PHYSICAL REVIEW E **67**, 010301(R) (2003)

Velocity distribution of inelastic granular gas in a homogeneous cooling state

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(Received 26 August 2002; published 15 January 2003)

The velocity distribution of inelastic granular gas is examined numerically on a two-dimensional hard disk system in nearly elastic regime using molecular dynamical simulations. The system is prepared initially in the equilibrium state with the Maxwell-Boltzmann distribution, then after several inelastic collisions per particle, the system falls in the state that the Boltzmann's equation predicts with the stationary form of velocity distribution. It turns out, however, that due to the velocity correlation the form of the distribution function does not stay time independent, but gradually returns to the Maxwellian immediately after the initial transient till the clustering instability sets in. It shows that, even in the homogeneous cooling state (Haff state), where the energy decays exponentially as a function of collision number, the velocity correlation in the inelastic system invalidates the assumption of molecular chaos and the prediction of the Boltzmann's equation fails.

DOI: 10.1103/PhysRevE.67.010301 PACS number(s): 45.70.−n, 45.50.−j, 51.10.+y

Free cooling of granular gas under no gravity has been attracting much interest as a subject of statistical mechanics, since people realized that the inelastic collisions between particles makes the system behave very different from the elastic system—the subject of the conventional statistical mechanics.

Besides the cooling, or loosing its kinetic energy due to the inelasticity, it has been well recognized by now that, as long as the system is large enough, the system shows series of instabilities, however, small the inelasticity may be. If the system is prepared in a highly agitated state, initially it cools down uniformly as

$$T=\frac{T_0}{(1+t/t_0)^2}, \tag{1}$$

which is called as the Haff state [1]. After a while, the vortex structure develops in the velocity field (the shearing instability) [2], then the uniformity of the particle density is broken-(the clustering instability) [3].

After the clustering instability, the clusters of particles collide with each other, merge, and split in a complex way [4]; the system eventually develops the high density region, where the inelastic collapse [5,6] is likely to happen if one consider the ideal hard sphere system with a constant restitution coefficient.

Regarding the velocity distribution, the Maxwell-Boltzmann distribution is an equilibrium velocity distribution for the elastic system, and the relaxation to the distribution is known to be very fast, i.e., within a several collisions per particles when the system is spatially uniform. In the case of the inelastic system, obviously any velocity distribution cannot be stationary because the system loses kinetic energy at every collision, but it is plausible that the form of distribution stays stationary, after a short transient if the velocity is scaled by the average speed $v_0(t)$:

$$f(\boldsymbol{v},t)=\frac{1}{v_0(t)^d}\hat{f}\left(\frac{\boldsymbol{v}}{v_0(t)}\right). \tag{2}$$

In fact, kinetic theories based on the Boltzmann's equation predicts that there is a stationary scaled solution for the velocity distribution that is different from the Gaussian [7,8], and after a several collisions per particle, the velocity distribution for the inelastic system falls into it [9,10].

In this report, I present results of large scale two-dimensional molecular dynamics (MD) simulations and shows that the form of the velocity distribution does not stay stationary in the inelastic gas, but after a short initial transient the distribution gradually getting back to the Gaussian till the clustering instability sets in. This gradual change starts at very early stage where the inhomogeneity in the system is hardly visible.

The system we examine is the two-dimensional system of hard disks that undergoes inelastic collisions with a constant normal restitution r. The rotational motion is ignored. If $\boldsymbol{v}_i$ and $\boldsymbol{v}_i'$ denote the velocity of the ith disk before and after the collision with the jth particle, respectively, then the collision rule is given by

$$\boldsymbol{v}_i'=\boldsymbol{v}_i-\frac{1+r}{2}[\boldsymbol{n}\cdot(\boldsymbol{v}_i-\boldsymbol{v}_j)]\boldsymbol{n},$$

$$\boldsymbol{v}_j'=\boldsymbol{v}_j+\frac{1+r}{2}[\boldsymbol{n}\cdot(\boldsymbol{v}_i-\boldsymbol{v}_j)]\boldsymbol{n},$$

where $\boldsymbol{n}$ is the unit vector parallel to the relative position of the colliding particles at the time of contact.

The average speed $v_0(t)$ for d-dimensional system, defined by

$$\frac{d}{2}v_0(t)^2=\int d\boldsymbol{v}\, f(\boldsymbol{v},t)\boldsymbol{v}^2, \tag{3}$$

decreases as the system looses energy; with this speed we scale the velocity distribution through Eq. (2). In order to see the time dependence of the scaled velocity distribution $\hat{f}$, it is convenient to expand it using the Sonine polynomial as

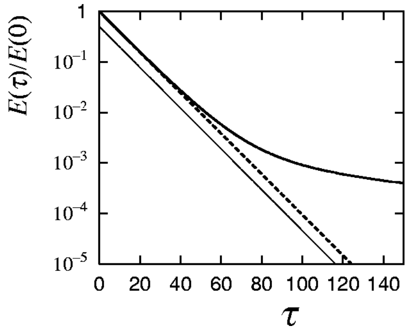

FIG. 1. Energy decay as a function of τ for $r=0.9$ and $n=0.25$ ($\phi=0.196$). The solid line denotes the result for the system with the ordinary inelastic dynamics and the dashed line for the system with the velocity shuffle (see the text). The exponential decay (5) with $2\gamma=0.093$ is also plotted by the thin solid line with an extra factor to avoid complete overlapping with the dashed line.

$$\hat{f}(\boldsymbol{c},t)=\frac{1}{\sqrt{\pi}^d}e^{-c^2}\sum_{\ell=0}^{\infty}a_\ell(t)S_\ell(c^2), \tag{4}$$

when the distribution is not very different from the Gaussian; the ℓth order Sonine polynomial is the ℓth order polynomial orthogonalized with the d-dimensional Gaussian weight function:

$$S_0(x)=1, \quad S_1(x)=-x+\frac{1}{2}d,$$

$$S_2(x)=\frac{1}{2}x^2-\frac{1}{2}(d+2)x+\frac{1}{8}d(d+2), \quad \text{etc.}$$

Due to the normalization and scaling of $\hat{f}$, we have $a_0=1$ and $a_1=0$, thus any deviation from the Gaussian distribution is seen in the nonzero values of a_ℓ for $\ell\geqslant 2$.

Simulations were performed by the event-driven method using the fast algorithm developed by Isobe [11]. Most of the simulations were done with the particle number $N=250\,000$, and the number density $n=0.25$; we have taken the disk diameter as the length unit, then the area fraction ϕ is given by $\phi\equiv\pi n/4=0.196$. I employed the periodic boundary condition and the initial state in the equilibrium state that is prepared by running the system for long enough with the restitution constant $r=1$. I focus on the nearly elastic regime where the system stays uniform for a substantial length of time and the distribution does not deviate very much from the Gaussian before the clustering instability occurs.

In the following, the time is measured by the collision time τ, which is defined as the number of collisions each particle experiences, i.e., $\tau\equiv 2N_{\rm coll}/N$ with $N_{\rm coll}$ being the total number of collisions (the factor of 2 comes from the fact that the collisions are binary).

Figure 1 shows the energy decay as a function of time τ for $r=0.9$ and $n=0.25$ in the semilogarithmic scale. In terms of τ, the decay in the Haff state given by Eq. (1) is expressed as

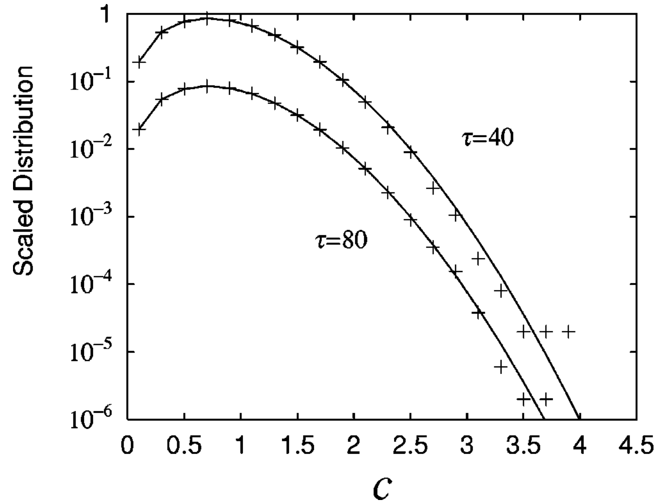

FIG. 2. The scaled speed distributions for $\tau=40$ and 80 with $r=0.9$ and $n=0.25$ ($\phi=0.196$). The plot for $\tau=80$ is shifted by the factor of 10^{-1}. The Maxwell-Boltzmann distributions are indicated by the solid lines for comparison.

$$E(\tau)=E(0)\exp[-2\gamma\tau], \tag{5}$$

where 2γ is a decay rate. The thin solid line in Fig. 1 shows the exponential function with $2\gamma=0.093$ (the line is shifted vertically to avoid complete overlapping). The initial τ dependence fits to the exponential decay very well with the decay rate very close to that obtained in the case of random collision: $2\gamma_0\equiv(1-r^2)/d=0.095$ for $r=0.9$. It eventually deviates from the exponential around $\tau\sim 70$, when the clustering instability sets in.

The speed distribution for this system is plotted in Fig. 2 for $\tau=40$ and 80. For both cases, the distribution is very close to the Gaussian and the deviation from it is hardly seen.

The deviation, however, is clearly seen in $a_2(\tau)$ plotted in Fig. 3, where the initial deviation from the Gaussian is shown for various values of restitution constant r. From this figure, it might seem that the scaled distribution becomes stationary after a several collisions per particle as is expected from the kinetic theories [9,10]. These ''stationary'' values of

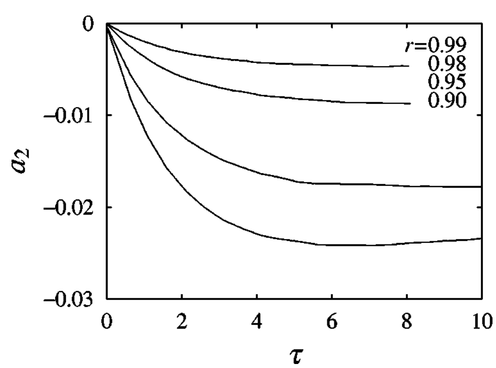

FIG. 3. The initial time dependence of a_2 for $r=0.99$ (top), 0.98, 0.95, and 0.90 (bottom) with $n=0.25$ ($\phi=0.196$). The data represent averages over 250 realizations.

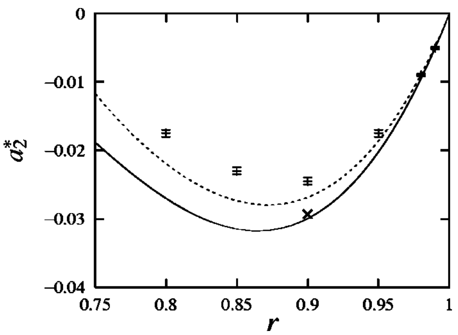

FIG. 4. The minimum values for a_2 vs the restitution constant r for $n=0.25$ ($\phi=0.196$). The lines show the estimate of a_2 by the Boltzmann's equation in the lowest approximation by Ref. [8] (the dashed line) and in the sixth order approximation by Ref. [10] (the solid line). (The latter is read off numerically from the original paper.) The cross at $r=0.9$ indicates the stationary value of a_2 for the velocity shuffling dynamics (see text).

a_2 agree very well with the results of the kinetic theory for the nearly elastic region $r \gtrsim 0.95$ in the case of $n=0.25$ (Fig. 4).

This form of distribution, however, is not really stationary as it may look in the initial stage data of Fig. 3. The τ dependence of Sonine coefficients over longer time scale is shown in Fig. 5 for $r=0.9$, 0.95, and 0.98 for $n=0.25$. In this time scale, the plateau is hardly seen and absolute values of all the coefficient show gradual decrease towards zero till the time when the clustering instability sets in; after that time the distribution deviates from the Gaussian drastically as has been reported [10].

The Sonine coefficient $a_2(\tau)$ for various r is plotted in Fig. 6 where the time is scaled by the clustering time τ^*

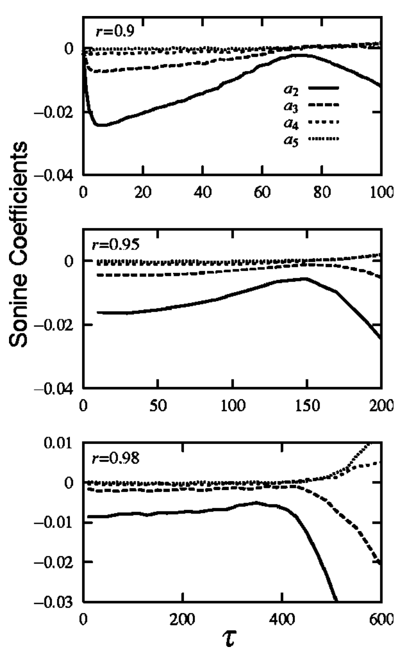

FIG. 5. The Sonine coefficients a_ℓ ($2 \geqslant \ell \geqslant 5$) for $r=0.9$ (top), 0.95 (middle), and 0.98 (bottom) as functions of τ for $n=0.25$ ($\phi=0.196$). The data represent averages over 100 realizations.

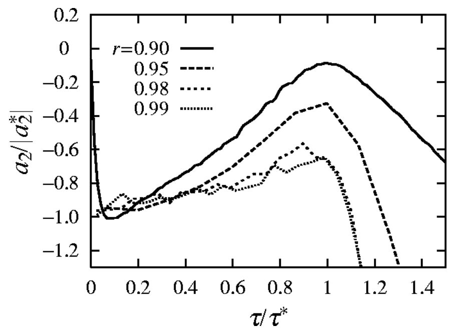

FIG. 6. The scaled Sonine coefficient $a_2/|a_2^*|$ vs the scaled time τ/τ^* for $r=0.90$, 0.95, 0.98, and 0.99 with $n=0.25$ ($\phi=0.196$). The data represent averages over 100 realizations.

when the clustering instability sets in and a_2 is scaled by its maximum absolute value $|a_2^*|$ for each r. The closer the value of r is to 1, the smaller the slope in the τ dependence becomes, but for all cases, the gradual return to the Gaussian starts almost immediately after the initial transient period finishes. It starts actually far before any instability becomes evident.

This behavior obviously contradicts to the results of the kinetic theories based on the Boltzmann's equation [9,10]; the theories predict that the distribution shows the stationary form after the short initial transient. The stationary form should last till the Boltzmann's equation becomes invalid due to correlations developed in the system. The fact that the distribution function starts to deviate from the stationary form at a quite early stage suggests that the correlation due to inelasticity becomes important much earlier than it is generally expected [12].

The correlation that is responsible for the behavior of the velocity distribution is the velocity correlation. This can be seen by examining the behavior of the system where the particle velocity is artificially randomized by the operation that the velocity of each particle is shuffled by exchanging them between pairs chosen randomly. By doing this, I destroy the spatial correlation of velocity while preserving the velocity distribution. The dashed line in Fig. 1 shows the energy decay with the velocity shuffling, and it indicates that the clustering is prevented by the velocity shuffle. From Fig. 7, we can see clearly that this system shows the stationary form of the velocity distribution whose Sonine coefficients are close to those predicted by the theories.

Some comparison with previous calculations is in order. Figures 3 and 4 correspond to Figs. 8 and 10 in Ref. [10], where the agreement with the theory looks much better than the present ones. The difference for these two sets of figures is in the particle density; $n=0.25$ ($\phi=0.196$) in the present work, but $n=0.0637$ ($\phi=0.05$) in Ref. [10]. The density dependence is examined in Fig. 7. It can be actually seen that the correspondence between the plot for $n=0.0625$ in Fig. 7 and that in Fig. 8 of Ref. [10] is quite good. The initial transient does not show the density dependence, but the gradual return to the Gaussian after it becomes slower for the dilute systems. Since the clustering time also becomes larger for the dilute system, it is not obvious how the system behavior converges to the uncorrelated one in the $n \to 0$ limit.

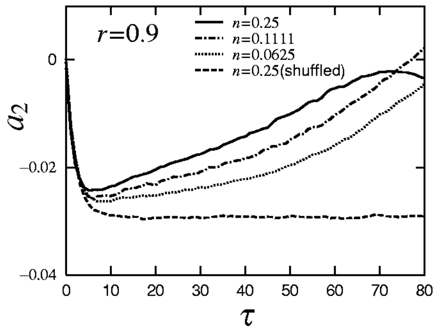

FIG. 7. The Sonine coefficient a_2 for $r=0.9$ as a function of τ for the ordinary dynamics (solid line) and the velocity shuffled dynamics (dashed line) for $n=0.25$ ($\phi=0.196$). a_2 for $n=0.1111$ ($\phi=0.0872$) and $n=0.0625$ ($\phi=0.049$) where original dynamics are also plotted by the dash-dotted line and the dotted line, respectively. The data represent averages over 100 realizations.

Looking at the data we have at the moment, the general behavior that $|a_2|$ decreases toward zero after the initial deviation is clear for all the density and they are all apparently different from the case with the velocity shuffling [13].

In one-dimensional systems, it has been reported that the distribution recovers the Gaussian form in the late stage of the clustering state after the velocity distribution shows a two peak structure [14,15]. This behavior has been analyzed in terms of the Burgers equation [14]. The difference, however, between this and that investigated in the present work is the stage that they occur; the present one starts far before the clustering, thus it is not obvious if the picture based on the Burgers equation is applicable to our case.

The kinetic theories have succeeded in explaining many aspects of granular gas, but the Boltzmann-Enskog equation, on which most of the theories are based, ignores the particle correlations except for the pair correlation factor of the position. This approximation is quite good in the equilibrium system thanks to the absence of the velocity correlation. In the inelastic systems, however, the system develops the velocity correlation, and the assumption of molecular chaos fails even at very early stage, where the system is generally regarded to be still in the homogeneous cooling state (HCS). This invalidates the prediction based on the Boltzmann's equation that the functional form of the velocity distribution of the inelastic system in HCS becomes stationary.

In summary, using large scale MD simulations, I have demonstrated that in the inelastic system the velocity distribution does not stay in a stationary form, contrary to the expectation by the kinetic theories based on the Boltzmann's equation. This is due to the velocity correlation developed through the inelastic collisions, and this effect manifests itself in the velocity distribution from the very early stage where any instabilities caused by the inelasticity are still hardly visible.

The author is grateful to N. Mitarai, U.M.B. Marconi, A. Puglisi, and T. Pöschel for stimulating discussions.

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