Long-Time Tails and Cage Effect in Driven Granular Fluids

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We study the velocity autocorrelation function of a driven granular fluid in the stationary state in three dimensions. As the critical volume fraction of the glass transition in the corresponding elastic system is approached, we observe pronounced cage effects in the velocity autocorrelation function as well as a strong decrease of the diffusion constant, depending on the inelasticity. At moderate densities the velocity autocorrelation function is shown to decay algebraically in time, like $t^{-3/2}$, if momentum is conserved locally, and like t^{-1}, if momentum is not conserved by the driving. A simple scaling argument supports the observed long-time tails.

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Strongly agitated granular fluids have attracted a lot of attention in recent years [1]. Generalizing kinetic theory to gases of inelastically colliding particles, most of the theoretical work which is based on microscopic dynamics has been done for either rather dilute or weakly inelastic systems. The velocity autocorrelation function [2] as well as transport coefficients [3] have been calculated for the homogeneous cooling state, which has also been simulated for a wide range of inelasticities [4].

Comparatively few studies have been performed on the stationary state of granular fluids in the moderate or high density regime. This is surprising, given the fact that the corresponding (elastic) molecular fluids have been studied in great detail [5] and have revealed several interesting features already in the dynamics of a single tagged particle: backscattering as indicated by a negative velocity autocorrelation, long-time tails due to the coupling of the tagged particle's density to a shear flow, and a glass transition at a volume fraction $\eta \approx 0.58$ accompanied by a strong decrease of the diffusion constant as a precursor to structural arrest. It is our aim to understand which of these features pertain to an inelastic gas and how they are destroyed by increasingly more dissipative collisions. This applies, in particular, to the glass transition, which has been conjectured to be related to the jamming transition in granular matter [6].

Several experimental groups have measured the velocity autocorrelation function (VACF) in dense granular flow [7–12]. The VACF in the steady state of a three-dimensional (3D) vibrofluidized bed [8] was shown to exhibit strong backscattering effects. In 2D vibrated layers, high-speed cameras have been used to measure the VACF. Even though long-time tails seem to be beyond the experimental resolution, these experiments give evidence for a nonexponential decay [11]. Caging effects have clearly been seen in air-fluidized beds [13] as well as in sheared granular materials [14]. In recent experiments [12] the development of a plateau in the mean square displacement has been observed but may be related to crystallization as seen in monodisperse vibrated layers [11,12].

Model.—We investigate a system of monodisperse hard spheres of diameter a and mass m. The time evolution is governed by instantaneous inelastic two-particle collisions. Given the relative velocity $\mathbf{g} := \mathbf{v}_1 - \mathbf{v}_2$, the change of $\mathbf{g}$ in the direction $\mathbf{n} := (\mathbf{r}_1 - \mathbf{r}_2)/|(\mathbf{r}_1 - \mathbf{r}_2)|$ is

$$(\mathbf{g} \cdot \mathbf{n})' = -\varepsilon(\mathbf{g} \cdot \mathbf{n}), \tag{1}$$

where primed quantities indicate postcollisional velocities and unprimed ones refer to precollisional ones. The coefficient of normal restitution ε characterizes the strength of the dissipation. For real systems, ε is a function of $\mathbf{n}$ and $\mathbf{g}$ [15]. Here we consider a simplified model with $\varepsilon = \text{const} \in [0, 1]$. The elastic system is characterized by $\varepsilon = 1$ and the sticky gas by $\varepsilon = 0$. The postcollisional velocities of the two colliding spheres are given by $\mathbf{v}_1' = \mathbf{v}_1 - \boldsymbol{\delta}$ and $\mathbf{v}_2' = \mathbf{v}_2 + \boldsymbol{\delta}$ with $\boldsymbol{\delta} = \frac{1+\varepsilon}{2}(\mathbf{n} \cdot \mathbf{g})\mathbf{n}$.

Because of the inelastic nature of the collisions, we have to feed energy into the system in order to maintain a stationary state. This can be done either by driving through the boundaries, for example, shearing the system or vibrating its walls [16], or alternatively by bulk driving, as in air-fluidized beds [13] or as in the experiments of Ref. [17]. Here we choose the simplest bulk driving [18] and kick a given particle, say, particle i, instantaneously at time t according to

$$\mathbf{v}_i'(t) = \mathbf{v}_i(t) + v_{\mathrm{Dr}}\boldsymbol{\xi}_i(t). \tag{2}$$

The driving amplitude v_{Dr} is constant, and the direction $\boldsymbol{\xi}_i(t)$ is chosen randomly with $\langle \xi_i^{(\alpha)}(t)\xi_j^{(\beta)}(t')\rangle = \delta_{ij}\delta_{\alpha\beta}\delta(t-t')$, with the Cartesian components $\xi_i^{(\alpha)}$, $\alpha = x, y, z$ distributed according to a Gaussian with zero mean. In practice we implement the stochastic process by kicking the particles randomly with frequency f_{Dr}.

If a single particle is kicked at a particular instant, momentum is not conserved. Because of the random direction of the kicks, the time average will restore the conservation of global momentum, but only on average. Momentum conservation is known to be essential for the appearance of long-time tails in elastic fluids. In fact the coupling of the tagged particle's density to the diffusion of transverse shear is responsible for the long-time tail of the VACF in elastic fluids. Hence we also study a second driving mechanism, in which pairs of particles are kicked in opposite directions [19]. However, even this kind of driving conserves momentum only globally. To ensure momentum conservation even on small scales, we choose pairs of neighboring particles and kick these in opposite directions. Our system is very close to an elastic fluid, in the sense that we provide the thermal energy "by hand." We regard this as a useful first step to investigate which features of an elastic molecular fluid pertain to a driven inelastic granular fluid.

We are interested in the time delayed correlation of a tagged particle's velocity $\Delta\mathbf{v}_i(t) = \mathbf{v}_i(t) - \overline{\mathbf{v}(t)}$ relative to the average $\overline{\mathbf{v}(t)} = 1/N\sum_i \mathbf{v}_i(t)$

$$\Phi(t) = \langle \Delta\mathbf{v}_i(t) \cdot \Delta\mathbf{v}_i(0)\rangle / \langle \Delta\mathbf{v}_i^2(0)\rangle \tag{3}$$

and its mean square displacement (MSD)

$$\Delta\mathbf{r}^2(t) = \langle [\mathbf{r}_i(t) - \mathbf{r}_i(0)]^2\rangle. \tag{4}$$

Here $\langle\ldots\rangle$ denotes an average over the random noise $\boldsymbol{\xi}_i(t)$. Of particular interest is the diffusion coefficient, which is expected to decrease as we increase the volume fraction towards close packing. It can be obtained in two alternative ways, either via the integral of the VACF $3D = \int_0^\infty dt\Phi(t)$ or as the time derivative of the MSD $6D = \lim_{t\to\infty} \frac{d\Delta\mathbf{r}^2(t)}{dt}$. Both definitions are equivalent in a stationary state.

Method.—In order to determine the MSD, the VACF, and the diffusion coefficient, we performed event driven molecular dynamics simulations for several system parameters: $0.5 \le \varepsilon \le 0.9$ and volume fractions $0.1 \le \eta \le 0.537\,25$. To detect long-time tails it is very important to have good statistics, since the tails occur at times when the correlations are already quite small. Hence we use a relatively small number of particles, $N \simeq 10^4$, but average each configuration over 1000 independent runs. Like Bizon *et al.* [20] we choose the driving frequency, f_{Dr}, of the order of the collision frequency. The balance of energy input and dissipation requires $v_{\mathrm{Dr}}^2 \approx \frac{1-\varepsilon^2}{4} T/m$. We choose v_{Dr} to achieve the same T for different ε. It is convenient to use dimensionless units such that $a = 2$, $m = 1$, and $T = 1$. Crystallization of the system has never been observed in the simulation, unless we prepare the system in a crystalline state initially, which was found to be stable in time only for $\varepsilon = 0.9$ and the highest density ($\eta = 0.537\,25$) investigated.

Event driven simulations of dense systems with a constant coefficient of restitution are known to undergo an inelastic collapse. Several mechanisms have been suggested to avoid the inelastic collapse. Here we proceed as follows: We introduce a virtual hull of very small width for each sphere. Two approaching spheres then collide 3 times—when the virtual hulls first touch each other, there is no change in momentum; then the real spheres collide elastically when they touch; finally the inelastic change of momentum takes place when the virtual hulls touch upon receding. Thus the dissipation takes place only when the colliding particles are sufficiently separated, i.e., by the width of the hull, which is taken to be 10^{-5} of the particles' diameter.

Results.—Backscattering effects are expected to be strongest for high densities, when cages have formed locally, enforcing reflection of the tagged particle by neighboring particles of the cage. In Fig. 1 we show the modulus of the VACF for volume fraction $\eta = 0.5$ and different inelasticities $0.7 \le \varepsilon \le 0.9$. The VACF becomes negative after a few collisions for all 3 of values of ε. It stays negative for about 10 collisions before the correlations become positive again for large times. For increasingly more inelastic collisions the range of negative correlations decreases and disappears completely for strongly inelastic systems, as demonstrated in Fig. 2 for $\eta = 0.45$. One clearly observes oscillations for $\varepsilon = 0.9$, whereas for $\varepsilon = 0.8$ the VACF stays positive, but shows a pronounced dint. For still smaller ε, backscattering disappears completely due to two effects. First, in the sticky limit a tagged particle is no longer reflected from its cage. Second, in order to achieve a stationary state of the same temperature, the driving force has to be increased for increasing inelasticity. Thereby the system is more strongly randomized, and the cages are destroyed more frequently.

Long-time tails are most easily observed for intermediate densities ($\eta = 0.2, 0.35$) and/or rather inelastic systems such that backscattering effects do not interfere significantly. In Fig. 3 we plot the modulus of the VACF for

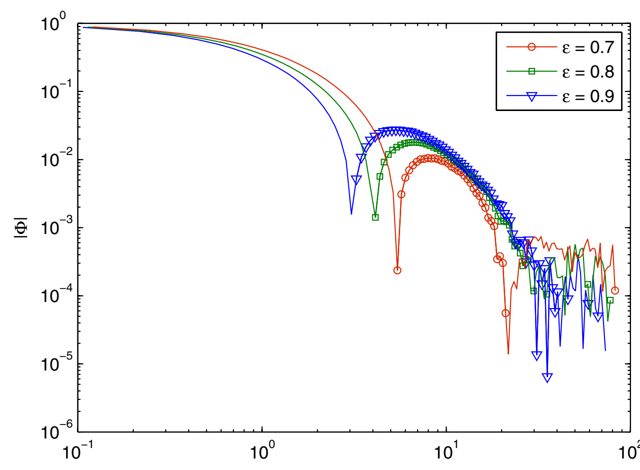

FIG. 1 (color online). Modulus of the VACF for $\eta = 0.50$ and different values for ε as a function of the mean number of collisions per particle, denoted by s. Symbols indicate negative values of the VACF.

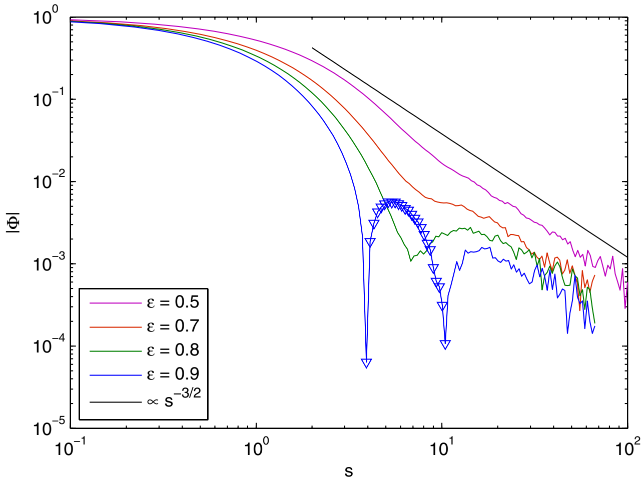

FIG. 2 (color online). Modulus of the VACF for $\eta = 0.45$ and $0.5 \leq \varepsilon \leq 0.9$ (from top to bottom). Symbols in the curve for $\varepsilon = 0.9$ indicate negative values of the VACF.

driving which conserves momentum locally. For a volume fraction of $\eta = 0.35$, an algebraic tail is clearly visible, and the exponent is approximately $-3/2$ as in the molecular fluid. For volume fraction $\eta = 0.2$, the algebraic decay is shifted to larger times. To observe long-time tails for higher volume fractions, one has to increase the inelasticity. In Fig. 2 a long-time tail $\propto s^{-3/2}$ is clearly visible only for the most inelastic system with $\varepsilon = 0.5$. In the inset of Fig. 3 we plot the VACF for a driving mechanism with random kicks of single particles, such that momentum is not conserved. One clearly observes an algebraic decay; however, the exponent is approximately -1 and clearly distinct from $-3/2$.

A simple scaling argument [5] yields the long-time tail of an elastic fluid and is easily generalized to the driven granular system with either momentum conservation or not. Let us assume that at $t = 0$ the tagged particle has velocity $v_{i,x}$ in the x direction. After a short time t the velocity is shared among the $N_t = \rho V_t$ particles in a small volume V_t around the tagged particle: $v_{i,x}(t) \sim v_{i,x}(0)/N_t$. If the driving conserves momentum locally, then the only process is diffusion of transverse momentum, which gives rise to a diffusive growth of the radius of V_t. This implies $V_t \sim t^{3/2}$ and consequently $v_{i,x}(t) \sim t^{-3/2}$. If on the other hand, momentum is not conserved by the driving, we have two competing processes. Collisions among the particles still conserve momentum and give rise to the same spread as above: $N_t \sim t^{3/2}$. At the same time, momentum builds up due to the random driving such that $P_t \sim t^{1/2}$. Considering both, the diffusive transport due to collisions and the build up of momentum due to driving, we find $v_{i,x}(t) = P_t/N_t \sim t^{-1}$.

The VACF has been studied previously for a freely cooling gas [21,22], which is not in a stationary state, so the VACF in general depends on two time arguments, the waiting time t_W and the delay t. For 2-dimensional systems a long-time tail of the form t^{-1} was observed [21]. Sheared granular gases were found to exhibit long-time tails in the VACF with an algebraic decay $\propto t^{-3d/2}$ [23] in spatial dimension $d = 2$ and $d = 3$.

In the inset of Fig. 4 we show a double logarithmic plot of the mean squared displacements for a system of inelasticity $\varepsilon = 0.7$ and volume fractions $\eta = 0.1$, 0.5, and 0.537 25. The ballistic regime can be clearly seen for up to one or two collision times. For larger times there is a

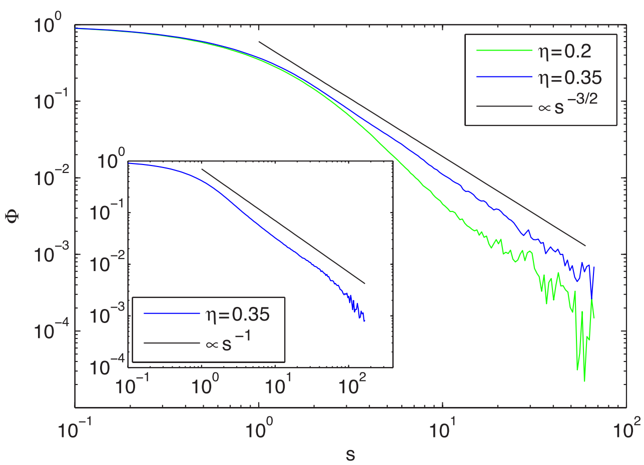

FIG. 3 (color online). The VACF for a system of inelasticity $\varepsilon = 0.7$ and volume fractions $\eta = 0.2, 0.35$ (from bottom to top) with local momentum conservation. Inset: without conservation of momentum.

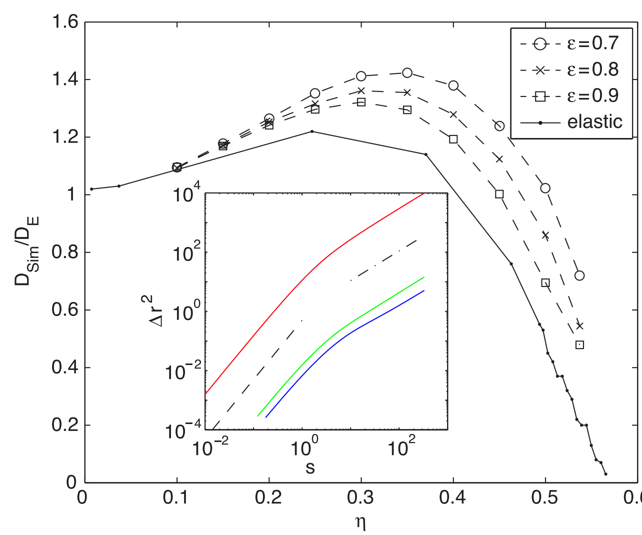

FIG. 4 (color online). Diffusion coefficients relative to the Enskog values as a function of η; reference values for the elastic system from [26]. Inset: MSD for $\varepsilon = 0.7$ and $\eta = 0.1$ (red solid line), 0.5 (green solid line), and 0.537 25 (blue solid line), from top to bottom, as a function of s; the dashed and the dash-dotted lines indicate ballistic (s^2) and diffusive (s) behaviors, respectively.

crossover to the linear regime. Even for the dense systems no plateau is visible, although a hint of a developing plateau may be observed for the highest density of $\eta = 0.537\,25$. For the longest times the MSD grows linearly with time, allowing us to extract the diffusion coefficient which decreases roughly by a factor of 20, when the volume fraction is increased from $\eta = 0.1$ to $\eta = 0.537\,25$.

The simplest kinetic theory for granular gases is the Enskog approximation, which has been employed extensively for free cooling dynamics [3]. It can be easily extended to driven systems [24], yielding an exponential decay of the VACF in the stationary state. This approximation implies for the diffusion coefficient

$$D_E = \frac{1}{\sqrt{\pi}} \frac{3}{8} \frac{1}{na^2 g(a)} \frac{1}{\frac{1+\varepsilon}{2}} \sqrt{\frac{T}{m}} \tag{5}$$

Here n denotes the number density, and $g(a)$ the pair correlation function at contact, which is usually approximated by the Carnahan-Starling formula [25]. We expect to observe deviations from the Enskog theory. To quantify these, we plot in Fig. 4 the diffusion coefficient D_{Sim}/D_E relative to the Enskog value as a function of volume fraction together with reference values for an elastic system [26].

As in the elastic case, the dependence of D_{Sim}/D_E on the volume fraction is not monotonic, but the maximum is shifted to higher volume fractions as compared to the elastic case. The increase over the Enskog value for intermediate densities is stronger, while the decrease over the Enskog value at high densities is smaller as compared to the elastic case. Nevertheless we see a pronounced decrease of the diffusion constant as the density of the glass transition in the elastic system is approached.

Conclusion.—We have investigated the dynamics of a tagged particle in a granular fluid, driven to a stationary state. Increasing the density we observe a strong decrease of the diffusion constant as the glass transition in the elastic system is approached. Cage effects are clearly visible at these high densities in the VACF, which was shown to oscillate as a function of time. As expected, backscattering becomes weaker as the fluid is made more inelastic. We have shown that long-time tails not only exist in the inelastic fluid but depend on whether or not the driving mechanism conserves momentum locally. If momentum is conserved locally, then momentum transport is diffusive, and the decay of the VACF is identical to the molecular fluid, like $t^{-3/2}$. If on the other hand momentum can build up locally, then the decay of the VACF is slowed down as compared to the conserved case, giving rise to a t^{-1} decay of the VACF.

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