Rheology of Dense Sheared Granular Liquids

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Abstract. The rheology of dense sheared granular liquids is investigated based on the mode-coupling theory (MCT). This extended MCT includes correlations for the density-current mode as well as the density-density correlation mode, and a self-consistent coupling equation for the energy balance condition. The extended MCT exhibits disappearance of the two-step relaxation of the density-density correlation function, and also successfully reproduces the density dependence of the shear viscosity for volume fractions between 0.50 and 0.60, if we use the renormalized density. However, it predicts unphysical tendency for the granular temperature. The cause of this drawback and the possibilities of its amendment are discussed.

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INTRODUCTION

Establishing a macroscopic description of granular materials has been a long-term challenge for both science and engineering. The problem extends to a vast range, from creep motion or force chain dynamics of frictional particles, two-phase flow of air-fluidized beds, to nonequilibrium transport of sheared granular flows [1]. Similar to solid-liquid transitions, critical features of the jamming transition in the vicinity of the random close packing and their relation to the glass transition have attracted much interest in the last decade [2, 3]. Even when we focus only on the classical problem of the flow properties well below the jamming transition density \( \phi_j \), which can be tracked back to Bagnold’s work [4], we have not yet understood the rheological properties of dense granular flows. One of the remarkable achievements is the extension of the Boltzmann-Enskog kinetic theory to inelastic hard disks and spheres [5, 6], which stimulated the following works [7, 8, 9]. Up to present, the kinetic theory is the unique continuum description of granular flows derived from first principles [10]. However, it has been recognized that the kinetic theory breaks down at high densities with volume fraction \( \phi > 0.5 \) [11, 12, 13], since there exists correlated motions of grains. Thus, a liquid theory which contains the effect of granular correlations is expected to be constructed for the regime \( 0.5 < \phi < \phi_j \).

On the other hand, a continuum description with long-time correlations has been constructed for thermal glassy liquids. The mode-coupling theory (MCT) exhibits the two-step relaxation of density correlation functions characteristic of glasses [14, 15, 16]. Although MCT has presented remarkable success [17, 18, 19, 20, 21], it is marred with problems; for instance, it predicts a non-ergodic transition which is not observed in experiments [15, 22], or its critical density \( \phi_{\text{MCT}} = 0.516 \) [23] is far below the glass transition density, which is observed to be \( \phi_g \approx 0.58 - 0.60 \) in numerical simulations [24, 25, 26, 27].

Despite these problems, it is still tempting to extend MCT to granular materials, because it might be the simplest method to include correlations. In MCT, these correlations are encoded in a memory kernel, which is absent in the kinetic theory. The extension of MCT to randomly driven granular systems has been proposed and analyzed [28, 29, 30]. However, the physics of sheared flows is completely distinct from random driving cases, and its study has to be addressed independently. Indeed, the characteristic plateau in the density correlation function for both glassy and randomly driven granular systems does not exist in sheared granular liquids [31, 32, 33]. The extension of MCT to sheared granular liquids can be traced back to Ref. [34], and an explicit calculation of time correlation functions has been reported in Ref. [35] without considering an energy balance condition. However, the problem of rheology and the characterization of the steady state have not been addressed so far. In this article, we demonstrate that the extended MCT reproduces the results of molecular dynamics (MD) simulations for the relaxation of time correlation functions and the density dependence of the shear viscosity.

The organization of this paper is as follows. We first explain the microscopic set up of the theory, in particular the Liouville equation and the steady-state condition. Then we derive the mode-coupling equations, without specifying the initial distribution function. We perform a concrete calculation for the case of a canonical initial distribution and evaluate the validity of the results. Finally, we discuss the problem of the formulation and the possibilities of its amendment.
MICROSCOPIC SETUP

Equations of motion

The starting point of our theory is an assembly of $N$ identical soft, smooth, inelastic spheres with the mass $m$ and the diameter $d$, contained in a box of the volume $V$. Thus, the number density is given by $n = N/V$. The interaction between the spheres are elastic as well as inelastic (dissipative), both of which are repulsive and emerge at contact. The system is subjected to a bulk shearing, which is uniform and constant with shear rate $\dot{\gamma}$. At first the system is equilibrated without shear and dissipation. Then, at $t = t_0$, shear is switched on, which eventually leads the system to a nonequilibrium steady state. The Newtonian equation of motion, Eqs. (1) and (2), to the form of the Liouville equation.

$$\begin{align*}
\dot{r}_i(t) &= \frac{p_i(t)}{m} + \dot{\gamma} \cdot r_i(t), \quad (1) \\
\dot{p}_i(t) &= F_i^{(el)}(t) + F_i^{(vis)}(t) - \dot{\gamma} \cdot p_i(t). \quad (2)
\end{align*}$$

Here, $\Gamma(t) = \{r_i(t), p_i(t)\}_{i=1}^N$ is a set of the positions and the momenta of all the grains at time $t$. $\dot{\gamma}$ is the shear rate tensor whose components are assumed to be given by $\dot{\gamma}_{\mu\nu} = \gamma \delta_{\mu\nu}$. $F_i^{(el)}(t)$, $F_i^{(vis)}(t)$ are the elastic and dissipative interactions, respectively. The Greek indices $\mu, \nu, \lambda, \cdots$ denote spatial components $\{x, y, z\}$, and the rule for the summation over repeated indices is implied. Here, the elastic force is given by $F_i^{(el)}(t) = -\sum_{j \neq i} \Theta(d - r_{ij}(t)) \partial u(r_{ij}(t)) / \partial r_{ij}(t)$, where $r_{ij}(t) = r_i(t) - r_j(t)$ and $r_{ij}(t) = |r_{ij}(t)|$ are, respectively, the relative position and distance between the $i$th and $j$th spheres. $u(r)$ is the two-body potential, and $\Theta(x)$ is a step function which is 1 for $x > 0$ and 0 for otherwise. Although a realistic potential might be Hertzian, it is assumed to be harmonic for simplicity. The dissipative force is given by $F_i^{(vis)}(t) = -\zeta \sum_{j \neq i} \Theta(d - r_{ij}) r_{ij} \cdot \dot{r}_{ij}$, where $\mathbf{r} \equiv r / |r|$ is a unit vector and $\zeta$ is a viscous constant corresponding to the harmonic potential.

Liouville equation

To formulate a theory, we rewrite the equations of motion, Eqs. (1) and (2), to the form of the Liouville equation [36]. In this formulation, the equation of motion for an arbitrary phase-space variable $A(\Gamma(t))$ is casted in the form

$$\frac{d}{dt} A(\Gamma(t)) = i\mathcal{L}(\Gamma)A(\Gamma(t)),$$

where $i\mathcal{L}(\Gamma)$ is referred to as the Liouvilian. The explicit form of $i\mathcal{L}(\Gamma)$ for Eqs. (1) and (2) is given by

$$i\mathcal{L}(\Gamma) = i\mathcal{L}_e^{(el)}(\Gamma) + i\mathcal{L}_s^{(vis)}(\Gamma),$$

where the elastic part $i\mathcal{L}_e^{(el)}(\Gamma)$, the shear part $i\mathcal{L}_s^{(vis)}(\Gamma)$, and the viscous part $i\mathcal{L}_s^{(vis)}(\Gamma)$ are given by

$$\begin{align*}
i\mathcal{L}_e^{(el)}(\Gamma) &= \sum_{i=1}^N \left[ \frac{p_i}{m} \cdot \frac{\partial}{\partial r_i} + F_i^{(el)}(t) \cdot \frac{\partial}{\partial p_i} \right], \quad (5) \\
i\mathcal{L}_s^{(vis)}(\Gamma) &= \sum_{i=1}^N \left[ (\mathbf{\gamma} \cdot \mathbf{r}_i) \cdot \frac{\partial}{\partial r_i} - (\mathbf{\gamma} \cdot p_i) \cdot \frac{\partial}{\partial p_i} \right], \quad (6) \\
i\mathcal{L}_s^{(vis)}(\Gamma) &= \sum_{i=1}^N F_i^{(vis)}(t) \cdot \frac{\partial}{\partial p_i}. \quad (7)
\end{align*}$$

On the other hand, the equation for the phase-space distribution function $\rho(\Gamma, t)$ reads

$$\frac{\partial}{\partial t} \rho(\Gamma, t) = -i\mathcal{L}^\dagger(\Gamma),$$

where the adjoint Liouvillian $i\mathcal{L}^\dagger(\Gamma)$ is defined as

$$i\mathcal{L}^\dagger(\Gamma) = i\mathcal{L}(\Gamma) + \Lambda(\Gamma),$$

together with the phase-space contraction factor,

$$\Lambda(\Gamma) = \frac{\partial}{\partial \Gamma} \cdot \dot{\Gamma} = -\frac{\zeta}{m} \sum_{i<j} \Theta(d - r_{ij}) < 0.$$

Here, we denote $\sum_{i,j}^N$ as $\sum_{i \neq j} \cdots$. The formal solution of Eqs. (3) and (8) are given by

$$\begin{align*}
\Lambda(\Gamma(0)) &= e^{t\mathcal{L}^\dagger} \Lambda(\Gamma(0)), \quad (11) \\
\rho(\Gamma, t) &= e^{-t\mathcal{L}} \rho(\Gamma, 0). \quad (12)
\end{align*}$$

To proceed, it is convenient to rewrite Eq. (12), by use of an identity [36], as

$$\rho(\Gamma, t) = \rho_{mi}(\Gamma) + \int_0^t ds e^{-i\mathcal{L}^\dagger s} \rho_{mi}(\Gamma),$$

where $\rho_{mi}(\Gamma) = \rho(\Gamma, 0)$ is the initial distribution function. Then, we can introduce the nonequilibrium work function, $\Omega(\Gamma)$, as the eigenvalue of of $i\mathcal{L}^\dagger$:

$$i\mathcal{L}^\dagger \rho_{mi}(\Gamma) = -\rho_{mi}(\Gamma) \Omega(\Gamma), \quad (14)$$

from which we obtain

$$\rho(\Gamma, t) = \rho_{mi}(\Gamma) + \int_0^t ds e^{-i\mathcal{L}^\dagger s} [\rho_{mi}(\Gamma) \Omega(\Gamma)]. \quad (15)$$

Note that $\Omega(\Gamma)$ includes the nonequilibrium information of the dynamics of the system because of the balance
between shearing and dissipation. In the remainder, we denote the ensemble average with respect to \( \rho_{mi}(\Gamma) \) by
\[
\langle \cdots \rangle = \int d\Gamma \rho_{mi}(\Gamma) \cdots
\] (16)

The nonequilibrium ensemble average of a phase-space variable \( A(\Gamma(t)) \), which we denote \( \langle A(t) \rangle \), can be expressed as
\[
\langle A(t) \rangle = \int d\Gamma \rho_{mi}(\Gamma) A(\Gamma(t)) = \int d\Gamma \rho(\Gamma,t) A(\Gamma(0)).
\] (17)

The equivalence of the two expressions can be shown by the adjoint relation of the Liouvillians [36]. From Eqs. (15), (17), and the adjoint relation, we obtain
\[
\langle A(\Gamma(t)) \rangle = \langle A(0) \rangle + \int_0^t ds \langle A(s) \Omega(0) \rangle,
\] which is referred to as the generalized Green-Kubo formula [37]. The steady-state average, \( A_{\infty} \), is obtained from this formula as
\[
A_{\infty} = \langle A(0) \rangle + \int_0^\infty ds \langle A(s) \Omega(0) \rangle. \tag{19}
\]

**Steady-state condition**

The steady state of a sheared granular flow is characterized by the balance of energy. The internal energy \( H_0(\Gamma) \) is given
\[
H_0(\Gamma) = \sum_{i=1}^N \left[ \frac{p_i^2}{2m} + \sum_{j \neq i} u(r_{ij}) \right]. \tag{20}
\]
The following equality can be shown from Eqs. (1) and (2),
\[
H_0(\Gamma) = -\gamma \sigma_{xy}(\Gamma) - 2\mathcal{R}(\Gamma), \tag{21}
\]
where
\[
\sigma_{xy}(\Gamma) = \frac{1}{V} \sum_{i=1}^N \left[ \frac{p_{ix}^2}{m} + r_{ij} F_i^x \right]
\] (22)
is the shear stress and
\[
\mathcal{R}(\Gamma) = -\frac{1}{4} \sum_{i,j} \hat{r}_{ij} \cdot F_{ij}^{(vis)} = \frac{1}{4V} \sum_{i,j} \Theta(d-r_{ij}) \langle \hat{r}_{ij} \cdot \hat{r}_{ij} \rangle
\] (23)
is the Rayleigh’s dissipation function. We can see from Eq. (21) that the steady state is characterized by the condition,
\[
\gamma \sigma_{xy} + 2\mathcal{R}_{\infty} = 0, \tag{24}
\]
where the steady-state values \( (\sigma_{xy})_{\infty} \) and \( \mathcal{R}_{\infty} \) can be evaluated by Eq. (19). Equation (24) implies the balance between the heating due to shear and the cooling due to dissipation. As will be discussed later, the time evolution of the temperature is not included in Eq. (24) in our MCT, and hence it will be imposed as a condition which determines the steady-state temperature.

**SHEARED GRANULAR MCT**

So far the formulation is exact but not solvable. To obtain a calculable theory for the low-frequency modes, Mori equations are approximated by MCT to derive a closed set of equations. MCT is also applied to the generalized Green-Kubo formula to discuss the stress formula. First we briefly review the essence of this procedure [35].

**MCT equations**

We identify the density and the current density fluctuations, which are \( n_q \equiv \sum_{i=1}^N e^{iq \cdot r^i} - N \delta_{q0} \) and \( j_q^\lambda \equiv \sum_{i=1}^N (p_{iq}^\lambda / m) e^{iq \cdot r^i} \) in Fourier space, as the slow modes. Fluid dynamics implies that the temperature fluctuation should also be considered on the same grounds as \( n_q \) and \( j_q^\lambda \). However, we attempt to formulate a theory without the temperature fluctuation, since otherwise it will be too complicated and almost untrackable. How to compensate the dynamics of the temperature will be discussed below.

The Mori equations for \( n_q \) and \( j_q^\lambda \) are obtained by applying the projection operator
\[
\mathcal{P}(t)X = \sum_k \frac{\langle X n_k(t) \rangle}{NS_k} n_k(t) + \sum_k \frac{\langle X j_k(t) \rangle}{Nv_k^2} j_k(t), \tag{25}
\]
where \( X(\Gamma) \) is an arbitrary phase-space variable. Here, \( S_k = \langle n_k n_k^* \rangle / N \) is the static structure factor, \( v_k^2 = \langle j_k^\lambda j_k^\lambda \rangle / (3N) \) is the equal-time correlation of the current, and \( k(t) \equiv (k_x, k_y - \gamma k_z, k_z) \) is the wave vector in the sheared frame. Note that \( \langle \cdots \rangle \) denotes the ensemble average with respect to the initial distribution function, Eq. (16). The orthogonality of \( n_k \) and \( j_k^\lambda \), i.e. \( \langle n_k j_k^\lambda \rangle = 0 \), is necessary for the idempotency, \( \mathcal{P}(t)^2 = \mathcal{P}(t) \). We assume that \( \rho_{mi}(\Gamma) \) is even with respect to the momentum, which is sufficient for \( \langle n_k j_k^\lambda \rangle = 0 \). Then, to obtain a closure for these equations, the second projection operator
\[
\mathcal{P}_{mc}(t) = \mathcal{P}_{mi}(t) + \mathcal{P}_{nj}(t), \tag{26}
\]
where
\[
\mathcal{P}_{mi}(t) = \sum_{k \neq p} \frac{\langle X n_k(t) n_p(t) \rangle}{N^2 S_k S_p} n_k(t) n_p(t), \tag{27}
\]
\[ \mathcal{P}_{ij}(t) = \sum_{k,p} \frac{\langle X n_{k(t)}^* \mu^i_{p(t)} \rangle}{N^2 S_{k(t)} V_T^2} \cdot j_{k(t)}^i \cdot j_{p(t)}^j, \]  

(28)

is applied to the memory kernels, which, together with the factorization approximation, expresses them in terms of four time correlation functions, \( \Phi_q(t) \equiv \langle \eta_q(t) \eta_q(0)^* \rangle / N \), \( H_q^2(t) \equiv i \langle \dot{q}_q(t) \eta_q(0)^* \rangle / N \), \( \dot{H}_q^2(t) \equiv i \langle \eta_q(t) \dot{q}_q(0)^* \rangle / N \), and \( C_q^{\mu\nu}(t) \equiv \langle \dot{q}_q(t) \dot{q}_q(0)^* \rangle / N \). However, we might expect that anisotropic effects are subdominant, considering that sheared colloidal systems are almost isotropic \([38, 39]\). Hence, we resort to the isotropic approximation, and reduce the time correlation functions to two scalar functions, \( \Phi_q(t) \) and \( \Psi_q(t) \), which depend only on the modulus of the wave vector, \( q \equiv |q| \). Here, \( \Psi_q(t) \) is introduced by the definition \( \dot{H}_q^2(t) \equiv -q^2(t) \Psi_q(t) \), and hence is essentially the density-current correlation. These two functions are related to the remaining two by the relations \( H_q^2(t) \approx |q^2(t)/q(t)^2| \cdot \dot{\Phi}_q(t) \) and \( C_q^{\mu\nu}(t) \approx \delta^{\mu\nu} \cdot \{ \frac{d}{dt} \Psi_q(t) + \frac{1}{2} [\Psi_q(t)/q(t)^2] \cdot \frac{d}{dt} q(t)^2 \} \). It should be noted that, while \( H_q^2(t) \) is obtained by the time derivative of \( \Phi_q(t) \), \( \dot{H}_q^2(t) \) cannot be derived from \( \Phi_q(t) \); i.e., the minimal set of time correlation functions is \( \{ \Phi_q, \Psi_q \} \). Then, the MCT equations for \( \Phi_q(t) \) and \( \Psi_q(t) \) read

\[
\frac{d^2}{dt^2} \Phi_q(t) = -Z_q(t) \Phi_q(t) - A_q(t) \frac{d}{dt} \Phi_q(t) + \int_0^t ds M_q(s)(t-s) \frac{d}{ds} \Phi_q(s),
\]

(29)

\[
\frac{d^2}{dt^2} \Psi_q(t) = -\frac{1}{3} Z_q(t) \Psi_q(t) - \frac{1}{3} A_q^{\lambda\lambda}(t) \frac{d}{dt} \Psi_q(t) - \frac{1}{3} \int_0^t ds M_q^{\lambda\lambda}(s)(t-s) \frac{d}{ds} \Psi_q(s),
\]

(30)

where the memory kernels \( M_q(t) \) and \( M_q^{\lambda\lambda}(t) \) are quadratic forms in terms of the time correlation functions. The coefficients \( Z_q, A_q, A_q^{\lambda\lambda} \) and the coefficients of the quadratic forms in the memory kernels are equal-time correlations, which originate from the projection operators. Hence, their explicit forms depend on the choice of \( \rho_{\text{ini}}(\Gamma) \), which we will discuss later. We simply note here that the memory kernels consist of elastic and dissipative terms. For instance, \( M_q(t) \) has the following form,

\[
M_q(t) = M_q^{(\text{el})}(t) + \frac{\zeta}{m\gamma} M_q^{(\text{vis})}(t),
\]

(31)

where \( M_q^{(\text{el})}(t) \) is the conventional term which induces the glass transition for sheared non-dissipative particles \([40]\), and \( M_q^{(\text{vis})}(t) \) represents the dissipative terms. These features also hold for the kernel \( M_q^{(d)}(t) \). It is significant that the dissipative kernels have negative contributions and are possible to suppress the glassy elastic term. The intuitive picture of this effect will be discussed below.

Accordingly, the second projection operator \( \mathcal{P}_{mc}(t) \) is applied to the time correlation \( \langle A(s) \Omega(0) \rangle \) in Eq. (19), which, together with the factorization approximation, expresses it as a quadratic form of the time correlation functions. Again, the explicit forms of the steady-state formulas for \( \sigma_{xy} \) and \( \mathcal{R} \) depend on \( \rho_{\text{ini}}(\Gamma) \), but exhibit the following forms in general,

\[
\langle \sigma_{xy} \rangle_{SS} = \langle \sigma_{xy}^{(el)} \rangle_{SS} + \frac{\zeta}{m\gamma} (\sigma_{xy}^{(vis)})_{SS},
\]

(32)

\[
\mathcal{R}_{SS} = \frac{\zeta}{m\gamma} \left[ \mathcal{R}^{(loc)}_{SS} + \Delta \mathcal{R}_{SS} \right].
\]

(33)

Here, \( (\sigma_{xy}^{(el)})_{SS} \) and \( (\sigma_{xy}^{(vis)})_{SS} / (m\gamma) \) are the elastic and the dissipative components of the shear stress, and \( \mathcal{R}^{(loc)}_{SS} \) and \( \Delta \mathcal{R}_{SS} \) are the local and the non-local contributions, which correspond to the first and the second terms of Eq. (19), respectively.

### Canonical initial distribution

To proceed to explicit calculations, it is necessary to specify the initial distribution function, \( \rho_{\text{ini}}(\Gamma) \). We consider the following form of \( \rho_{\text{ini}}(\Gamma) \),

\[
\rho_{\text{ini}}(\Gamma) = \frac{e^{-I(\Gamma)}}{\int d\Gamma e^{-I(\Gamma)}},
\]

(34)

where \( I(\Gamma) \) is the effective potential. Then, from Eq. (14), the work function \( \Omega(\Gamma) \) is expressed as

\[
\Omega(\Gamma) = i \mathcal{L}(\Gamma) I(\Gamma) - \Lambda(\Gamma) = I(\Gamma) - \Lambda(\Gamma).
\]

(35)

The most naive choice of \( I(\Gamma) \) is

\[
I(\Gamma) = \frac{H_0(\Gamma)}{T},
\]

(36)

which corresponds to the canonical initial distribution. In this case, the system is equilibrated at temperature \( T \) at \( t < t_0 = 0 \), and shear and dissipation are switched on at \( t = t_0 = 0 \). In this section, we show the results for the case of canonical initial distribution and discuss its validity.

### Interpretation and determination of the temperature

A simple feature of \( \rho_{\text{ini}}(\Gamma) \) under \( I(\Gamma) \) of Eq. (36) is that the momentum integral in Eq. (16) is a Gaussian and hence can be performed straightforwardly. Then, the
canonical temperature $T$ in Eq. (36) appears in the coefficients of the MCT equations and the memory kernels. This poses a problem, since the dynamics governed by the MCT equations, and hence the steady-state averages, apparently depend on $T$, while it is expected to be independent from physical grounds. The origin of this problem resides in our treatment where the dynamics is projected onto the density and the current density correlations, but not on the temperature fluctuation, and hence the time evolution of the temperature is not included.

To remedy this problem, we identify $T$ with the steady-state temperature, and determine it from the energy balance condition, Eq. (24). As shown below, $T$ appears in the coefficients of the time correlation functions via the projection operators; that is, it appears in MCT equations, Eqs. (29) and (30), as well as in the energy balance condition, Eq. (24). We solve MCT equations iteratively until the temperature $T$ is determined self-consistently with the energy balance condition. The initial conditions for Eqs. (29) and (30) are $\Phi_q(0) = S_q$, $\frac{d}{dt}\Phi_q(0) = 0$ and $\Psi_q(0) = 0$, $\frac{d}{dt}\Psi_q(0) = v_T^2$.

**Explicit expressions**

For the case of the canonical initial distribution, we can explicitly calculate the coefficients $Z_q$, $A_q$, and $A^{\lambda\lambda}_q$ in Eqs. (29), (30), and the coefficients which appear in the memory kernels $M_q(t)$, $M^{\lambda\lambda}_q(t)$ and the steady-state formulas for $\sigma_{xy}$ and $\mathcal{R}$, i.e. Eqs. (32) and (33).

**Coefficients**– The coefficients $Z_q$, $A_q$, and $A^{\lambda\lambda}_q$ are given by

$$Z_q = \frac{v_T^2 q^2}{S_q},$$

$$A_q = \frac{4\pi \zeta_H}{m} \left[ 1 - j_0(qd) + 2j_2(qd) \right],$$

$$A^{\lambda\lambda}_q = \frac{4\pi \zeta_H}{m} \left[ 1 - j_0(qd) \right],$$

where $v_T = \sqrt{T/m}$ is the thermal velocity, $j_j(qd)$ is the spherical Bessel function of the $l$-th order, and

$$\frac{\zeta_H}{m} = 4\sqrt{\pi} \left( 1 - \epsilon^2 \right) c(d)n^2 \sqrt{\frac{T}{m}}$$

is the effective frequency of the dissipation in the hard-core limit. Here, $\epsilon$ is the normal restitution coefficient, and $g(d)$ is the contact value of the equilibrium radial distribution function. We take this limit because we address the rheology below the jamming point.

**Memory kernels**– The memory kernel for $\Phi_q(t)$, $M_q(t)$, is given up to linear order in $\zeta/(m\gamma)$ by

$$M_q(t) = M^{(el)}_q(t) + \frac{\zeta}{m\gamma} \sum_{i=1}^2 M^{(vis)i}_q(t),$$

where $M^{(el)}_q(t)$, $M^{(vis)}_q(t)$, and $M^{(vis2)}_q(t)$ are given by

$$M^{(el)}_q(t) = \frac{nv_T^2}{32\pi^2 q^2} \int_0^\infty dk \int_{|q-k|}^{q+k} dp \left[ \Phi_q(t) \Phi_p(t) \right],$$

$$M^{(vis)}_q(t) = \frac{\gamma}{4\pi mq^2} \int_0^\infty dk \int_{|q-k|}^{q+k} dp \left[ \Phi_q(t) \Phi_p(t) \right] \times \left[ \Phi_q(t) \alpha(t) \beta(t) V^{(el)}_M(k, p) \right],$$

$$M^{(vis2)}_q(t) = \frac{\gamma}{4\pi mq^2} \int_0^\infty dk \int_{|q-k|}^{q+k} dp \left[ \Phi_q(t) \Phi_p(t) \right] \times \left[ \Phi_q(t) \alpha(t) \beta(t) V^{(el)}_M(k, p) \right] \times \left[ \Phi_q(t) \alpha(t) \beta(t) \right],$$

Here, $\tilde{k}(t) = \hat{k}(t)$ with $h(x) = \sqrt{1 + x^2/3}$ is the modulus of the advected wavevector in the isotropic approximation, and the vertex functions are given by

$$V^{(el)}_M(k, p) = c_k \left( q^2 + k^2 - p^2 \right) + c_p \left( q^2 + p^2 - k^2 \right),$$

$$V^{(vis)}_M(k, p, \alpha, \beta) = \frac{1}{2} \sin \alpha \sin(\alpha + \beta) \cdot ml^{(1)}(k)$$

$$\times \left[ \cos \alpha \cos(\alpha + \beta) - \frac{1}{2} \sin \alpha \sin(\alpha + \beta) \right] \cdot ml^{(2)}(k)$$

$$- \cos \beta \cdot ml^{(2)}(p),$$

where $l^{(1)}(q) = 2 [1 - j_0(qd)]$ and $l^{(2)}(q) = \frac{q}{3} [1 - j_0(qd) + 2j_2(qd)]$, and the angles $\alpha$, $\beta$ are defined by $\cos \alpha = \left( q^2 + k^2 - p^2 \right)/(2qk)$, $\cos \beta = \left( q^2 + p^2 - k^2 \right)/(2qp)$. Note that $V^{(el)}_M(k, p)$ is the vertex function of the equilibrium MCT [14]. Note also that $\Psi_q(t)$ couples to the MCT equation of $\Phi_q(t)$, Eq. (29), only via $M^{(vis2)}_q(t)$, so $\Psi_q(t)$ decouples from $\Phi_q(t)$ in the limit $\zeta \rightarrow 0$. Hence, our theory reduces to the sheared MCT of thermal glassy systems in the limit $\zeta \rightarrow 0$, together with appropriate thermostats, e.g. Gaussian Isokinetic thermostat, which controls the temperature.

Similarly, the memory kernel $M^{\lambda\lambda}_q(t)$ is given up to linear order in $\zeta/(m\gamma)$ by

$$M^{\lambda\lambda}_q(t) = M^{(el)\lambda\lambda}_q(t) + \frac{\zeta}{m\gamma} \sum_{i=1}^2 M^{(vis)i\lambda\lambda}_q(t),$$

where $M^{(el)\lambda\lambda}_q(t)$, $M^{(vis)1\lambda\lambda}_q(t)$, and $M^{(vis2)\lambda\lambda}_q(t)$ are

$$M^{(el)\lambda\lambda}_q(t) = \frac{m v_T^2}{8\pi^2 q^2} \int_0^\infty dk \int_{|q-k|}^{q+k} dp \left[ \Phi_q(t) \Psi_p(t) \right] \times \left[ \Phi_q(t) \alpha(t) \beta(t) \right],$$

$$M^{(vis)1\lambda\lambda}_q(t) = \frac{\gamma}{2\pi mq} \int_0^\infty dk \int_{|q-k|}^{q+k} dp \left[ \Phi_q(t) \Psi_p(t) \right] \times \left[ \Phi_q(t) \alpha(t) \beta(t) \right] \times \left[ \Phi_q(t) \alpha(t) \beta(t) \right],$$

$$M^{(vis2)\lambda\lambda}_q(t) = \frac{\gamma}{4\pi mq^2} \int_0^\infty dk \int_{|q-k|}^{q+k} dp \left[ \Phi_q(t) \Psi_p(t) \right] \times \left[ \Phi_q(t) \alpha(t) \beta(t) \right] \times \left[ \Phi_q(t) \alpha(t) \beta(t) \right]$$
\[ M_q^{(vis2)}(\lambda) (t) = -\frac{\dot{\gamma}}{2\pi m q} \int_0^\infty \int_{q-k}^{q+k} dk \frac{dp}{p^2} \times \left\{ k c_k \sigma^{(vis1)}(k, p, \alpha, \beta) + p c_{\rho(t)} \right\} \]

\[ W^{(vis2)}(k, p, \alpha, \beta) = \frac{1}{2} \sin^2(\alpha + \beta) \cdot ml^{(1)}(k) + \frac{3}{2} \cos^2(\alpha + \beta) \cdot ml^{(2)}(k) - ml^{(2)}(p), \]

\[ W^{(vis3)}(k, \alpha, \beta) = \frac{1}{2} \sin^2(\alpha + \beta) \cdot ml^{(1)}(k) - ml^{(2)}(k) . \]

Note that \( M_q^{(vis2)}(\lambda) \) is the purely dissipative contribution which exists even in the absence of shear, among which \( \Delta \mathcal{R}(\Gamma) \) is the contribution from the energy dissipation due to inelastic collisions.

The steady-state shear stress reads

\[ (\sigma_{xy})_{SS} = (\sigma_{xy}^{(el)})_{SS} + \frac{\zeta_{ld}}{m \gamma} \sum_{i=1}^{N} (\sigma_{xy}^{(vis)})_{SS} , \]

where \( (\sigma_{xy}^{(el)})_{SS} \), \( (\sigma_{xy}^{(vis)})_{SS} \), and \( (\sigma_{xy}^{(vis2)})_{SS} \) are given by

\[ (\sigma_{xy}^{(el)})_{SS} = \frac{\gamma T}{60 \pi^2} \int_0^\infty \frac{dt}{h(\gamma t)} \int_0^\infty dk \frac{k^4}{k} \times V_{\sigma}^{(el)}(k(t)) V_{\sigma}^{(el)}(k(t))^2 , \]

\[ (\sigma_{xy}^{(vis)})_{SS} = -\frac{\gamma^2}{60 \pi^2} \int_0^\infty \frac{dt}{h(\gamma t)^3} \int_0^\infty dk \frac{k^4}{k} \times V_{\sigma}^{(vis)}(k(t)) V_{\sigma}^{(vis)}(k(t)) \frac{d}{dt} \Phi_k(t) , \]

\[ (\sigma_{xy}^{(vis2)})_{SS} = -\frac{\gamma^2}{60 \pi^2} \int_0^\infty \frac{dt}{h(\gamma t)} \int_0^\infty dk \frac{k^4}{k} \times V_{\sigma}^{(vis2)}(k(t)) V_{\sigma}^{(vis2)}(k(t)) \Phi_k(t) \Psi_k(t) . \]

The vertex functions \( V_{\sigma}^{(el)}(q) \) and \( V_{\sigma}^{(vis)}(q) \) are given by

\[ V_{\sigma}^{(el)}(q) = \frac{1}{S_q} \frac{\partial }{\partial q} \ln S_q , \]

\[ V_{\sigma}^{(vis)}(q) = -\frac{1}{m} \left[ I_1^{(el)}(q) - 3 I_2^{(el)}(q) \right] , \]

\[ I_1^{(el)}(q) = 2 d j_1(qd) , \]

\[ I_2^{(el)}(q) = \frac{4}{5} d \left[ \frac{3}{2} j_3(qd) - j_3(qd) \right] . \]

Note that \( (\sigma_{xy}^{(el)})_{SS} \), Eq. (62), is coincident to the steady-state shear stress in the sheared MCT of thermal glassy systems [41, 38].

The steady-state energy dissipation rate is given by

\[ \dot{\mathcal{R}}_{SS} = \frac{\zeta_{ld}}{m \gamma} \left[ \dot{\mathcal{R}}_{SS}^{(loc)} + \sum_{i=1}^{3} \dot{\mathcal{R}}_{SS}^{(i)} \right] , \]

where \( \dot{\mathcal{R}}_{SS}^{(loc)} \) is the local contribution,

\[ \dot{\mathcal{R}}_{SS}^{(loc)} = \frac{1}{2} \gamma g(d) N d^3 T , \]

and \( \dot{\mathcal{R}}_{SS}^{(i)} (i = 1, 2, 3) \) are the non-local contributions,

\[ \dot{\mathcal{R}}_{SS}^{(i)} = \frac{\gamma^2 T}{60 \pi^2} \int_0^\infty \frac{dt}{h(\gamma t)} \int_0^\infty dk \frac{k^4}{k} \times \frac{1}{2} \left[ I_1^{(el)}(k) V_{\sigma}^{(el)}(k(t)) \Phi_k(t) \right]^2 , \]
the physical contents are quite different. However, Eq. (70) is formally coincident to the kinetic theory wave number given by Eqs. (65), (66), and (67). Note that the vertex functions are consistent with the results of MD reported previously [31, 32, 33]. The result of MD for the density-current correlation is multiplied by a factor 30 to be comparable with the results of MCT in a single figure.

\[
\mathcal{R}_{SS}^{(2)} = -\frac{\gamma^3}{30\pi^2} \int_0^\infty \frac{dt}{h(\gamma t)^3} \int_0^\infty dk k^2 \\
\times V_{\sigma}^{(vis)}(\bar{k}(t)) V_{\bar{\sigma}}^{(el)}(k) \Phi_k(t) \frac{d}{dt} \Phi_k(t),
\]

\[
\mathcal{R}_{SS}^{(3)} = \frac{\gamma^3}{3\pi^2} \int_0^\infty dt \frac{\gamma}{h(\gamma t)} \int_0^\infty dk k^4 \\
\times \frac{1}{2} I_{\sigma}^{(1)}(k) V_{\sigma}^{(vis)}(\bar{k}(t)) \Phi_k(t) \Psi_{\bar{k}(t)}(t).
\]

The vertex functions \( V_{\sigma}^{(el)}(q) \), \( V_{\sigma}^{(vis)}(q) \), and \( I_{\sigma}^{(1)}(q) \) are given by Eqs. (65), (66), and (67). Note that \( \mathcal{R}_{SS}^{(loc)} \), Eq. (70), is formally coincident to the kinetic theory expression of the energy dissipation rate [7]. However, the physical contents are quite different.

**Numerical calculations**

In our calculation of MCT, the unit of mass, length, and time are chosen as \( m, d, \) and \( \dot{\gamma} \). The inputs necessary for the calculation are \( S_q \) and \( g(d) \), both at equilibrium. We adopt for \( S_q \) the Percus-Yevick solution for the hard spheres [42] (\( \varphi \leq 0.52 \)) and the numerical results from the MD simulation (\( \varphi > 0.52 \)), \( S_q \), and \( g(d) \) the interpolation formula valid in the range \( 0.49 < \varphi < 0.64 \) [43].

In order to verify the validity of our theory, we also perform MD simulations of the Slloq equations for soft spheres, Eqs. (1) and (2), under the Lees-Edwards boundary condition [36]. The equations are integrated by the Verlet algorithm. The conditions are: the time step \( \Delta t = 0.01\sqrt{m/\kappa} \), where \( \kappa \) is the spring constant, the number of particles \( N = 2000 \), and the dimensionless shear rate \( \dot{\gamma} \sqrt{m/\kappa} = 1.0 \times 10^{-4} \). The values of \( \zeta \) are determined by \( \kappa \) and \( e \). The results are averaged from 10 independent samples.

**Time correlation functions**– The left (right) figure of Fig. 1 is the relaxation of the density-density (density-current) time correlation function \( \Phi_q(t) \) (\( \Psi_q(t) \)). Refer to the caption for the conditions. The result of MCT for \( \Phi_q(t) \) shows a clear two-step relaxation in the nearly elastic cases (\( e = 0.99, 0.98 \)), while it cannot be seen for the dissipative cases (\( e = 0.94, 0.92 \)). This is qualitatively consistent with the result of the MD simulations, though the plateau is suppressed even for \( e = 0.999 \) in MD. Note that our results for MCT and MD which exhibit no plateau in \( \Phi_q(t) \) are consistent with the results of MD reported previously [31, 32, 33]. The result of MCT for \( \Psi_q(t) \) shows a clear peak and a shoulder for the dissipative cases, while it has only a peak in short time scales for the nearly elastic cases. This is again qualitatively consistent with MD, though the amplitude of MD is much smaller than that of MCT. It is interesting to note that a plateau or a shoulder appears complementarily in \( \Phi_q(t) \) and \( \Psi_q(t) \). This is an evidence of the significant role of \( \Psi_q(t) \) in sheared granular liquids. From this result, we can derive the following intuitive picture when the dissipation is significant. The spheres lose density correlations because they cease to collide with the surrounding caging spheres at the time scale \( \sim m/\zeta H \) due to inelasticity. On the other hand, the spheres "meme" the information of the current at the onset of shearing and inelastic collisions, since they lose the kinetic energy more rapidly when they interact with currents which have larger relative velocity. The spheres become crowded where the dissipation rate is large, which results

![FIGURE 1. The relaxation of the time correlation functions. The left (right) figure is for the density-density (density-current) time correlation function \( \Phi_q(t) (\Psi_q(t)) \). The results of MCT for \( \varphi = 0.52 \) and \( e = 0.99, 0.98, 0.94, 0.92 \) are shown in thick solid, broken, dashed, and thin solid lines. The results of MD for \( \varphi = 0.63 \) and \( e = 0.9999, 0.999 \) are shown in triangles and diamonds. The wave number \( qd = 7.4 \) is chosen for both MCT and MD, which corresponds to the first peak of the static structure factor measured in MD. The results of MD for the density-current correlation \( \Psi_q(t) \) is multiplied by a factor 30 to be comparable with the results of MCT in a single figure.](image-url)

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in a density fluctuation; i.e., the density fluctuation is correlated with the initial current, even at the time scales of slow motions. This correlation is eventually destroyed by shearing at the time scale $\sim \gamma^{-1} > m/\zeta_{H}$. In contrast, for elastic or driven cases, the information of the initial current is lost and no density fluctuation is generated.

Shear viscosity—The density dependence of the shear viscosity $\eta = \sigma_{xy}/\dot{\gamma}$ is shown in Fig. 2. In this figure, we also plot the result of MD for hard spheres [12]. We find a remarkable agreement between MCT and MD for $\varphi < 0.60$ by renormalizing the density in MCT as $\varphi \rightarrow \varphi_{\text{eff}} = \varphi + \Delta \varphi$ with $\Delta \varphi = 0.11$. This leads to the renormalized MCT transition density, $\varphi_{\text{MCT,eff}} = \varphi_{\text{MCT}} + \Delta \varphi \simeq 0.626$. Although this value is higher than the glass transition density, $\varphi_{g} \simeq 0.58 - 0.60$, it is close to the renormalized density 0.62, which is determined to explain the result of the simulations for colloidal hard-sphere dispersions by MCT, for both the long-time self-diffusion coefficient [44, 45, 46] and the shear viscosity [47]. The results of MCT approximately scales as $\eta \propto (\varphi_{i} - \varphi_{\text{eff}})^{-\alpha}$ for $\varphi_{\text{eff}} < 0.60$, where a cross-over from $\alpha = 3$ to 1 can be observed as reported in Ref. [48], depending on the choice of $\varphi_{i}$. However, for $\varphi_{\text{eff}} > 0.60$, $\alpha$ becomes smaller and MCT fails to reproduce the divergence observed in MD. In fact, the result of MD shows a cross-over at $\varphi \simeq 0.60$ to a stronger divergence as $\varphi \rightarrow \varphi_{i}$. Comparison with the related works on the cross-over of the exponent from 1 to 4 for 2D disks [49] and understanding the cross-over itself is a future task. The divergent feature for $\varphi \rightarrow \varphi_{i}$ is expected to originate in the contact network of the spheres, which is not considered in the present MCT. Hence, it is reasonable to find a discrepancy between MCT and MD in the vicinity of the jamming point.

Temperature—The density dependence of the temperature is shown in Fig. 3, together with the granular temperature measured in MD. The results of MCT show monotonically increasing tendency up to $\varphi \simeq 0.58 - 0.59$ in accordance with MD, although the magnitudes are approximately twice larger. However, qualitative discrepancies are found around $\varphi \simeq 0.58 - 0.59$; peculiar peaks appear, and $T$ decreases in denser regions. This indicates that there is difficulty in identifying $T$ as the steady-state granular temperature in this framework.

DISCUSSIONS

Problem of canonical initial distribution

First we discuss the problem of the canonical initial distribution. From the result of the temperature shown in Fig. 3, we can infer that the correct balance between the shearing and the dissipation is not realized in MCT. To inspect in detail, let us observe the steady-state energy dissipation rate $\mathcal{P}_{\text{SS}}$, Eq. (69). While the local contribution $\zeta_{H}\mathcal{P}_{\text{SS}}^{(\text{loc})}/(m\dot{\gamma})$ is independent of $\dot{\gamma}$, the non-local contributions with time integrations, $\zeta_{H}\mathcal{P}_{\text{SS}}^{(i)}/(m\dot{\gamma})$ ($i = 1, 2, 3$), are proportional to $\dot{\gamma}$ or $\dot{\gamma}^{2}$. This indicates that the purely dissipative contribution is absent in $\zeta_{H}\mathcal{P}_{\text{SS}}^{(i)}/(m\dot{\gamma})$ ($i = 1, 2, 3$), which is physically unacceptable, since inelastic collisions are expected to exhibit non-local, as well as local, time correlations.

The origin of this problem can be traced back to the choice of the canonical initial distribution as follows. In MCT, the time correlation $\langle A(t)\Omega(0) \rangle$ in the steady-state formula, Eq. (19), is approximated as

$$\langle A(t)\Omega(0) \rangle \approx \int [\mathcal{P}_{0}(t, 0)\mathcal{P}_{\text{mc}}^{0}(t)A(t)] [\mathcal{P}_{\text{mc}}^{0}(0)\Omega(0)] \, dt,$$

(74)
where $U_{m}(t,0)$ is the time evolution operator in the space orthogonal to the projected space [50], and $P_{mc}^{0}(t)$ is the second projection operator, Eq. (26), restricted to zero-wavevector. The specific feature of the canonical initial distribution is that the purely dissipative contribution in the work function, i.e. $ΔR$ of Eq. (59), is projected out by $P_{mc}^{0}$.

$$P_{mc}^{0}(0)ΔR(0) = 0, \quad (75)$$

which results in

$$⟨A(t)ΔR(0)⟩ = 0. \quad (76)$$

This indicates that the purely dissipative effect is missing in the steady-state formula. This observation leads us to adopt an initial distribution other than the canonical distribution.

In general, it is expected that the steady-state averages are insensitive to the choice of the initial distribution. In fact, it is shown explicitly that this is true for some special cases [51]. However, this feature is violated in the approximate formulation of MCT. This is because MCT is intended to describe long-time dynamics, and sacrifices the accuracy for the description of the initial relaxation. One evidence we have already seen is its dependence on the initial temperature, which appears in the coefficients. Thus, the choice of the initial distribution is crucial in MCT. A basic idea to remedy this problem is to choose the initial distribution which is much closer to the steady-state distribution. To obtain an exact steady-state distribution is of course an extremely difficult task which is out of our scope at present. However, we might be able to speculate a valid distribution.

**Relation to previous works**

Next we discuss the relation of this work and the previous related works. In the former MCTs for thermal sheared glassy systems [41, 52] or randomly driven granular systems [28, 29, 30], only the projection to the pair-density modes, i.e. $P_{nn}$ of Eq. (27), has been included. In fact, we have already shown in Ref. [53] that the effect of the projection to the density-current modes, i.e. $P_{nj}$ of Eq. (28), is negligible in thermal sheared underdamped systems [50]. However, we have figured out that including the correlations to the density-current modes, or, equivalently, considering $Ψ_{Ψ}(t)$ as well is crucial to take into account the dissipation effect for sheared granular liquids. This can be convinced by observing that the dissipative force is proportional to the relative velocity of spheres, and hence dissipation is correlated with current fluctuations.

**Scaling of the shear stress**

As for the scaling of the shear viscosity with the shear rate, we only obtain the Bagnold scaling $η ∝ γ$. This seems to originate from the hard-core limit we have adopted. To reproduce a departure from the Bagnold scaling, which is significant near the jamming transition point, we should take into account the soft-core nature in our theory [48]. More specifically, the soft-core formulation alone might be insufficient, and it might be necessary to further incorporate the information of the contact networks formed between the particles. However, constructing a theory based on the generalized Green-Kubo formula is still promising, because it holds even above the jamming transition point [54].

**CONCLUSION**

We have succeeded in predicting the time correlations and the shear viscosity of dense sheared granular liquids by extending MCT, although the prediction of time correlations requires refinement to improve quantitative accuracy. It has been demonstrated that, in contrast to thermal glassy systems, the density-current correlation plays an essential role. Its validity for $φ > 0.60$ has been verified by comparing it with MD. This scheme is expected to be further extended to higher densities $φ > 0.60$ by incorporating the soft-core nature of the spheres. On the other hand, our theory fails to predict the appropriate tendency of the granular temperature. We have discussed that this problem seems to reside in the choice of the canonical initial distribution. To remedy this problem, it seems to be crucial to adopt a distribution which is expected to be close to the steady-state distribution.

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