Glass Transition for Driven Granular Fluids

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We investigate the dynamics of a driven system of dissipative hard spheres in the framework of mode-coupling theory. The dissipation is modeled by normal restitution, and driving is applied to individual particles in the bulk. In such a system, a glass transition is predicted for a finite transition density. For increasing inelasticity, the transition shifts to higher densities. Despite the strong driving at high dissipation, the transition persists up to the limit of totally inelastic normal restitution.

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The celebrated jamming diagram of Liu and Nagel [1] generated a lot of interest in recent years. The conjecture is that in the space spanned by the parameters packing fraction \( \varphi \), temperature \( T \), and external stress \( \sigma \), there is a region where the material is solid like or jammed, cf. Fig. 1. This perspective unifies the concepts of jamming of macroscopic, athermal particles and of the glass transition of microscopic, thermal particles. A lot of work has been devoted to the point \( J \) — the arrest of static or quasi static granular assemblies [2]. Similarly, the glass transition of a supercooled molecular liquid has been studied extensively, corresponding to a transition line in the \( \varphi-T \)-plane, which in the case of hard spheres is parallel to the \( T \)-axis. In such a system of elastic hard spheres, the glass transition is described well by the mode-coupling theory (MCT) [3, 4]. Whether or not the unified picture of the jamming diagram holds is still a matter of debate, though.

![Fig. 1: a) The jamming diagram for sheared systems as a function of inverse density \( \varphi^{-1} \), temperature \( T \), and shear stress \( \sigma \). b) Jamming diagram for driven inelastic hard spheres where the driving power \( \varepsilon_{Dr} \) replaces the shear stress. In this latter case, the temperature dependence is trivial for \( T > 0 \), and the origin of the graph lies at random-close packing (rcp).](image)

It was shown by theory and computer simulation that both Newtonian and Brownian equations of motion yield the same glassy dynamics [5, 6]. The situation is different when the system is subject to shear. MCT has been extended recently to the case of colloidal suspensions under shear [7], and for this case it was shown that any finite shear rate is able to destroy the glass transition. While remnants of the glass transition are still affecting the dynamics, full arrest is no longer possible. Another scenario is proposed by the above mentioned jamming diagram where applied shear stress unjams the system but can be compensated by higher density or lower temperature, cf. Fig. 1(a).

It is the objective of the present paper to investigate the possibility of a glass transition in a granular fluid in a steady state when dissipation is balanced by bulk driving. Experiments by Abate and Durian [8] and Reis et al. [9] showed indications of a granular glass transition in such fluidized granular systems in two dimensions. These observations would fit into a modified jamming diagram, where the shear-stress axis \( \sigma \) is replaced by an axis that quantifies the driving force \( \varepsilon_{Dr} \) used to compensate for the dissipative interactions among the granular particles. In the following, we shall investigate if a granular glass transition can exist and how such a transition can be described by an appropriate theory. It will be demonstrated that (1) the combination of MCT [6] with granular kinetic theory [10] predicts a glass transition for a driven dissipative system, (2) the nature of the transition depends on the degree of dissipation, and (3) granular dynamics cannot be scaled onto Brownian or Newtonian dynamics.

We consider the non-equilibrium stationary state of a driven granular fluid comprised of \( N \rightarrow \infty \) identical hard spheres of diameter \( d \) and mass \( m \) in a volume \( V \). Energy dissipation in binary collisions is modeled by a coefficient of normal restitution \( \varepsilon \). Due to the energy loss in the collisions the system needs to be driven in order to achieve a stationary state. We use a simple bulk driving mechanism, e.g., as in air fluidized beds [3]. The
particles are kicked with frequency $\omega_{\text{Dr}}$, 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 of the kick, $\xi_i(t)$, is chosen randomly from a Gaussian distribution, $P(\xi)$, with unit variance. To ensure momentum conservation, we choose pairs of neighboring particles and kick them in opposite directions [12]. A stationary state is reached, when the energy loss due to collisions is balanced by the energy input due to driving.

A simple estimate relates the properties of the driving $(\omega_{\text{Dr}}, v_{\text{Dr}})$ to the collision frequency $\omega_{\text{coll}}$:
\[ \omega_{\text{coll}}(1 - \varepsilon^2) \frac{T}{4} = \omega_{\text{Dr}} v_{\text{Dr}}^2. \]
The time evolution of the system consists of ballistic motion in between binary collisions and random kicks. These can be formally incorporated in a pseudo-Liouville operator $L_+$ [11,13], which generates the time evolution of an observable, such as the density
\[ \rho_q(t) = \frac{1}{N} \sum_i \exp(iq \cdot r_i(t)) = \exp(itL_+)\rho_q(0). \]
For the discussion of the long-time dynamics, the central quantity of interest is the density correlation function,
\[ F(q,t) = \int d^3 \xi P(\xi) \int d\Gamma w(\Gamma) \rho_{q,0}(0) \rho_{q,t}(t) =: \langle \rho_{q,0}(0) | \rho_{q,t}(t) \rangle, \]
which is directly accessible from computer simulations and experiments. Here, $w(\Gamma)$ is the stationary $N$-particle distribution and $\Gamma = \{ r_i, v_i \}_{i=1}^N$ denotes a point in phase space.

Following Mori and Zwanzig, the normalized correlation function, $\phi_q(t) = F(q,t)/S(q) = F(q,t)/F(q,0)$, can be represented in terms of restoring forces and a memory kernel [14],
\[ (\partial_t^2 + \nu_q \partial_t + \Omega_q^2) \phi_q(t) = -\int_0^t d\tau M_q(t - \tau) \partial_\tau \phi_q(\tau), \]
with
\[ \nu_q = N \frac{v_0}{\Omega_q^2} \langle j_q^t | L_+ j_q^t \rangle, \quad \Omega_q^2 = \frac{N^2}{v_0 S_q} \langle \rho_q | L_+ j_q^t \rangle \langle j_q^t | L_+ \rho_q \rangle. \]
The thermal velocity $v_0 = \sqrt{T/m}$ and initial conditions are $\phi_q(0) = 1, \partial_\tau \phi_q(0) = 0$.

Detailed balance does not hold and consequently, the transition rates of forward and backward reactions are not simply related, $\langle \rho_q | L_+ j_q^t \rangle \neq \langle j_q^t | L_+ \rho_q \rangle^*$, as it would be the case in equilibrium systems. For the same reason, the memory kernel, $M_q(t) = \langle R_q^t | R_q(t) \rangle$, is now given by the cross-correlation of two unequal fluctuating forces, $R_q \neq R_q^\dag$, driven by the reduced dynamics. Details of the calculation can be found elsewhere [15]. The representation in Eq. (1) is exact. It correctly accounts for the conservation laws for the density, $\rho_q(t)$ and the longitudinal momentum, $qj_q(t) = \partial_\tau \rho_q(t)$. Energy is not conserved in a granular medium and transverse momentum is decoupled. Hence the representation guarantees the correct hydrodynamic limit of $\phi_q(t)$.

To proceed, we have to resort to approximations. First, we need an approximate form of the $N$-particle distribution to compute static (equal time) correlations. We assume that positions and velocities are uncorrelated $w(\Gamma) = w_r(\{ r_i \})w_v(\{ v_i \})$ and that the velocity distribution factorizes into a product of one-particle distributions, $w_v(\{ v_i \}) = \prod_i w_v(\{ v_i \})$. The precise form of $w_v(\{ v_i \})$ is not needed, it only has to satisfy $\langle v \rangle = 0$ and $\langle v^2 \rangle = 3T/m < \infty$. Furthermore, the system is assumed to be isotropic and homogeneous except for the excluded volume: $w_r(\{ r_i \}) = \prod_{i<j} \theta(r_{ij} - d)$. For the restoring forces we find
\[ \nu_q = -i \frac{\nu_E}{2} [1 - j_0(qd) + 2j_2(qd)], \]
\[ \Omega_q^2 = \frac{q^2 v_0^2}{S_q} \left( \frac{1 + \varepsilon}{2} + \frac{1 - \varepsilon}{2} S_q \right), \]
with $\nu_E$ the Enskog frequency for the elastic case.

An additional approximation is necessary to compute the memory kernel. The success of MCT for the description of dense molecular and colloidal fluids motivates its application also to dissipative granular fluids. First, we project the fluctuating forces onto products of densities. Second, the resulting higher order correlations are factorized into pair correlations. Thereby, one generates an explicit expression for $M_q(t) = m_q(t) \Omega_q^2$ in terms of $\phi_q(t)$ [12],
\[ m_q[\phi](t) \approx A_q(\varepsilon) \frac{n S_q}{q^2} \int d^3 k V_{qk} \phi_k(t) \phi_{q-k}(t) \]
with $V_{qk}$ given by
\[ V_{qk} = S_k S_{q-k} |\hat{q} \cdot \hat{k} c_k + \hat{q} \cdot (\hat{q} - \hat{k}) c_{q-k}|^2 \]
The direct correlation function, $c_q$, is simply related to the static structure factor via the Ornstein-Zernike equation $n c_q \equiv 1 - S_q^{-1}$ and $A_q(\varepsilon) = [1 + (1 - \varepsilon) S_q/(1 + \varepsilon)]^{-1}$ depends on $\varepsilon$ explicitly. Inserting the mode coupling approximation, Eq. (2), into Eq. (1), we get a self-consistency equation for the scattering function $\phi_q(t)$.

The only further input that is required is the static structure factor $S_q$. For simplicity, we use the elastic Percus-Yevick expression [12] here. Future work [15] will study the influence of a more precise structure factor that depends on the coefficient of restitution $\varepsilon$.

A memory function under driving is not necessarily positive and might not even be a real function [16]. Hence, it is surprising that for a driven granular fluid the only change compared to the elastic case is the $\varepsilon$-dependent prefactor $A_q(\varepsilon) > 0$, see Eq. (2). Consequently, the memory kernel itself is positive and a vast
A glass transition is signaled by the appearance of a time persistent part of the density correlations $f_q := \lim_{t \to \infty} \phi_q(t)$ in Eq. (1). In this limit, Eq. (1) reduces to the algebraic equation $f_q/(1-f_q) = m_q[f]$ which is solved readily by standard procedures \cite{17}. For all values of the coefficient of restitution, $0 \leq \varepsilon \leq 1$, an ideal glass transition of the driven granular fluid is found with a transition density $\varphi^c(\varepsilon)$, cf. Fig. 2. For increasing dissipation, i.e., smaller $\varepsilon$, the glass transition is shifted to higher densities. This can be understood as follows: For increased dissipation, $\varepsilon < 1$, the prefactor $A_q(\varepsilon)$ in Eq. (2) becomes smaller than unity. Dissipation and driving hence weaken the memory effects and destabilize the glass. This needs to be compensated by a higher density. The resulting compensation of enhanced dissipation and driving by increased density can be represented in a corresponding jamming diagram as shown in Fig. 1A, where for simplicity the mean field relation $v_D^2 \propto (1-\varepsilon)^2/4$ was used. It might be reassuring that, although the critical density increases with increasing dissipation, it stays below the density of random-close-packing.

The full dynamics of Eq. (1) is shown in Fig. 3. The time dependent scattering function $\phi_q(t)$ with a density close to the glass transition density $\varphi^c$ shows the generic two step relaxation. After an initial fast relaxation, the scattering function approaches a plateau $\phi_q(t) \simeq f_q$ and decays to zero only for very long times, provided the density is still below the critical one. Close to the transition point a critical decay is found onto these plateaus, $\phi_q(t) - f_q \propto t^{-a}$. The variation of the critical exponent $a$ is shown in the inset of Fig. 2. For values below the transition, $\varphi < \varphi^c$, a second power law describes the decay from the plateau, known as the von-Schweidler law, $\phi_q(t) - f_q \propto t^b$. The exponent $b$ (not shown here) also varies with the coefficient of restitution $\varepsilon$, and is uniquely related to $a$.

At the transition point and beyond, $\varphi > \varphi^c$, the correlation function assumes a finite long-time limit $f_q > 0$ which sets in at a critical plateau value $f_q^c$. These values are shown in Fig. 4 for various values of $\varepsilon$. The increasing dissipation has three noticeable effects: (1) correlations at small wavenumbers are enhanced, (2) oscillations re-
reflecting the local structure become less pronounced, and (3) the localization length (indicated by the inverse of the width of the \( f_R \) distribution) decreases. The last finding is a consequence of the glass transition taking place at a higher density, cf. Fig. 2.

It was shown earlier that Newtonian (N) and Brownian (B) systems show the same glassy dynamics. This is shown for the MCT dynamics in Fig. 5 for curves N and B, where N only needed to be shifted along the time axis to match B. In contrast, due to the explicit dependence on \( \varepsilon \) in Eq. (2), for any \( \varepsilon < 1 \), the granular long-time dynamics (G) cannot be scaled on top of the Newtonian or Brownian results. In addition, for granular dynamics at different \( \varepsilon \) there also exists no single master curve, cf. Fig. 6. Therefore, granular dynamics leads to a fundamentally different long-time behavior.

In conclusion, we have shown that MCT can be extended to granular fluids, which are in a steady state far from equilibrium. It can be shown that the resulting memory kernel in Eq. 2 is positive, and this allows that most mathematical theorems from equilibrium MCT carry over to the driven granular case. An ideal glass transition is observed for all values of the dissipation or equivalently all values of the driving. Since the balance between dissipation and driving implies that the driving amplitude is proportional to the inelasticity \( \epsilon^2 \), the glass transition defines a line in the \( \varphi^{-1} \)-versus-\( \epsilon^2 \) plane of a generalized jamming diagram, cf. Fig. 1. The universality known for Newtonian and Brownian dynamics is broken in the granular case – however, the predicted differences in the critical exponents, cf. inset of Fig. 2 and glass form factors, cf. Fig. 1 are relatively small. Comparably large changes with increased dissipation are expected in the transition densities as shown in Fig. 2. This prediction can be supported by looking at a precursor of the glass-transition line in computer-simulation data: For increasing dissipation, points of equal diffusivity are found to be shifted to higher densities (inset of Fig. 5) in accordance with our predictions for the glass transition in Fig. 2. Therefore, we expect our results to be testable in further computer simulation studies and also in experiments.

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![Graph](image-url)

FIG. 5: Dynamic scattering function \( \phi_q(t) \) for \( qd = 4.2 \) at the glass transition, \( \varphi = \varphi_c \), and for slightly lower volume fraction, \( \varphi = 0.999\varphi_c \), for Newtonian dynamics (N) with \( \sigma_q = 0 \), Brownian dynamics (B), and granular dynamics (G) with coefficient of restitution \( \epsilon = 0.5 \). The Newtonian dynamics is scaled along the time axis to match the Brownian dynamics at long times. No such rescaling is possible for the granular dynamics. The inset shows three lines of equal diffusivity (from top to bottom: \( D = 0.7, 0.8, \) and 0.9 in relative units) taken from the data of a computer simulation [12].

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