Long-time tails and cage effect in driven granular fluids

Andrea Fiege, Timo Aspelmeier, and Annette Zippelius
Georg-August-Universität Göttingen, Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen and
Max-Planck-Institut für Dynamik und Selbstorganisation, Bunsenstr. 10, 37073 Göttingen

(Dated: September 25, 2008)

We study the velocity autocorrelation function (VACF) of a driven granular fluid in the stationary state in 3 dimensions. As the critical volume fraction of the glass transition in the corresponding elastic system is approached, we observe pronounced cage effects in the VACF as well as a strong decrease of the diffusion constant. At moderate densities the VACF is shown to decay algebraically in time \((t^{-3/2})\) like in a molecular fluid, as long as the driving conserves momentum locally.

PACS numbers: 45.70.-n, 51.20.+d, 47.10.-g

Strongly agitated granular fluids have attracted a lot of attention in recent years [1]. Most of the theoretical work which is based on microscopic dynamics has been done for either rather dilute or weakly inelastic systems, generalising kinetic theory to gases of inelastically colliding particles. 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 revealed several interesting features already in the dynamics of a single tagged particle:

1. backscattering as indicated by a negative velocity autocorrelation
2. long-time tails due to the coupling of the tagged particle’s density to a shear flow and
3. a glass transition at a volume fraction \(\phi \approx 0.58\) 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 VACF in dense granular flow [7, 8, 9, 10, 11, 12]. Positron emission particle tracking allows to determine the location of a tracer particle and hence to measure its VACF in 3-dimensional space. Thereby the VACF in the steady state of a vibro-fluidized bed has been measured [8] and was shown to exhibit strong backscatter effects. In 2 dimensional 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]. More recent experiments [12] on 2 dimensional vibrated layers show strong caging effects like the development of a plateau in the mean square displacement. These effects may, however, be related to crystallization, which is observed 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 \(g := v_1 - v_2\), the change of \(g\) in the direction \(n := (r_1 - r_2) / |r_1 - r_2|\) is

\[
(g \cdot n)' = -\varepsilon (g \cdot n)
\]

where primed quantities indicate postcollisional velocities and unprimed refer to precollisional ones. The coefficient of normal restitution \(\varepsilon\) characterizes the strength of the dissipation. For real systems, \(\varepsilon\) is a function of \(n\) and \(g\) [13]. 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 \(v_1' = v_1 - \delta\) and \(v_2' = v_2 + \delta\) with \(\delta := \frac{1+\varepsilon}{2\varepsilon} (n \cdot g)n\).

Due to 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, like shearing the system or vibrating its walls [14], or alternatively by bulk driving like on an air table or the experiments of ref. [15]. Here we choose the simplest bulk driving [16] and kick a given particle, say particle \(i\), instantaneously at time \(t\) according to

\[
v_i'(t) = v_i(t) + v_{\text{Dr}} \xi_i(t).
\]

The driving amplitude \(v_{\text{Dr}}\) is constant and the direction \(\xi_i(t)\) 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 \(\xi_i^{(\alpha)} \cdot \alpha = x, y, z\) distributed according to a Gaussian with zero mean. In practice we implement the stochastic process by kicking the particles randomly with frequency \(f_{\text{Dr}}\).

If a single particle is kicked at a particular instant, momentum is not conserved. Due to 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
The quantities we are interested in are the VACF of a tagged particle
\[
\Phi(t) = \langle \mathbf{v}_i(t) \cdot \mathbf{v}_i(0) \rangle / \langle \mathbf{v}_i^2(0) \rangle
\]  
(3)

and its mean square displacement (MSD)
\[
\Delta r^2(t) = \langle (\mathbf{r}_i(t) - \mathbf{r}_i(0))^2 \rangle
\]  
(4)

Here \(\langle \ldots \rangle\) denotes an average over the random noise \(\xi_i(t)\).

Of particular interest is the diffusion coefficient, which requires good statistics, since the tails occur at times of elastic molecular fluid pertain to a driven inelastic granular fluid.

The strength of the driving force is chosen depending on \(\varepsilon\) such that the granular temperature attains the value 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 \((\phi = 0.53725)\) 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. Each of these collisions is counted separately and we therefore divide the total number of collisions by three. In the simulations the width of the hull is taken to be \(10^{-5}\) of the particle's diameter. The balance of energy input and dissipation requires \(v_{Dr}^2 \approx \frac{1-\varepsilon^2}{4} T/m\). We choose \(v_{Dr}\) to achieve the same \(T\) for different \(\varepsilon\). It is convenient to use dimensionless units such that \(\alpha = 2, m = 1\) and \(T = 1\).

Results—Backscattering effects are expected to be strongest for high densities, when locally a cage has formed, enforcing reflection of the tagged particle colliding with neighbouring particles forming the cage. In Fig. 1 we show the modulus of the VACF for volume fraction \(\phi = 0.45\) and for different inelasticities \(\varepsilon = 0.7, 0.8, 0.9\). For \(\varepsilon = 0.9\) and \(\phi = 0.45\) we clearly observe oscillations in the VACF as a function of time measured in number of collisions: The VACF first becomes negative at \(t = 4\), stays negative until \(t = 10\) and becomes positive again before the signal disappears in the noise. The oscillations are suppressed by the inelasticity. For smaller \(\varepsilon\) the VACFs stay positive but show a dip, which is very pronounced for \(\varepsilon = 0.8\). We expect backscattering to disappear completely as the inelasticity is further increased due to two effects. First, in the steady 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.

For a higher volume fraction of \(\phi = 0.5\) the VACF crosses the time axis for all investigated inelasticities to
become positive again, as can be seen in Fig. 2. For \( \varepsilon = 0.9 \), the range of negative VACF is wider than for \( \phi = 0.45 \), starting shortly after the firstcollision and lasting for about 10 collisions. For larger inelasticities, \( \varepsilon = 0.8, 0.7 \), the range decreases.

Due to strong backscattering effects at high densities it is difficult to investigate long-time tails at these densities. Hence we plot in Fig. 3 the modulus of the VACF for intermediate volume fractions \( \phi = 0.1, 0.2, 0.35 \)and inelasticity \( \varepsilon = 0.7 \). For a volume fraction of \( \phi = 0.35 \) an algebraic tail is clearly visible and the exponent is approximately \(-3/2\) as in the molecular fluid. For volume fraction \( \phi = 0.2 \), the algebraic decay is shifted to larger times and for \( \phi = 0.1 \) this tail seems to vanish in noise.

The issue of long-time tails in elastic fluids has been exhibited long-time tails in the VACF with an algebraic decay \( \propto t^{-3/2} \) in spatial dimension \( d = 2 \) and \( d = 3 \).

Fig. 4 shows a double logarithmic plot of the mean squared displacements for a system of inelasticity \( \varepsilon = 0.7 \) and volume fractions \( \phi = 0.1 \) and 0.5. The ballistic regime can be clearly seen for up to one or two collision times. For larger times there is a 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 \( \phi = 0.53725 \). For the longest times the MSD grows linearly with time allowing us to extract the diffusion coefficient from the data. Fig. 4 reveals that the diffusion constant decreases roughly by a factor of 20, when the volume fraction is increased from \( \phi = 0.1 \) to \( \phi = 0.5 \).
and a stationary Maxwellian velocity distribution. Both assumptions are known to break down in granular fluids so that we expect to observe deviations from the Enskog theory. To quantify these, we plot in Fig. 5 the diffusion coefficient $D_{\text{Sim}}/D_{\text{E}}$ relative to the Enskog value as a function of volume fraction together with reference values for an elastic system.

As in the elastic case, the dependence of $D_{\text{Sim}}/D_{\text{E}}$ 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 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 exist in the inelastic fluid and are most clearly seen at intermediate densities. The issue of long-time tails is strongly tied to momentum conservation. Coupling to shear flow is one mechanism leading in the elastic case to an algebraic decay in time like $t^{-d/2}$ which pertains to the inelastic system provided momentum is conserved locally.

**Acknowledgments**

We thank Till Kranz, Matthias Sperl and Katharina Vollmayr-Lee for many interesting discussions.

---

[1] For a recent review see e.g. N. V. Brilliantov and T. Pöschel, "Kinetic Theory of Granular Gases", Oxford University Press, Oxford, 2004;
[2] J. W. Dufty, J. J. Brey and J. Lutsko, Phys. Rev. E 65, 051303, 2002;
[3] J. J. Brey, M. J. Ruiz-Montero, D. Cubero and R. Garcia-Rojo, Phys. Fluids 12, 876, 2000;
[4] J. Lutsko, J. J. Brey and J. W. Dufty, Phys. Rev. E 65, 051304, 2002;
[5] For a review see e.g. J.-P. Hansen and I. R. McDonald, "Theory of simple liquids", Academic Press, London, 1996;
[6] A. J. Liu and S. R. Nagel, Nature 396, 21, 1998;
[7] N. Menon and D. J. Durian, Science 275, 1920, 1997;
[8] R. D. Wildmann, J.-P. Hansen and D. J. Parker, Phys. Fluids 14, 232, 2002;
[9] J. Choi, A. Kudrolli, R. R. Rosales and M. Z. Bazant, Phys. Rev. Lett. 92, 174301, 2004;
[10] A. V. Orpe and A. Kudrolli, Phys. Rev. Lett. 98, 238001, 2007;
[11] P. Melby, F. Vega Reyes, A. Prevost, R. Robertson, P. Kumar, D. A. Egolf and J. S. Urbach, J. Phys. C 17, S2698, 2005;
[12] P. M. Reis, R. A. Ingale and M. D. Shattuck, Phys. Rev. Lett. 98, 188301, 2007;
[13] N. V. Brilliantov and T. Pöschel, Phys. Rev. E, 61, 1716, 2000; N. V. Brilliantov and T. Pöschel, Chaos 15, 026108, 2005;
[14] A. Puglisi, F. Cecconi and A. Vulpiani, J. Phys. Cond. Matt., 17, 82715, 2005;
[15] M. Schroeter, D. I. Goldman and H. L. Swinney, Phys. Rev. E, 71, 030301(R), 2005;
[16] D. R. M. Williams and F. C. MacKintosh, Phys. Rev. E, 54, R9, 1996;
[17] T. P. C. van Noije, M. H. Ernst, E. Trizac and I. Pagannabarraga, Phys. Rev. E 59, 4326, 1999
[18] T. Kranz, T. Aspelmeier and A. Zippelius, preprint 2008;
[19] Such a driving has been suggested in the context of dissipative particle dynamics, see e.g. P. Espanol and P. Warren, Europhys. Lett. 30, 191, 1995
[20] T. Kranz, T. Aspelmeier and A. Zippelius, preprint 2008;
[21] C. Bizon, M. D. Shattuck, J. B. Swift and H. L. Swinney, Phys. Rev. E 60, 4340, 1999;
[22] S. R. Ahmad and S. Puri, Phys. Rev. E 75, 031302, 2007;
[23] H. Hayakawa and M. Otsuki, Phys. Rev. E 76, 051304, 2007;
[24] V. Kumar, Phys. Rev. Lett. 96, 258002, 2006;
[25] A. Fiege, diploma thesis, University of Göttingen 2007;
[26] N. F. Carnahan and K. E. Starling, J. Chem. Phys. 51, 635, 1969;
[27] R. J. Speedy, Mol. Phys. 62, 509, 1987;