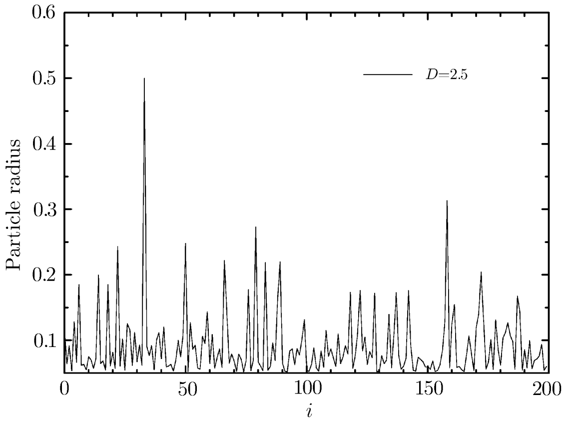

Fig. 1 The granular radii randomly chosen by Eq. (2) using the given parameters $N = 200$, $r_{\max} = 0.5$, $n_0 = 1$, and $D = 2.5$, respectively.

Then, we simulate the hard particles colliding and Brownian motion between collisions. In all simulations, we use $N = 5000$, $L = 5000$, $\rho = N/L = 1$, $m_{\max} = 20$, $r_{\max} = 0.5$, $n_0 = 1$, $T_b = 1$, and $\gamma = 0.02$, and perform the simulations by the molecular dynamics method. The simulations have been performed using a fixed time step Δt integration of Eqs. (4) and (5) where $\Delta t \ll \tau_c$, and an event driven check of collisions during every time step. The motion between two consecutive collisions is governed by the dynamics Eqs. (4) and (5). Thus, we determine the instant when the first collision among the N particles occurs and the change of its velocities and positions according to these equations of motion. The effect of the collision is taken into account by updating the velocities according to Eqs. (6) and (7). After a long evolution time, the system of randomly given choice of e and D reaches a stationary state. At last we discuss the steady-state dynamic properties of the system.

3.1 *Velocity Distribution*

Figures 2 and 3 show the distributions of velocities, obtained by sampling the velocities of all particles after a very long evolution time, when the system has reached a statistically stationary state. There are two different dynamic regimes (an elastic case with $e = 1.0$ and an inelastic case with $0 < e < 1$). In the elastic regime, the velocity distributions for different fractal dimension D which are limned in rotundities, are well fitted by a Gaussian. However, in the inelastic case, as a general result, the velocity distributions which are described by circles, cease to be Gaussian, and display strong deviations both at low and high velocities. The quantitative information of the deviations is given as follows.

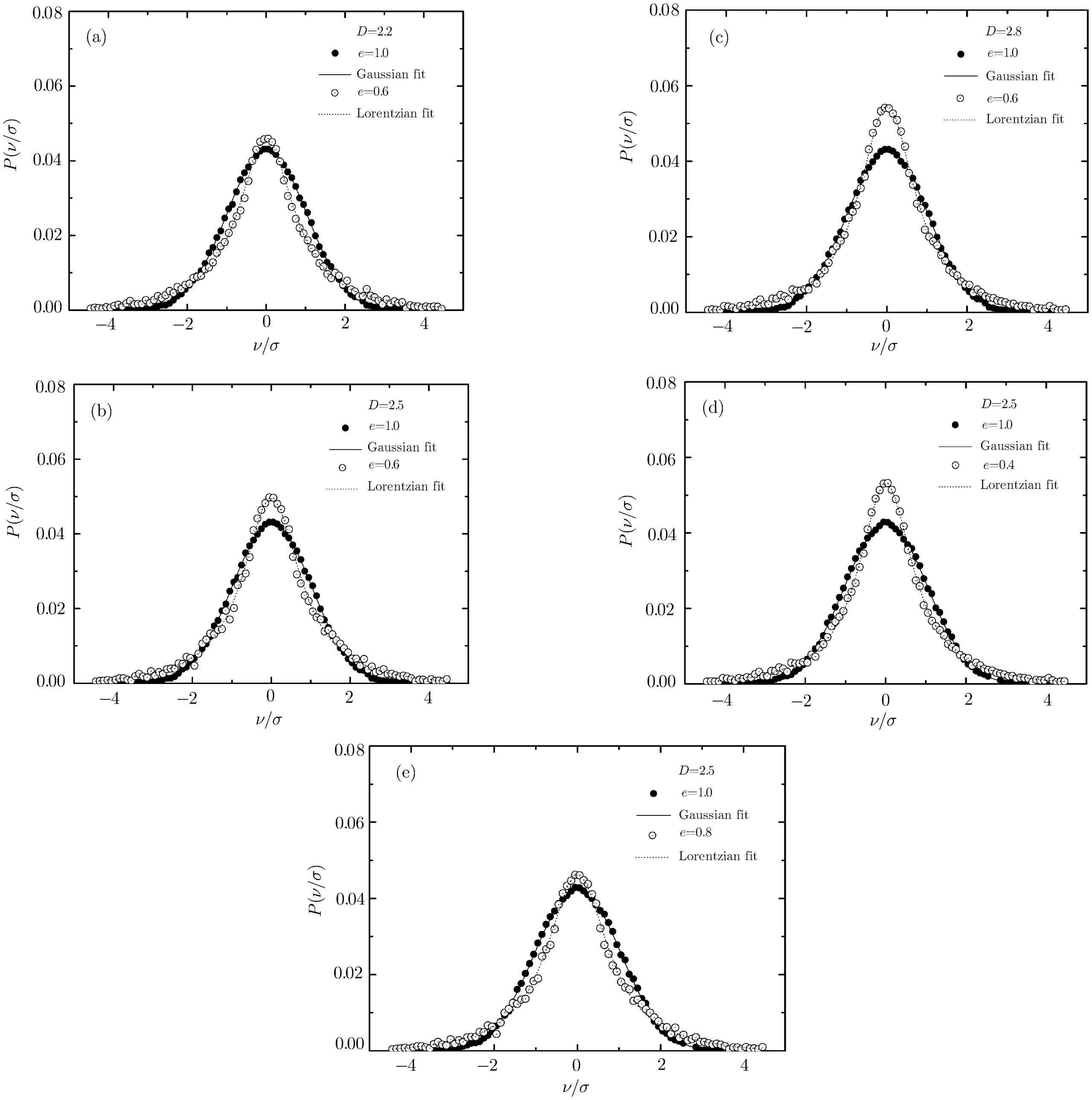

Fig. 2 The rescaled velocity distribution $P(\nu/\sigma)$ vs. ν/σ for two different regimes (an elastic case with $e = 1.0$ and an inelastic case with $0 < e < 1$) on a linear-linear scale. In both cases, rotundities are simulation data in the elasticity case, and circles are simulation data in the inelasticity case. The solid-line represents the Gaussian fit, while the dot-line represents the Lorentzian fit.

In Fig. 2, non-Gaussian velocity distributions display low-velocity and high-velocity overpopulated regions. By plotting the distributions on a linear scale, we display the more statistically significant deviations from the Gaussian velocity distribution. Apparently, the kurtosis of the velocity distribution functions (VDFs) increases higher as the fractal dimension D increases at the same restitution coefficient $e(0 < e < 1)$. This phenomenon is consistent with our previous simulation results.[11−13] Also, the kurtosis distinctly increases higher as the restitution coefficient e decreases at the same fractal dimension D, and it is similar to Ref. [4]. For further discussion, we quantitatively calculate the kurtosis of the VDFs. The kurtosis is obtained by the following equation:[5]

$$\beta = \frac{\langle \nu^4 \rangle}{\langle \nu^2 \rangle^2} \,. \tag{9}$$

If the velocity distribution is a Gaussian, $\beta = 3$, while if it is non-Gaussian, β exceeds 3. We also find that the calculated values of the kurtosis changing with the fractal dimension D or the restitution coefficient e have the same evolution as the above observation.

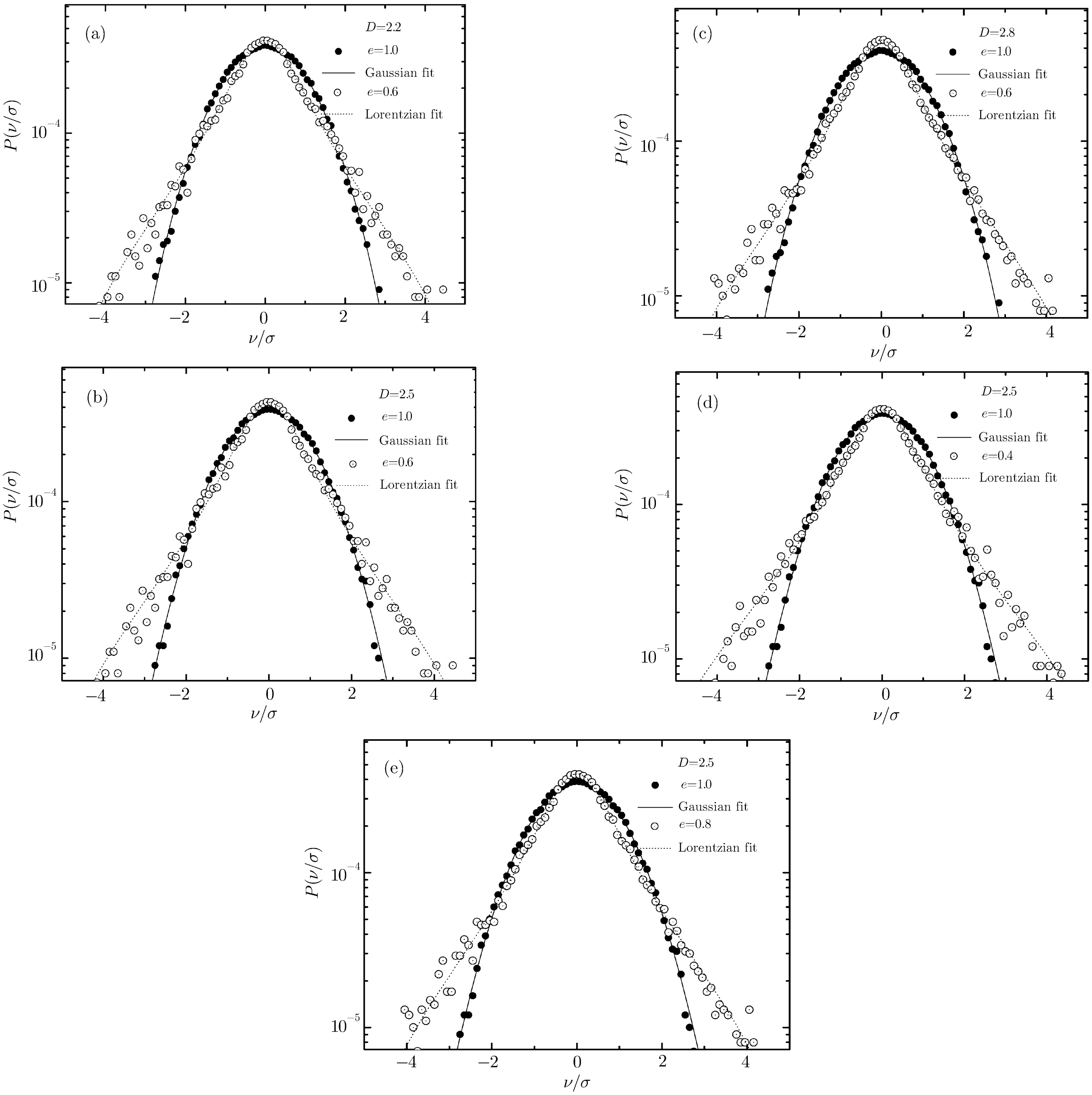

Fig. 3 The rescaled velocity distribution $P(\nu/\sigma)$ vs. ν/σ for two different regimes (an elastic case with $e = 1.0$ and an inelastic case with $0 < e < 1$) on a log-linear scale. In both case, rotundities are simulation data in the elasticity case, and circles are simulation data in the inelasticity case. The solid-line represents the Gaussian fit, while the dot-line represents the Lorentzian fit.

Also, we normally display the distributions of velocities in a log-linear fashion to accentuate the tails of the VDF; however, this suppresses the deviations at low velocities. From Fig. 3, we observe that non-Gaussian velocity distributions exhibit fatter tails. As the restitution coefficient e decreases, the tails become more overpopulated at the same fractal dimension D, and this is also similar to Refs. [4] and [6]. But, when the restitution coefficient e $(0 < e < 1)$ is fixed, the deviations of the fat tails change unobviously with the increasing fractal dimension D.

In particular, the deviations of the stationary velocity distribution function from the Gaussian can be quantitatively investigated through the Sonine expansion. The first nonvanishing correction a_2 to the Gaussian can be computed neglecting non-linear contributions of $O(a_2^2)$; in one-dimensional case, it has the expression[6]

$$a_2 = 4\Big(\frac{\langle \nu^4 \rangle}{3\langle \nu^2 \rangle^2} - 1\Big)\,. \tag{10}$$

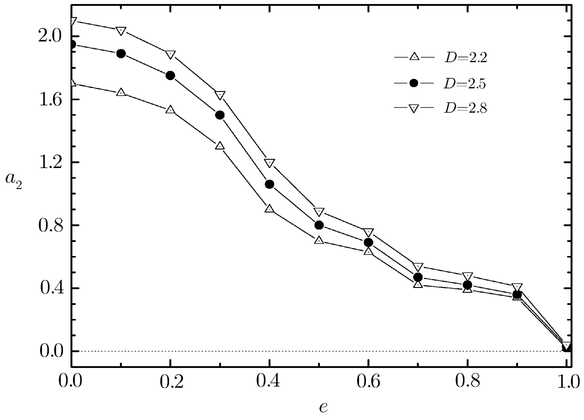

Fig. 4 The fourth cumulant a_2 vs. the restitution coefficient e for different fractal dimension D.

Figure 4 illustrates the variation of the fourth cumulant a_2 (the first correction to the Gaussian) as a function of the inelasticity for three different values of the fractal dimension D. We find that the coefficient a_2 is a monotonic decreasing function of the restitution coefficient e at the same fractal dimension D; on the contrary, when the restitution coefficient e $(0 < e < 1)$ is fixed, the coefficient a_2 increases with the increasing value of the fractal dimension D, and the smaller the restitution coefficient e is, the larger the magnitude of the coefficient a_2 is. In the limit $e \to 1$, a_2 does not vanish, and the fractal dimension D has a little effect on a_2. Therefore, we find a peculiarity of one-dimensional case: a_2 does not vanish as $e \to 1$. It is a hint that the quasi-elastic limit is singular in one-dimensional case, and this phenomenon is similar to Ref. [6].

3.2 *Distribution of Interparticle Spacing*

The probability distribution, $p(\delta x)$, of distances between nearest-neighbor particles $\delta x = x_i - x_j$, shown in Fig. 5, provides information about the spatial arrangement of the system. In the elastic case, one easily finds

$$P(\delta x) = \frac{1}{\lambda}\exp\Big\{-\frac{1}{\lambda}[\delta x - (r_i + r_j)]\Big\}\,, \tag{11}$$

for $\delta x \geq (r_i + r_j)$ and 0 for $\delta x < (r_i + r_j)$ with $\lambda = (L - \sum_{i=1}^{N} 2r_i)/N$. The presence of inelasticity modifies such a simple exponential law in the way shown in Fig. 5. In this case, the probability of finding two particles at small separation increases together with that of finding large voids. Such a picture is consistent with the idea of the spatial clustering phenomenon: Two particles, after the inelastic collision, have a smaller relative velocity and therefore reach smaller distances, eventually producing dense clusters and leaving larger empty regions with respect to elastic case.

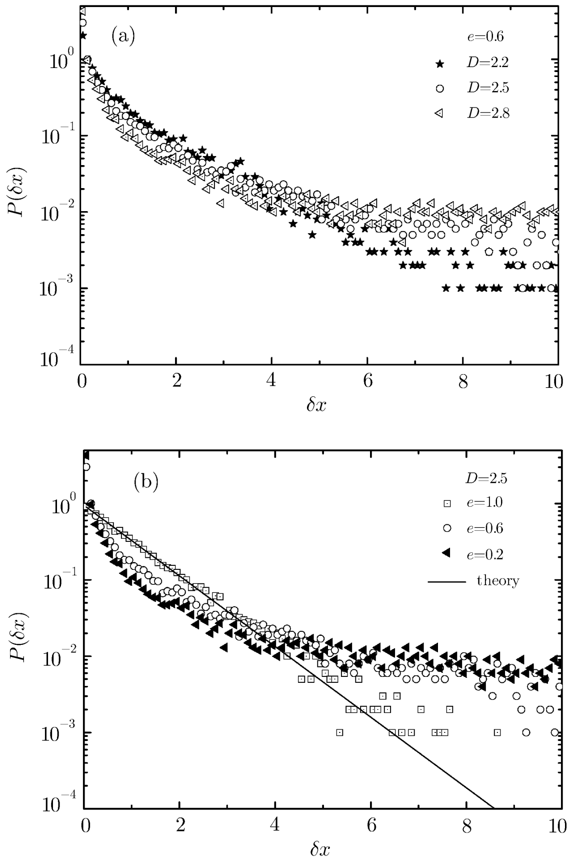

Fig. 5 Distributions of distances between nearest-neighbor particles $\delta x = x_i - x_j$, for elastic and inelastic non-uniform systems, in (a) $e = 0.6$, $D = 2.2, 2.5, 2.8$ respectively, and in (b) $D = 2.5$, $e = 1.0, 0.6, 0.2$ respectively. The solid line indicates the exponential expected in the elastic case (see the text).

It is seen from Fig. 5 that, as the fractal dimension D increases with respect to the same restitution coefficient e $(0 < e < 1)$, the probability of finding two particles at small separation increases together with that of finding large voids. This indicates that when the value of the fractal dimension D augments in the inelasticity case, the system becomes more and more clusterized. From Fig. 5 it can be also found that, at the same fractal dimension D, when the restitution coefficient e decreases, the probability of finding two particles at small separation also increases together with that of finding large voids. Also, this suggests that the spatial clusterization becomes more and more pronounced with decreasing value of the restitution coefficient e. Only when $e = 1$, is the probability distribution $P(\delta x)$ of theoretical predictions found to be in excellent agreement with those of the numerical simulations. This shows that the spatial density is nearly homogeneous.

The clusterization may quantitatively be characterized by means of an entropy defined as[3]

$$h_{_M} = -\sum_{j=1}^{M} \frac{m_j}{N} \ln \frac{m_j}{N}\,, \tag{12}$$

where the ring of length L is divided into M equal boxes (i.e., segments) and m_j is the number of particles in the $j_{\rm th}$ box. The entropy $h_{_M}$ attains its maximum value $h_{_M} = \ln m$ when $m_j = N/M$ for every box j. $h_{_M}$ decreases as the density distribution becomes more and more clusterized.

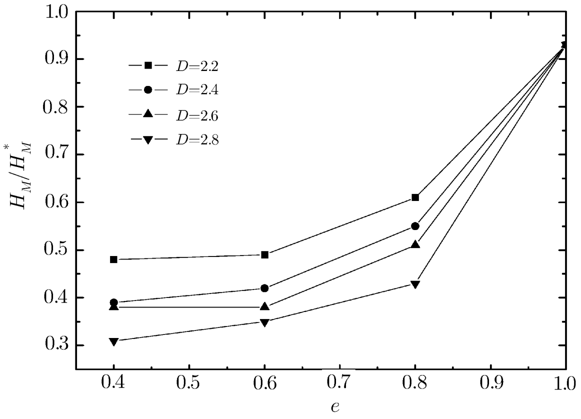

Fig. 6 H_M/H_M^* vs. the restitution coefficient e for different fractal dimension D, with $N = 500$, $M = 500$.

In Fig. 6 many measurements of H_M/H_M^* are presented, where $H_M = \exp(\langle h_{_M}\rangle)$, $H_M^* = \exp(\langle h_{_M}^*\rangle)$, $h_{_M}^*$ is the effective entropy for homogeneous regime ($e = 1.0$) and $\langle\rangle$ is the time average. The quantity H_M/H_M^* basically gives an indication of the fraction of non-empty boxes in a typical snapshot. The figure shows that H_M/H_M^* decreases as the fractal dimension D increases with respect to the same restitution coefficient e. Namely, the system becomes more and more clusterized. When $e = 1$, all the curves reach one point and H_M/H_M^* attains its maximum value. The spatial density is homogeneous and there is not energy dissipation as the collisions between particles are elastic. Therefore, the energy dissipation induces clusterization.

4 Analysis

As Ref. [15] Zhang discussed the relationship between the granular size dispersion of non-uniform granular system and the fractal dimension D of the size distribution according to the experimental granulometric analysis. The experimental data show that both in a simplex non-uniform granular system and in a mixed granular system, the higher D implies greater dispersion of the finer particles, which leads to more inhomogeneity in the particle size distribution due to the formation of relatively fine particles. That is to say, the fractal dimension D can be considered as a measurement of the inhomogeneity of the size distribution. Moreover, a larger fractal dimension D implies a more inhomogeneous granular system.

It is believed that the energy dissipation due to the inelastic collisions in granular gas system causes the instantaneous energy balance invalid, which leads to the non-Gaussian velocity distribution and spatial clustering. From Eqs. (6) and (7), the energy dissipation due to the inelastic collisions during one collision is

$$\begin{aligned}\Delta E &= \frac{(1-e^2)(v_i-v_j)^2}{2}\frac{m_i m_j}{m_i+m_j}\\ &= \frac{(1-e^2)(v_i-v_j)^2}{2}\cdot\frac{m_i(m_i+\Delta m_{ij})}{2m_i+\Delta m_{ij}}\,,\end{aligned} \tag{13}$$

where $\Delta m_{ij} = m_j - m_i$. Obviously, in the inelasticity case, when the fractal dimension D does not change, the smaller the value of the restitution coefficient e is, the more dissipation of energy is caused by the collisions among particles. Therefore, with the decreasing value of the restitution coefficient e, the movement of particles deviates from the Brownian motion more distinctly, then the velocity distribution deviates more obviously from the Gaussian and the spatial clusterization is more pronounced.

On the other hand, if the restitution coefficient e ($0 < e < 1$) remains the same, the greater the difference of the mass between the two colliding particles is, the more the dissipation of energy ΔE is. Customarily, the larger value of D represents that there are more numbers of finer particles in the system and the inhomogeneity of the particle size distribution is more prominent, which makes the difference of the mass between any two colliding particles greater. So the larger the value of D is, the more the energy dissipation in the system is. Therefore, in the inelasticity case, with the increasing value of the fractal dimension D, the velocity distribution deviates more obviously from the Gaussian one and the system becomes more and more clusterized.

5 Conclusions

In summary, we present a one-dimensional dynamic model for the non-uniform inelastic driven granular system, whose granularity distribution has the fractal characteristic. The fractal dimension D of granularity distribution is considered to be a measurement of the inhomogeneity of the particle size distribution. The higher the D is, the more inhomogeneous the granularity distribution will be.

By molecular dynamics simulations, we further study the influences of the inhomogeneity and the inelasticity on the velocity distribution and distribution of interparticle spacing. When the system reaches the stationary state, some novel results are found as follows:

(i) When the restitution coefficient e ($0 < e < 1$) is fixed, the deviation from the Gaussian velocity distribution is more obvious with the increasing fractal dimension D, such as the higher kurtosis of the VDFs and the larger fourth cumulant a_2, but the deviations of the fat tails change unobviously. In contrast, as the restitution coefficient e decreases, the deviation also becomes more pronounced at the same fractal dimension D, such as the higher kurtosis, the fatter tails and the larger fourth cumulant a_2. However, in the limit $e \rightarrow 1$, a_2 does not vanish, and the fractal dimension D has a little effect on a_2. This indicates that the quasi-elastic limit is singular in one-dimensional case.

(ii) When the value of the fractal dimension D augments, the system becomes more and more clusterized in the inelasticity case. Also, the spatial clusterization becomes more and more pronounced with decreasing value of the restitution coefficient e at the same fractal dimension D. Only when $e = 1$, is the spatial density nearly homogeneous. Also, the clusterization is quantitatively characterized by means of an entropy h_M.

All the results indicate that the steady-state dynamic properties of the inelastic driven non-uniform granular system are prominently influenced by the inhomogeneity and the inelasticity.

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