Divergence of viscosity in jammed granular materials: a theoretical approach

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**Introduction**

- Granular materials behave as unusual solids and liquids.
- Jamming is an athermal solid-liquid transitions.

Flow of mustard seeds @Chicago group  
Kamigamo shrine (Kyoto!)
• Above the critical density, the granular material has rigidity and behaves as a solid.
• Jamming transition is similar to glass transition.
Differences between jamming and glass transitions

• Although both describes the freezing of motion, there are some differences between two.

• Most important differences is that the jamming is the phase transition, but glass is not.

• There is no plateau of time correlation in the jamming.

• There is the divergence of the first peak.

(Pica Ciamarra, Coniglio, 2009)
Divergence of viscosity

- Approach from below the jamming, the most important characteristics is the divergence of the viscosity at the jamming.

\[ \eta \sim (\varphi_J - \varphi)^{-\lambda} \text{ with } \lambda \approx 2 \]

- Kawasaki et al estimated as \(1.67 < \lambda < 2.5\).
- This divergence with \(\lambda = 2\) is known even in colloid systems (see e.g. Brady 1993).
- However, some people indicated that \(\lambda\) for granular materials is larger than the estimated value.
Granular systems under uniform steady shear (SLLOD dynamics and Lees-Edwards boundary condition)
Limitation of Kinetic Theory

- Kinetic theory of Garzo-Dufty works well for $\phi < 0.5$ (around Alder transition point).
- So we need to construct a new approach for dense sheared granular flow.

S. Chialvo and S. Sundaresan, Phys. Fluid. 25, 0706503 (2013), where $\gamma$ is the shear rate.

N. Mitarai and H. Nakanishi, PRE75, 031305 (2007)

The agreement of the temperature is poor.
Equation of motion

- Newton’s equation (equivalent to Liouville equation)

\[ m \ddot{r}_i = F_i^{(el)} + F_i^{(vis)} \quad (i = 1, \ldots, N), \]

\[ F_i^{(el)} = -\frac{\partial U}{\partial r_i} = \sum_{i \neq i} F_{ii}^{(el)} \]

\[ F_{ij}^{(el)} = -\frac{\partial u(r_{ij})}{\partial r_{ij}} = \Theta(d - r_{ij}) f(d - r_{ij}) \hat{r}_{ij} \]

\[ f(x) = \kappa x \quad (\kappa > 0) \]

\[ F_{ij}^{(vis)} = -\zeta \Theta(d - r_{ij}) \hat{r}_{ij} (g_{ij} \cdot \hat{r}_{ij}). \quad g_{ij} \equiv \mathbf{v}_i - \mathbf{v}_j \]

\[ \Lambda(\Gamma) = -\frac{\zeta}{m} \sum_{i,j} \Theta(d - r_{ij}) < 0 \]
Liouville equation

• Liouville equation is equivalent to Newton’s equation.

• An arbitrary observable $A(\Gamma(t))$ satisfies

$$\Gamma(t) = \{r_i(t), p_i(t)\}_{i=1}^N$$

$$\frac{d}{dt} A(\Gamma(t)) = \dot{\Gamma} \cdot \frac{\partial}{\partial \Gamma} A(\Gamma(t)) \equiv i\mathcal{L}A(\Gamma(t)).$$

• The distribution function satisfies

$$\frac{\partial \rho(\Gamma, t)}{\partial t} = -\frac{\partial}{\partial \Gamma} \cdot \left[ \dot{\Gamma} \rho(\Gamma, t) \right] = - \left[ \dot{\Gamma} \cdot \frac{\partial}{\partial \Gamma} + \Lambda(\Gamma) \right] \rho(\Gamma, t)$$

Phase volume contraction due to dissipation
Energy balance equation

- Hamiltonian

$$\mathcal{H}(\Gamma) = \sum_{i=1}^{N} \frac{p_{i}^2}{2m} + \sum_{i,j}^{'} u(r_{ij})$$

- Satisfies the energy balance equation

$$\dot{\mathcal{H}} = -\dot{\gamma} V \sigma_{xy} - 2R.$$

$$\sigma_{\mu\nu}(\Gamma) = \frac{1}{V} \sum_{i}^{N} \left[ \frac{p_{i}^{\mu} p_{i}^{\nu}}{m} + r_{i}^{\nu} \left( F_{i}^{(el)\mu} + F_{i}^{(vis)\mu} \right) \right]$$

$$R(\Gamma) = -\frac{1}{2} \sum_{i=1}^{N} \dot{r}_{i} \cdot F_{i}^{(vis)} = -\frac{1}{4} \sum_{i,j}^{'} g_{ij} \cdot F_{ij}^{(vis)}$$
Perturbation of the Liouville equation

- Liouville equation contains $6N$ dimensional distribution.
- This cannot be exactly solved because it contains too many degrees of freedom.
- Unperturbed state: canonical distribution (no dissipation)
  - This corresponds to the degenerated unperturbed state.
  - Zero-eigenmodes correspond to the density, momentum and energy conservations.
- Perturbation: inelasticity + shear $\Rightarrow$ constant energy
Expansion parameters & restitution constant

- Perturbation parameter

\[ \epsilon = \frac{\zeta}{\sqrt{\kappa m}} \ll 1. \]

- Restitution constant

\[ e = \exp\left[-\frac{\zeta t_c}{m}\right] \]

\[ t_c = \frac{\pi}{\sqrt{2\kappa/m - (\zeta/m)^2}} \]

\[ \epsilon \approx \frac{\sqrt{2(1 - e)}}{\pi} \text{ for } e \approx 1 \]
Perturbative spectrum analysis

\[ \Psi_n(\Gamma) = \int_{-\infty}^{0} dt \, e^{-z_n t} \rho(\Gamma, t) \]

\[ \Psi_n^*(\Gamma) = \rho_{eq}^*(\Gamma) \left[ \Psi_n^{(0)*}(\Gamma) + \epsilon \tilde{\Psi}_n^{(1)}(\Gamma) \right] + \mathcal{O}(\epsilon^2) \]

\[ z_n^* = z_n^{(0)*} + \epsilon \tilde{z}_n^{(1)} + \mathcal{O}(\epsilon^2), \]

Unperturbed canonical state

\[ i \mathcal{L}^{(eq)*}(\Gamma) \rho_{eq}^*(\Gamma) = 0 \]

Zero-eigenmodes

\[ i \mathcal{L}^{(eq)*}(\Gamma) \phi_n^*(\Gamma) = 0 \quad (\alpha = 1, \ldots, 5). \]

\[ \phi_n^*(\Gamma) \propto \left\{ 1, \sum_{i=1}^{N} p_i^{*x}, \sum_{i=1}^{N} p_i^{*y}, \sum_{i=1}^{N} p_i^{*z}, \mathcal{H}^*(\Gamma) \right\} \]
Eigenvalue

• Lowest eigenvalues are easily obtained as

\[ \tilde{\zeta}_1^{(1)} = 0, \]
\[ \tilde{\zeta}_\alpha^{(1)} = -\frac{2}{3} \mathcal{G} \quad (\alpha = 2, 3, 4, 5), \]

• Where

\[ \mathcal{G} = n^* \int d^3 r^* g(r^*, \varphi) \Theta(1 - r^*). \]

• In the hard-core limit, the relaxation time is

\[ \tau_{\text{rel}}^* \approx -\frac{1}{\varepsilon \tilde{\zeta}_\alpha^{(1)}} = \left[ \frac{2}{3} \varepsilon \mathcal{G} \right]^{-1} \]

\[ \mathcal{G} \to \sqrt{\pi} \omega_E^*(T^*), \]
Steady distribution

\[ \rho_{SS}^{(ex)}(\Gamma) = \exp \left[ \int_{-\infty}^{0} d\tau \Omega_{eq}(\Gamma(-\tau)) \right] \rho_{eq}(\Gamma(-\infty)) \]

\[ \exp \left[ \int_{-\infty}^{0} d\tau \Omega_{eq}(\Gamma(-\tau)) \right] \approx e^{\tau_{rel} \Omega_{SS}(\Gamma)} \]

\[ \tau_{rel} = \left[ \frac{2\sqrt{\pi}}{3} \epsilon \omega_{E}^{*}(T^{*}) \right]^{-1} \]

\[ \tilde{\Omega}_{SS}(\Gamma) = -\beta_{SS}^{*} \left[ \tilde{\gamma} V^{*} \tilde{\sigma}_{xy}^{(el)}(\Gamma) + 2\Delta \tilde{\mathcal{R}}_{SS}^{(1)}(\Gamma) \right] \]

\[ \Delta \mathcal{R}_{eq}^{(1)}(\Gamma) \equiv \mathcal{R}^{(1)}(\Gamma) + \frac{T_{eq}}{2} \Lambda(\Gamma) \quad \mathcal{R}^{(1)}(\Gamma) \equiv \frac{\zeta}{4} \sum_{i,j} \left( \frac{p_{ij}}{m} \cdot \hat{r}_{ij} \right)^{2} \Theta(d - r_{ij}) \]

Thus, we obtain the effective Hamiltonian in NESS.
Average under NESS

- Average is calculated by

\[
\langle \cdots \rangle_{SS} \equiv \int d\Gamma \, \rho_{SS}(\Gamma) \cdots
\]

\[
\rho_{SS}(\Gamma) = \frac{e^{-I_{SS}(\Gamma)}}{\int d\Gamma e^{-I_{SS}(\Gamma)}} \quad I_{SS}(\Gamma) = \beta_{SS} \mathcal{H}(\Gamma) - \tau_{rel} \Omega_{SS}(\Gamma)
\]

- \( \beta_{SS} \) is determined by the energy balance equation.

\[
\rho_{SS}(\Gamma) \approx \frac{e^{-\beta_{SS}^* \mathcal{H}^*(\Gamma)}}{\mathcal{Z}} \left[ 1 + \tilde{\tau}_{rel} \tilde{\Omega}_{SS}(\Gamma) \right]
\]

\[
\mathcal{Z} \approx \int d\Gamma \, e^{-\beta_{SS}^* \mathcal{H}^*(\Gamma)} \left[ 1 + \tilde{\tau}_{rel} \tilde{\Omega}_{SS}(\Gamma) \right]
\]
Shear stress

\[ \langle A(\Gamma) \rangle_{ss} \approx \langle A(\Gamma) \rangle_{eq} + \tilde{\tau}_{rel} \langle A(\Gamma) \tilde{\Omega}_{ss}(\Gamma) \rangle_{eq} \]

\[ \langle \cdots \rangle_{eq} = \int d\Gamma e^{-\beta_{ss}^* \mathcal{H}^*(\Gamma)} \cdots \]

\[ \langle \tilde{\sigma}_{xy}(\Gamma) \rangle_{ss} \approx -\tilde{\tau}_{rel} \tilde{\gamma} / \beta_{ss}^* V^* \langle \tilde{\sigma}_{xy}^{(el)}(\Gamma) \tilde{\sigma}_{xy}^{(el)}(\Gamma) \rangle_{eq} \]

- This corresponds to Kubo formula under the exponential relaxation.

\[ \langle \tilde{R}(\Gamma) \rangle_{ss} \approx \langle \tilde{R}^{(1)}(\Gamma) \rangle_{eq} - 2\tilde{\tau}_{rel} \beta_{ss}^* \langle \tilde{R}^{(1)}(\Gamma) \Delta \tilde{R}_{ss}^{(1)}(\Gamma) \rangle_{eq} \]
The evaluation of multi-body correlations

• We have to evaluate 3-body and 4-body static correlation functions.
• We adopt the Kirkwood approximation in which the multi-body correlation can be represented by a product of two-body correlations.
Radial distribution at contact

- We use the empirical formula for the radial distribution at contact

\[ g(\varphi) = G_{CS}(\varphi_f)(\varphi_f - \varphi_J)/(\varphi - \varphi_J) \]

\[ G_{CS}(\varphi) = (1 - \varphi/2)/(1 - \varphi)^3 \]

\( \varphi_f < \varphi < \varphi_J \), where \( \varphi_f = 0.49 \) and \( \varphi_J = 0.639 \)
Granular temperature and shear stress

- From the energy balance and Kirkwood approximation, we obtain

\[ T_{SS}^* = \frac{3 \tilde{\gamma}^2}{32\pi} \frac{S}{R} \]

where \( S \) and \( R \) are given by

\[ S = 1 + \mathcal{I}_2 n^* g(\varphi) + \mathcal{I}_3 n^* g(\varphi)^2 + \mathcal{I}_4 n^* g(\varphi)^3 \]

\[ R = \mathcal{R}_2' n^* g(\varphi) + \mathcal{R}_3' n^* g(\varphi)^2, \]

with \( \mathcal{R}_2' = -3/4 \), \( \mathcal{R}_3' = 7\pi/16 \)

\[ \langle \tilde{\sigma}_{xy}(\Gamma) \rangle_{SS} = -\frac{3}{8\pi} \tilde{\gamma} T_{SS}^{1/2} \frac{S}{g(\varphi)} = -\frac{3\sqrt{6}}{64\pi^{3/2}} \tilde{\gamma}^2 \frac{S^{3/2}}{R^{1/2} g(\varphi)}. \]
Near the jamming point

- Near the jamming point, the radial distribution function diverges linearly. Thus, we extract the most divergent term:

\[ T_{SS}^* \approx \frac{3\tilde{\gamma}^2}{32\pi} \mathcal{L}_4 \mathcal{R}_3 n^* g(\varphi) = \frac{9\pi}{2240} \tilde{\gamma}^2 n^* g(\varphi), \]

\[ \langle \tilde{\sigma}_{xy}(\Gamma) \rangle_{SS} \approx -\frac{9\pi^2}{1280} \tilde{\gamma} T_{SS}^{1/2} n^3 g(\varphi)^2 \]

\[ = -\frac{27\pi^{5/2}}{10240\sqrt{35}} \tilde{\gamma}^2 n^{7/2} g(\varphi)^{5/2}. \]

- The power law dependences are

\[ T_{SS}^* \sim g(\varphi) \sim (\varphi_J - \varphi)^{-1} \]

\[ \tilde{\eta}' = -\langle \tilde{\sigma}_{xy} \rangle_{SS} / \tilde{\gamma}^2 \propto -\langle \tilde{\sigma}_{xy} \rangle_{SS} / (\tilde{\gamma} \sqrt{T_{SS}^*}) \sim (\varphi_J - \varphi)^{-2} \]
To verify the validity of our theoretical prediction, we perform MD (or DEM) for frictionless grains.

Parameters: \( N = 2000, \quad \epsilon = 0.018375 \ (e = 0.96) \)

\( \dot{\gamma}^* = 10^{-3}, \ 10^{-4}, \ 10^{-5} \)

Sllod + Lees-Edwards boundary condition
Viscosity

(\phi_j - \phi)^{-2}

\dot{\gamma} \to 0
Granular temperature & relaxation time

• Agreement of granular temperature is relatively poor.
• Agrees well ($\varphi < 0.62$)
• MD result: extracted from fitting the relaxation due to inelastic collisions
• Relaxation time $\tau_{rel} =$ eigenvalue of Liouville eq. 
  $\Rightarrow$ Enskog (collision) frequency
Discussion

• Constitutive equation still obeys Bagnold’s scaling.

• For example, if we assume $\sigma_{xy} \sim |\varphi - \varphi_J|$, then $\sigma_{xy} \sim \dot{\gamma}^{4/7}$, which is close to the simulation value.

• Based on the nonequilibrium steady distribution, we may discuss above the jamming point (by using replica) => Now in progress.

• The effects of rotation and tangential friction mainly appear in the radial distribution at contact. => Now in progress

• Our method is generic. Thus, we can apply it to many other systems.

• Can the relaxation time described by the eigenvalue?
No critical slowing down which is consistent with the theory. This can change the critical exponents.
We have developed the theory of dense sheared granular flow (frictionless grains).

We obtain the steady distribution, which can be regarded as the effective Hamiltonian in the non-equilibrium steady state.

Then, we can evaluate the viscosity and the granular temperature analytically.

The result of the viscosity gives the quantitatively precise result.

The granular temperature is not good.