Integration through transients for inelastic hard sphere fluids

W. Till Kranz,1,∗Fabian Frahsa,2 Annette Zippelius,3 Matthias Fuchs,2 and Matthias Sperl1,4
1Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany
2Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany
3Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany
4Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany

The Integration Through Transients (ITT) formalism provides a kinetic theory to go beyond the linear response regime of low density and shear rate. Its main advantage is to express observables under shear as expectation values in the quiescent system. Here we show that the quiescent fluid does not have to be in thermal equilibrium. Considering a fluidized granular medium under shear, we introduce a granular ITT formalism (gITT) providing quantitative predictions for the flow curves that reflect the rich phenomenology of granular fluids.

I. INTRODUCTION

Understanding the rheology of granular fluids from a kinetic theory point of view has been of interest from the earliest days of granular physics [1–8]. It has been established that the granular Boltzmann, or Boltzmann-Enskog equation [9, 10] is a useful starting point to understand granular gases at low density [4, 7, 9–12]. Various methods to extract the transport coefficients in linear response, originally developed for molecular gases have been generalized to non-equilibrium granular gases [7, 13–15]. The general understanding is that the Navier-Stokes equations of hydrodynamics (with small modifications [16]) provide a useful description of granular gas flow. Unfortunately, the range of natural phenomena involving flow at low density and infinitesimal perturbations is much smaller for granular media than it is for classical gas flow. Most granular flows occur at both high volume fraction and significant shear rates. Indeed every gravity driven granular flow will start from a granular solid at rest [6, 17, 18] with a packing fraction around the random close packing density of the respective material. Only recently, first proposals to extend granular kinetic theory to relevant densities have appeared [19–23].

Qualitative considerations have shown that the dynamic state diagram characterizing the rheological response of a granular fluid to shear (Fig. [1]) is determined by several timescales [24]. The Newtonian behavior where shear stress $\sigma = \eta \dot{\gamma}$ is linearly related to the shear rate $\dot{\gamma}$ extends to higher densities and shear rates as long as the shear rate is smaller than the intrinsic structural relaxation rate $\tau^{-1}_\alpha$. Beyond that, the shear stress becomes approximately independent of shear rate, indicated by shear thinning behavior. For even higher shear rates, shear heating will become important which appears as shear thickening behavior. Ultimately, Bagnold scaling, $\sigma \sim \dot{\gamma}^2$, holds for the largest shear rates.

For thermalized colloidal dispersions, the Integration Through Transients (ITT) formalism provides a framework to calculate flow curves, i.e., shear stress $\sigma$ as a function of shear rate

∗ till.kranz@dlr.de
FIG. 1. **Protocol H**: Dynamic state diagrams in the plane spanned by shear rate, $\dot{\gamma}$, and packing fraction, $\varphi$, for several values of the coefficient of restitution, $\varepsilon$, as indicated. The effective exponent $R$ quantifying the shear rate dependence of the viscosity, $\eta(\dot{\gamma}) \sim \dot{\gamma}^R$, is color coded.

$\dot{\gamma}$ beyond the linear response regime. In contrast to the low-density, Boltzmann-Enskog approaches, ITT works best around the glass transition density, i.e., in the range $0.5 \lesssim \varphi \lesssim 0.6$ and is therefore especially well suited to describe dense flows. In this contribution we will demonstrate an ITT approach which extend the calculations for thermalized colloidal suspensions to far-from-equilibrium (driven) granular fluids comprised of inelastic hard spheres.

A first generalization of the ITT formalism from the overdamped Brownian dynamics of colloidal suspensions to inertial, Newtonian dynamics has been obtained by Chong and Kim and later updated to the refined formulation of Fuchs and Cates by Suzuki and Hayakawa. In both cases the lack of viscous damping in the inertial description necessitates the explicit introduction of a thermostat. At least for the Gaussian isokinetic thermostat used in the above references, the details of the artificial thermostat explicitly appear in the final results. Suzuki and Hayakawa where the first to propose an ITT calculation for inelastic soft spheres. Unexpectedly they found that no dissipative effects remain after applying the standard ITT approximations. Only after including current correlation functions in addition to the density correlator did they find results that depend on the inelasticity of the particles. The substantially increased complexity due to the additional observables has so far made applications of this approach difficult. On the upside employing dissipative interactions removes the need for an artificial thermostat.

In the following we will show that using inelastic hard spheres, it is much simpler to retain dissipative effects and this allows us to develop a granular ITT formalism that captures the qualitative behavior introduced above. The paper is organized as follows. We will start with a description of the model in Sec. II. In Sec. III we will introduce the microscopic
observables, equations of motion and distribution functions used to formulate the coarse
gained description in Sec. IV. The generalized Green-Kubo relations that form the central
part of the granular ITT formalism (gITT) will be introduced in Sec. V. To evaluate the
Green-Kubo relations, we introduce a suitable equation of motion for the transient correlator
in Sec. VI. In Sec. VII we will present a number of results that can be derived from the
formalism developed here before concluding in Sec. VIII.

II. MODEL

We consider a monodisperse fluid of inelastic smooth hard spheres with diameter \(d\), mass
\(m = 1\), and coefficient of normal restitution \(\varepsilon \in [0, 1]\) \cite{2, 34}. The system is prepared at
a prescribed volume fraction \(\varphi = \pi nd^3 / 6\) where in the thermodynamic limit, the number
of particles \(N \rightarrow \infty\) such that the density, \(n = N/V\), remains finite. Here \(V\) denotes the
volume. To mimic fluidization, each particle \(i\) is subjected to a random driving force \(\xi_i(t)\)
\cite{35, 36} with zero mean, \(\xi_i = 0\), and variance

\[
\overline{\xi_i^\alpha(t)\xi_j^\beta(t')} = 2P_D \delta_{ij} \delta^{\alpha\beta} \delta(t-t'),
\]

where \(P_D\) characterizes the driving power and the Greek superscripts denote the Cartesian
components. To implement the shear, we prescribe a perfectly linear shear profile,
\(u_x(y) = \dot{\gamma} y\), with a fixed shear rate \(\dot{\gamma}\) on the level of the coarse grained flow field \(u(r)\).

It is convenient to use the particle diameter, \(d\), as a length scale and the inverse of
the collision frequency, \(\omega_c^{-1}\), as a time scale. Then the shear rate is given in terms of the
dimensionless Péclet number \(Pe = \dot{\gamma} / \omega_c\).

A. Experimental Protocol

We envisage to describe the following experimental situation: Initially, a monodisperse
granular assembly is homogeneously fluidized at a prescribed packing fraction \(\varphi\) until a
non-equilibrium steady state is reached where the dissipative collisions balance the energy
input due to driving,

\[
P_D = \Gamma \omega_c(T_0)T_0,
\]

and the temperature \(T_0\) becomes constant. Here \(\Gamma(\varepsilon) := (1 - \varepsilon^2)/3\) quantifies the dissipation
\cite{2}. In the following we will refer to this state as the reference system. The reference system
undergoes a glass transition at a critical packing fraction \(\varphi_c(\varepsilon)\) and freezes into an amorphous
solid for densities \(\varphi > \varphi_c\) \cite{31, 37–39}. The collision frequency, \(\omega_c(\varphi, T_0) \propto \sqrt{T_0}\), increases
with temperature and packing fraction \cite{40}.

Starting at time \(t = 0\) the prescribed shear rate \(\dot{\gamma}\) is applied until the fluid reaches a new
stationary state, i.e., we focus on a shear rate controlled protocol at fixed packing fraction.
Shear heating, \(\sigma \dot{\gamma}\), needs to be considered in the power balance which now reads \cite{24}

\[
\sigma \dot{\gamma} + nP_D = n\Gamma \omega_c(T)T.
\]

Regarding the control of the driving force, we will consider two protocols:
Protocol H: A straightforward procedure (employed in Ref. [24]) sets a shear rate and leaves the driving fixed, $P_D = \text{const}$. Then the shear heating adds to the power balance

$$\sigma \dot{\gamma} + n \Gamma \omega_c(T_0) T_0 = n \Gamma \omega_c(T) T$$

resulting in a higher temperature in the sheared steady state

$$T(\text{Pe}) = \frac{T_0}{[1 - \hat{\sigma}(\text{Pe}) \text{Pe} / \Gamma]^{2/3}} = \frac{T_0}{(1 - \text{Pe} / \text{Pe}_\infty)^{2/3}}$$

where $\hat{\sigma}(\text{Pe}, \varphi, \varepsilon) \equiv \sigma / n T$ is the dimensionless shear stress, independent of the temperature for dimensional reasons. The stationary temperature, $T(\text{Pe})$, diverges for the Péclet number reaching its maximum value, $\text{Pe} \rightarrow \text{Pe}_\infty$ [24].

Protocol T: Alternatively, we can regulate the driving power from the initial value $P_D = P_D^{(i)}$ to a lower, final value $P_D = P_D^{(f)} < P_D^{(i)}$ such that the temperature in the sheared stationary state is equal to the initial temperature $T \equiv T_0$. Note that shear heating will increase with shear rate while we cannot reduce the driving below $P_D^{(f)} \equiv 0$. That is, for Protocol T we are limited to shear rates $\dot{\gamma} \leq \dot{\gamma}_\infty$ smaller than a maximal value which is attained when the driving is completely turned off. The maximum shear, $\dot{\gamma}_\infty = \omega_c(T_0) \text{Pe}_\infty$, corresponds to the maximal Péclet number, $\text{Pe}_\infty$, where the temperature diverges in Protocol H.

III. MICROSCOPIC DESCRIPTION

A. Dynamics

An established, albeit artificial, method to enforce a shear profile $u(r) = r \cdot k$ on the microscopic level are the Sllod equations [33, 41],

$$\dot{r}_i = c_i + r_i \cdot k$$

$$\dot{c}_i = F_i - c_i \cdot k - F_{\text{thermo},i}$$

(6a)

(6b)

Here $F_i$ is the total interaction force acting on particle $i$ and $F_{\text{thermo},i}$ is a necessary thermostating force to dissipate shear heating. To be concrete, we define the velocity gradient tensor $k \equiv \nabla u = \dot{\gamma} \delta_{\alpha\beta} \delta_{x\beta}$.

For inelastic hard spheres the inelastic interactions also afford the dissipation such that the interaction and thermostat combine to

$$\dot{c}_i = \frac{dc_i}{dt}|_{\text{coll}} - c_i \cdot k$$

(6b')

where $dc_i / dt|_{\text{coll}}$ indicates the discontinuous momentum change in a hard sphere collision [34]. Finally, the initial condition

$$\sum_i c_i(0) = 0,$$

(6c)

has to be imposed to avoid an unphysical buildup of total momentum [41].

Note that the velocities $c_i$ are defined relative to the mean flow, $u(r_i)$, and are not the velocities seen in the laboratory frame, $v_i \equiv \dot{r}_i$. As for $u \equiv 0$ in the reference system, $c_i = v_i$ trivially, we can consider the phase space to be spanned by the set of positions $\{r_i\}$ and peculiar velocities $\{c_i\}$, throughout.
B. Stress Tensor

The stress tensor of inelastic hard spheres \[42, 43\] \(\sigma_{\alpha\beta} = \sigma_{\alpha\beta}^{\text{kin}} + \sigma_{\alpha\beta}^{\text{int}}\) is given microscopically as the sum of a kinetic part \(\sigma_{\alpha\beta}^{\text{kin}} = \sum_i v_i^\alpha v_i^\beta\) and an interaction part,

\[
\sigma_{\alpha\beta}^{\text{int}} = \frac{1 + \epsilon}{4} d \sum_{i<j} (\hat{r}_{ij} \cdot v_{ij})^2 r_{ij}^\alpha r_{ij}^\beta \Theta(-\hat{r}_{ij} \cdot v_{ij}) \delta(r_{ij} - d).
\] (7)

Here \(\Theta(x)\) denotes the Heaviside step-function.

IV. COARSE-GRAINED DESCRIPTION

We will be concerned with a continuum description of the particle density and momentum current using the following definitions

\[
\rho(r, t) = \frac{1}{N} \sum_i \delta(r - r_i(t)), \quad j(r, t) = \frac{1}{N} \sum_i c_i \delta(r - r_i(t)).
\] (8)

Note that the current \(j\) is defined with respect to the peculiar velocities \(c_i\) [27, 32]. We will use the spatial Fourier transforms \(\rho_q(t) = \text{FT}[\rho](q, t)\), and \(j_q(t) = \text{FT}[j](q, t)\) [44].

To maintain a continuum description, we need to require that the Knudsen number \(Kn < 1\). Here we can take the Péclet number as a proxy for the Knudsen number [45] and the fact that the Péclet number is limited \(Pe \leq Pe_\infty\) [24] ensures that we are not limited in shear rates as long as the density is sufficiently high such that \(Pe_\infty < 1\).

A. Reference System

1. Dynamics

In the reference system, the dynamics can be described by a (forward in time) effective pseudo Liouville operator \(\mathcal{L}^{+}_{\text{ref}}(P_D) = \mathcal{L}_0 + \mathcal{L}^+_I + \mathcal{L}^+_D(P_D)\) [39]. Here \(i\mathcal{L}_0 = \sum_j c_j \cdot \nabla j\) describes free streaming. The interaction is made up of pairwise inelastic collisions, \(i\mathcal{L}^+_I = \sum_{j<k} i\mathcal{T}^+_{jk}\), where

\[
i\mathcal{T}^+_{jk} = -(\hat{r}_{jk} \cdot v_{jk})\Theta(-\hat{r}_{jk} \cdot v_{jk}) \delta(r_{jk} - d)(b^+_{jk} - 1)
\] (9)

denotes the inelastic binary collision operator [34]. Here the operator \(b^+_{jk}\) implements the inelastic collision rule [46]. The driving term, \(\mathcal{L}^+_D(P_D) = P_D \sum_j \partial^2_{c_j}\), is parameterized by the driving strength \(P_D\). Strictly speaking, the binary collision operator \(\mathcal{T}^+_{jk}\) is defined in terms of relative laboratory-frame velocities \(v_{jk} = v_j - v_k\). Here we will assume that we can replace \(v_{jk}\) by \(c_{jk}\). This is a good approximation as long as the relative shear speed between two touching particles which is at most \(d^\gamma\) is much smaller than the typical relative speed of said particles which is proportional to the thermal speed \(\sqrt{T}\). This is automatically fulfilled for small Knudsen number \(Kn < 1\).
2. Phase Space Distribution

In contrast to the canonical distribution of an equilibrium colloidal suspension, the phase space distribution function \( \varrho_{\text{ref}}(X) \) of the randomly driven granular fluid reference state is not known exactly. To make progress, we make the same minimal assumptions as in Ref. [39]. Namely, (i) that the distribution factorizes into a spatial distribution function and a velocity distribution function; and (ii) that the (precollisional) velocity distribution factorizes into single particle distributions with zero mean and a finite second moment

\[
\langle c^2 \rangle := \int dX \varrho_{\text{ref}}(X) c^2 = 3T < \infty.
\]

Writing the ensemble average of an observable \( A(X) \) as a scalar product

\[
\frac{d}{dt} \langle A \rangle = \langle i \mathcal{L}^+_{\text{ref}} A \rangle = \int dX \varrho_{\text{ref}}(X) \mathcal{L}^+_{\text{ref}} A(X) =: (\varrho_{\text{ref}}, \mathcal{L}^+_{\text{ref}} A)
\]

we can introduce the f-Liouvillean \( \mathcal{T}^+_{\text{ref}} \) as the adjoint of the p-Liouvillean \( \mathcal{L}^+_{\text{ref}} \),

\[
(\mathcal{T}^+_{\text{ref}} \varrho_{\text{ref}}, A) = (\varrho_{\text{ref}}, \mathcal{L}^+_{\text{ref}} A),
\]

acting on the phase space distribution \( \varrho_{\text{ref}} \). With respect to two observables \( A_1(X), A_2(X) \), we write correlations functions as another scalar product,

\[
\langle A_1 | A_2 \rangle := \int dX \varrho_{\text{ref}}(X) A_1^*(X) A_2(X),
\]

where the asterisk denotes complex conjugation.

B. Sheared System

1. Dynamics

Formally encoding the Sllod equations in terms of a Liouville operator yields \( \mathcal{L}^+_{PD} = \mathcal{L}^+_{\text{ref}}(PD) + \mathcal{L}_r \) where \( \mathcal{L}_r = \mathcal{L}_{ir} + \mathcal{L}_{ic} \),

\[
i \mathcal{L}_{ir} = \sum_j r_j \cdot k \cdot \nabla_j, \quad i \mathcal{L}_{ic} = \sum_j c_j \cdot k \cdot \frac{\partial}{\partial c_j}.
\]

A more careful consideration, however, reveals that we are interested in applying the Liouville operator to the coarse grained fields \( \rho(r, t) \) and \( \mathbf{j}(r, t) \). It is not obvious, how to systematically coarse grain the momentum constraint, Eq. (6c), and we will come back to this point in the end (Sec. VIII). In analogy with the concept of local thermodynamic equilibrium, we assume that the constraint holds locally for every volume element used to define the local values of the fields. This implies that \( \sum_i c_i = 0 \), locally and for all times and amounts to dropping \( \mathcal{L}_{ic} \) as a spurious contribution. We will consequently use

\[
\mathcal{L}^+_P := \mathcal{L}^+_{\text{ref}}(PD) + \mathcal{L}_{ir}
\]

as the p-Liouvillean of the sheared state.
2. Low Density Linear Response

At low density, ϕ ≪ 1, and small shear rate, ˙γ → 0, we expect Newtonian rheology [24], σ0 = ηγ, with a viscosity η(ϕ ≪ 1) that is well approximated by the Enskog predictions, ηE(ϕ, ε), of Garzó and Montanero [13]. A natural scale to compare viscosities to is the Boltzmann viscosity,

\[ \eta_0 := \eta(\varphi \to 0, \varepsilon = 1) = \frac{5}{16d^2} \sqrt{\frac{T}{\pi}}, \]

(15)
of a hard sphere gas at vanishing density [40].

3. Translational Invariance

It is natural to assume that the fluid is translationally invariant in the comoving frame \( \hat{r} = r - k^t \cdot rt \) [26]. Therefore, we define the Fourier Transform of an observable \( A(r, t) = A(\hat{r}, t) \) in this frame as

\[ A_q(t) = \int d^3\hat{r} A(\hat{r}, t) e^{-iq \cdot \hat{r}}. \]

(16)

Performing a coordinate transform,

\[ A_q(t) = \int d^3r \det(\partial \hat{r}/\partial r) A(r, t) e^{-iq \cdot (1-k^t) \cdot r} = \int d^3r A(r, t) e^{-iq \cdot (1-k^t) \cdot r}, \]

(17)

we use the invariance of \( A \) under a change of reference frame. With the identification \( q(t) = q \cdot (1-k^t) \) this is formally equivalent to a Fourier Transform in the laboratory frame with a time-dependent wave vector \( q(t) \),

\[ A_{q(t)}(t) = \int d^3r A(r, t) e^{-iq(t) \cdot r}. \]

(18)

V. GENERALIZED GREEN-KUBO RELATION

In the spirit of the ITT formalism [26], we rewrite the sheared steady state phase space density \( \varrho_{ss} \) in the following exact form,

\[ \varrho_{ss} = \varrho_{ref} + \int_0^\infty dt \exp(-it\Delta t^+ i\Delta t^+ \varrho_{ref}), \]

(19)

where \( \Delta t^+ = \mathcal{L}^+(\Delta P_D) \), and \( \Delta t^+(\Delta P_D) = -\Delta P_D \sum_j \varrho_{c_j}^2 \). To minimize the change of the boundary conditions to the fluid, we assume that we choose the driving power in the reference state, \( P_D^{(e)} \), for time \( t < 0 \) such that it yields the same stationary temperature \( T \) as in the sheared stationary state, i.e., \( \Delta P_D = P_D^{(f)} - P_D^{(e)} \).

To make progress, we have to make assumptions on the action of \( \Delta t^+ \) on \( \varrho_{ref} \). For a canonical distribution, \( \varrho_{ref}^{-1} \mathcal{L}_{\gamma_r} \varrho_{ref} = -\gamma \sigma_{xx}^{int}/T \) [26] and with the assumptions we made for the non-equilibrium granular distribution \( \varrho_{ref} \), this will still serve as a good approximation. With the same assumptions we find for the effect of the change in driving power \( \varrho_{ref}^{-1} \Delta t^+ \varrho_{ref} = -3\Delta P_D \delta K/T \) where

\[ \delta K = 1 - \frac{1}{N} \sum_j \frac{c_j^2}{3T}. \]

(20)
Using Eq. (19) to calculate the expectation value, \( \langle A \rangle_{ss} := \int dX q_{ss}(X) A(X) \), of any observable \( A(X) \) in the sheared steady state, we find

\[
\langle A \rangle_{ss} = \langle A \rangle - \frac{\dot{\gamma}}{T} \int_{0}^{\infty} dt \langle \sigma_{xy}^{\text{int}} | A(t) \rangle - \frac{3 \Delta P_{D}}{T} \int_{0}^{\infty} dt \langle \delta K | A(t) \rangle. \tag{21}
\]

For any \( A \) analytic in the velocities, the last term, \( \langle \delta K | A(t) \rangle \), will vanish. Non-Gaussian corrections to the single particle velocity distribution will lead to corrections of the order \( a_{2} \) \( \cite{10} \) that will be discussed in future work. Formally, we recover the established generalized Green-Kubo relation \( \cite{25, 26} \)

\[
\langle A \rangle_{ss} = \langle A \rangle - \frac{\dot{\gamma}}{T} \int_{0}^{\infty} dt \langle \sigma_{xy}^{\text{int}} | A(t) \rangle. \tag{22}
\]

Adapting an argument by Chong and Kim \( \cite{27} \), we can show that for any observable \( A \), we have

\[
\langle \sigma_{xy}^{\text{int}} | \exp(it \mathcal{L}_{+}) A \rangle = \langle \sigma_{xy}^{\text{int}} Q | \exp(it \mathcal{Q} \times \mathcal{Q}) QA \rangle, \tag{23}
\]

where \( Q = 1 - \mathcal{P} \) and

\[
\mathcal{P} = \frac{N}{S_{q}} \sum_{q} |\rho_{q}\rangle \langle \rho_{q}| + \frac{N}{T} \sum_{q} |j_{q}\rangle \langle j_{q}| \tag{24}
\]

projects onto the hydrodynamic fields. Here \( S_{q} = N \langle \rho_{q} | \rho_{q} \rangle \) denotes the static structure factor \( \cite{47} \). Now, making a mode-coupling approximation,

\[
\exp(it \mathcal{Q} \mathcal{L}_{+} \mathcal{Q}) \approx N^{2} \sum_{k, p} |\rho_{k(-t)} \rho_{p(-t)}\rangle \frac{\Phi_{k(-t)}(t) \Phi_{p(-t)}(t)}{S_{k} S_{p}} \langle \rho_{k} \rho_{p} |, \tag{25}
\]

we can express the Green-Kubo relation in terms of the transient correlator \( \Phi_{q}(t) := N \langle \rho_{q} | \rho_{q}(t) \rangle / S_{q} \),

\[
\langle A \rangle_{ss} \approx \langle A \rangle - \frac{\dot{\gamma}}{2T} \sum_{k} \int_{0}^{\infty} dt \mathcal{V}_{k(-t)}^{A} \mathcal{W}_{k}^{*} \Phi_{k(-t)}^{2}(t), \tag{26}
\]

where

\[
\mathcal{W}_{k}^{A} = N \langle \rho_{k} \rho_{-k} | A \rangle / S_{k}^{2}, \tag{27}
\]

\[
\mathcal{V}_{k}^{*} = N \langle \sigma_{xy}^{\text{int}} | \rho_{k} \rho_{-k} \rangle = -\frac{1 + \epsilon}{2} \varphi T k_{x} k_{y} C_{k}. \tag{28}
\]

Here \( C_{k} := 6 \chi j_{0}''(kd)/k \) (see appendix \( \ref{A} \)) where \( \chi = \chi(\varphi) \) indicates the value of the pair correlation function at contact \( \cite{47} \) and \( j_{0}(x) \) is a spherical Bessel function \( \cite{48} \). Primes denote derivatives with respect to the wave number. For soft spheres \( \varphi C_{k} \equiv S_{k}^{*} \) is given as the derivative of the structure factor \( \cite{26} \). For hard spheres, \( \varphi C_{k} \neq S_{k}^{*} \), as only binary collisions contribute to the vertex \( \mathcal{V}_{k}^{*} \). The wave vectors \( \pm k \) of the modes involved in the vertices above add up to zero as a manifestation of momentum conservation.

In particular we find for the macroscopic shear stress

\[
-\langle \sigma_{xy} \rangle_{ss} / V = \dot{\gamma} \varphi^{2} T \frac{(1 + \epsilon)^{2}}{8} \int \frac{d^{3}k}{(2\pi)^{3}} \int_{0}^{\infty} dt \frac{k_{x}^{2} k_{y}^{2} \delta(t)}{kk(-t)} \times \frac{C_{k(-t)} C_{k}}{S_{k}^{2}} \Phi_{k(-t)}^{2}. \tag{29}
\]
where only the interaction part, \( \sigma_{xy}^{\text{int}} \), yields a finite contribution and the expectation value of the kinetic part, \( \langle \sigma_{xy}^{\text{kin}} \rangle \), vanishes due to parity. Once we know the transient correlator \( \Phi_k(t) \), this allows us to determine the shear stress for a given shear rate \( \dot{\gamma} \). In terms of the dimensionless time \( \tau = \omega_c t \) and the dimensionless wave number \( k^* = kd \) we find a dimensionless stress

\[
- \langle \sigma_{xy} \rangle_{ss} / NT = \text{Pe} \varphi \frac{(1 + \epsilon)^2}{4} \int \frac{d^3k^*}{96\pi^2} \int_0^\infty d\tau \frac{k^*_{x}k^*_{y}k^*_{y}(-\tau)}{k^*k^*(-\tau)} \times \frac{C_{k^*}(-\tau)C_{k^*}}{S_{k^*}^2} \Phi_{k^*}^2(-\tau)(\tau)
\]

manifestly temperature independent.

VI. MODE-COUPLING THEORY FOR THE TRANSIENT CORRELATOR

A. Separating the Slow Dynamics

For the observables \( A_q \in \{ \rho_q, j_q \} \) we define the propagator \( U(t) \) via

\[
A_q(t) = \exp(itL_+)\exp(-it\mathcal{L}_{\gamma})A_q =: U(t)A_q
\]

where \( U(t) \neq \exp[it(L_+ - \mathcal{L}_{\gamma})] \) because \( L_+ \) and \( \mathcal{L}_{\gamma} \) do not commute. Following Suzuki and Hayakawa \[32\] we write

\[
\frac{d}{dt}U(t) = \exp(itL_+)i\tilde{\mathcal{L}}_+ \exp(-it\mathcal{L}_{\gamma})
\]

where \( \tilde{\mathcal{L}}_+ = L_+ - \mathcal{L}_{\gamma} \). In order to separate the slow dynamics, we define the projectors

\[
\mathcal{P}(t) := N \sum_k |\rho_k(t)\rangle \langle \rho_k(t)| / S_k(t) + N \sum_k |j_k(t)\rangle \langle j_k(t)| / T,
\]

and \( \mathcal{Q}(t) = 1 - \mathcal{P}(t) \). Next, we can expand the time derivative of the propagator as follows,

\[
\frac{d}{dt}U(t) = U_S(t)i\tilde{\mathcal{L}}_+ \exp(-it\mathcal{L}_{\gamma}) + \mathcal{Q}(0)\dot{U}(t,0)R(t) + \int_0^t d\tau U_S(\tau)i\tilde{\mathcal{L}}_+ \mathcal{Q}(\tau)\dot{U}(t,\tau)R(t),
\]

where

\[
U_S(t) := U(t)\exp(it\mathcal{L}_{\gamma})\mathcal{P}(t)
\]

\[
= N \sum_k |\rho_k(t)\rangle \langle \rho_k(t)| / S_k(t) + N \sum_k |j_k(t)\rangle \langle j_k(t)| / T
\]

is the propagator of the slow modes,

\[
\dot{U}(t, \tau) := \exp(-i\tau \mathcal{L}_{\gamma}^\dagger)\tilde{U}(t, \tau) \exp(it\mathcal{L}_{\gamma}),
\]

\[
\tilde{U}(t, \tau) := \exp_- \left[ \int_{\tau}^t dt' \mathcal{Q}(t')i\tilde{\mathcal{L}}_+ \exp(-it'\mathcal{L}_{\gamma}) \right]
\]

and \( \exp_- \) is the time ordered exponential. Finally, \( R(t) := \mathcal{Q}(t)i\tilde{\mathcal{L}}_+ \exp(-it\mathcal{L}_{\gamma}) \), is the fluctuating force operator. In the last term of Eq. \(34\), the conventional small strain approximation \(20\) \( \exp(-it\mathcal{L}_{\gamma}) \approx \exp(-it\mathcal{L}_{\gamma}^\dagger) \) has been employed. Besides this approximation, Eq. \(34\) is exact. Note that the second term in Eq. \(34\) will never contribute due to the orthogonal projector \( \mathcal{Q}(0) \).
B. Equation of Motion for the Transient Correlators

The continuity equation for the density, \( i \tilde{\mathcal{L}} + \rho_q(t) = i \mathbf{q}(t) \cdot \mathbf{j}_q(t) \), implies

\[
\frac{d}{dt} \Phi_q(t) = \mathbf{q}(t) \cdot H_q(t) / S_q
\]

(38)

where

\[
H_q(t) := iN \langle \rho_q | j_q(t) \rangle
\]

(39)

is the transient density-current correlator. Next, we expand

\[
\frac{d}{dt} H_q(t) = iN \langle \rho_q | \frac{d}{dt} \mathbf{U}(t) \mathbf{j}_q \rangle
\]

(40)

in terms of Eq. (34). For the first term we find

\[
U_S(t) i \tilde{\mathcal{L}} j_q(t) = \Omega_q^{ji}(t) \rho_q(t) + j_q(t) \cdot \Omega_q(t)
\]

(41)

where

\[
\Omega_q^{ji} := N \langle \rho_q | i \tilde{\mathcal{L}} j_q \rangle / S_q, \quad \Omega_q^{\lambda \mu} := N \langle j_q^\lambda | i \tilde{\mathcal{L}} j_q^\mu \rangle / T
\]

(42a, 42b)

The third term yields for the fluctuating force \( R_q(t) := R(t) \mathbf{j}_q \)

\[
U_S(t) i \tilde{\mathcal{Q}}(t) \mathbf{U}(t, \tau) R_q(t) = -L_q(t, \tau) \rho_q(t) - j_q(t) \cdot M_q(t, \tau)
\]

(43)

where

\[
L_q(t, \tau) := -N \langle \rho_q(t) | i \tilde{\mathcal{Q}} \mathbf{U}(t, \tau) R_q(t) \rangle / S_q(t), \quad M_q^{\lambda \mu}(t, \tau) := -N \langle j_q^\lambda(t) | i \tilde{\mathcal{Q}} \mathbf{U}(t, \tau) R_q^{\mu}(t) \rangle / T
\]

(44a, 44b)

are two memory kernels.

The elements of the frequency matrices are known from the literature: \( \Omega_q^{ji} = i \mathbf{q} C_q^2 \) where

\[
C_q^2 = \frac{T}{S_q} \left[ \frac{1 + \epsilon}{2} + \frac{1 - \epsilon}{2} S_q \right]
\]

(45)

is the (squared) speed of sound \([39]\), and

\[
\Omega_q^{\lambda \mu} = i \mu_q \delta^{\lambda \mu} \quad \text{where} \quad \mu_q = \frac{1 + \epsilon}{3} \omega_c [1 - j_0(qd)]
\]

(46)

and \( j_0(x) \) is the zeroth order spherical Bessel function \([48]\).

The equations of motion for the correlators, \( \Phi_q(t) \) and \( H_q(t) \) can be written as

\[
S_q \frac{d}{dt} \Phi_q(t) = \mathbf{q}(t) \cdot H_q(t)
\]

(47a)
and
\[
\frac{d}{dt} H_q(t) + q(t) C^2_{q(t)} S_q \Phi_q(t) + \mu_q(t) H_q(t) \\
+ \int_0^t d\tau L_q(t, \tau) S_q(\tau) \Phi_q(\tau) + \int_0^t d\tau H_q(\tau) \cdot M_q(t, \tau) = 0.
\] (47b)

With \( S_q \Phi_q(t) = -q(t) \cdot k \cdot H_q(t) + q(t) \cdot \dot{H}_q(t) \) \[50] we can express Eq. (47a) also in the form
\[
\ddot{\Phi}_q(t) + \nu_q(t) \dot{\Phi}_q(t) + q^2(t) C^2_{q(t)} \Phi_q(t) + q \cdot k \cdot H_q(t)/S_q \\
+ q(t) \cdot \int_0^t d\tau L_q(t, \tau) S_q(\tau) \Phi_q(\tau) + q(t) \cdot \int_0^t d\tau M_q(t, \tau) \cdot H_q(\tau)/S_q = 0
\] (48)

where \[39\]
\[
\nu_q = \frac{1 + \epsilon}{3} \omega_c [1 + 3 j_0'(qd)]
\] (49)
is known as the Enskog term \[51\] and the double primes denote the second derivative. The first three terms in Eq. (48) describe sound waves with an advected wave vector \( q(t) \). The fourth term is proportional to \( \ddot{q} \) and vanishes in the limit of no shear. All effects not local in time are contained in the memory kernels \( L_q \) and \( M_q \). To make progress we evaluate the memory kernels in terms of a mode-coupling approximation.

C. Mode-Coupling Approximation

We approximate \( \dot{U}(t, \tau) \) with a mode-coupling ansatz \[26\],
\[
\dot{U}(t, \tau) \approx P_2(\tau) \dot{U}(t, \tau) P_2(t) \\
\approx N^2 \sum_{k,p} |\rho_{k(\tau)}\rho_{p(\tau)}| \frac{\Phi_{k(\tau)}(t-\tau)\Phi_{p(\tau)}(t-\tau)}{S_{k(t)}S_{p(t)}} \langle \rho_{k(t)}\rho_{p(t)} \rangle,
\] (50)

where
\[
P_2(t) := N^2 \sum_{k,p} |\rho_{k(t)}\rho_{p(t)}| \langle \rho_{k(t)}\rho_{p(t)} \rangle / S_{k(t)}S_{p(t)}.
\] (51)

This immediately yields \( L_q(t, \tau) \approx 0 \) as the left vertex \( \propto \langle \rho_{q(\tau)} | i\tilde{L}_+ Q(\tau) \rho_{k(\tau)}\rho_{p(\tau)} \rangle = 0 \) due to parity. For the second memory kernel we find
\[
M^\lambda_{q}(t, \tau) \approx \frac{N}{T} \sum_{k,p} \frac{S_{k(t)}}{S_{k(t)}} \nu^\lambda_{qkp}(\tau) \nu^\mu_{qkp}(t) \Phi_{k(\tau)}(t-\tau)\Phi_{p(\tau)}(t-\tau)
\] (52)

where the vertices,
\[
\nu^\lambda_{qkp}(t) = N \left\langle j^\lambda_{q(t)} | i\tilde{L}_+ Q(t) \rho_{k(t)}\rho_{p(t)} \right\rangle / S_{k(t)},
\] (53a)
\[
\nu^\lambda_{qkp}(t) = N \left\langle \rho_{k(t)}\rho_{p(t)} | Q(t) i\tilde{L}_+ j^\lambda_{q(t)} \right\rangle / S_{p(t)}.
\] (53b)
are, again, known from the literature \[ [V_{qkp}(t) \equiv V_{q(t)k(t)p(t)}], \]
\[
i V_{qkp}^\lambda(t) = \frac{T}{N} S_p[k^\lambda n c_k + p^\lambda n c_p] \delta_{q,k+p}, \tag{54a} \]
\[
i V_{qkp}^{-\lambda}(t) = \frac{1 + \epsilon}{2} \frac{T}{N} S_k[k^\lambda n c_k + p^\lambda n c_p] \delta_{q,k+p}. \tag{54b} \]

This closes the equations of motion as soon as we know the static structure factor \( S_q \). Solving the full set of equations, (47a,b) and (52), constitutes a major challenge that we will not attempt here. Instead, we assume that the sheared system is still reasonably isotropic and employ a respective approximation.

### D. The Isotropic Approximation

Assuming an isotropic state \[ [26], \] we have \( \Phi_q(t) = \Phi_0(t) \), and
\[
\begin{align*}
\mathbf{H}_q(t) &= q(t) S_q \dot{\Phi}_q(t)/q^2(t), \\
\mathbf{k} \cdot \mathbf{H}_q(t) &= |\gamma| q(t) S_q \dot{\Phi}_q(t)/q^2(t).
\end{align*} \tag{55} \]

Moreover, \( M_q(t, \tau) = q(t) q(\tau) C_{q(t)}^2 m_q(t, \tau) \), where the odd normalization is for later convenience. This allows us to eliminate \( \mathbf{H}_q(t) \) completely and write a closed equation for \( \Phi_q(t) \),
\[
\dot{\Phi}_q(t) + [\nu_q(t) + |\gamma|] \dot{\Phi}_q(t) + q^2(t) C_{q(t)}^2 \Phi_q(t) + q^2(t) C_{q(t)}^2 \int_0^t d\tau m_q(t, \tau) \Phi_q(\tau) = 0, \tag{56} \]

where the shear rate appears as an additional damping term. Here
\[
m_q(t, \tau) = A_q(t) \epsilon \frac{S_q(t)}{n q^2} \int \frac{d^3k}{(2\pi)^3} S_k(\tau) S_p(\tau) \times [(\hat{q} \cdot \mathbf{k}) n c_k(t) + (\mathbf{q} \cdot \mathbf{p}) n c_p(t)][(\hat{q} \cdot \mathbf{k}) n c_k(\tau) + (\mathbf{q} \cdot \mathbf{p}) n c_p(\tau)] \times \Phi_k(\tau)(t - \tau) \Phi_p(\tau)(t - \tau) \tag{57} \]

and we have used the approximate relations \([\hat{q}(t) \cdot \mathbf{k}(t)]/q(t) \simeq \hat{q} \cdot \mathbf{k}/q \) and \( k(t) \simeq k \sqrt{1 + (\dot{\gamma}t)^2/3} \tag{26}. \) For vanishing shear, \( \dot{\gamma} \to 0 \), the memory kernel reduces to the one calculated in Ref. \[ [39], \] where
\[
A_q^{-1}(\epsilon) = 1 + \frac{1 - \epsilon}{1 + \epsilon} S_q. \tag{58} \]

Eqs. (56,57) can also be made manifestly temperature independent by writing them in terms of the dimensionless time \( \omega_s t \) and the dimensionless wave number \( k_d \). Applying the isotropic approximation to the shear stress, Eq. (29), we find as our central result the shear stress [see Eq. (4) in Ref. \[ [24], \] for a dimensionless form]
\[
\sigma := \sigma_0 + \dot{\gamma} \varphi^2 T \frac{1 + \epsilon}{4} \int_0^\infty \frac{dt}{\sqrt{1 + (\dot{\gamma}t)^2/3}} \int_0^\infty \frac{dk k^4}{60 \pi^2} \times \frac{C_{k(t)} C_k}{S_k^2} \Phi_k(\tau)(t), \tag{59} \]

where we have added the Enskog term \( \sigma_0 \) (cf. Sec. IV B 2) to obtain a finite low density limit not recovered by the ITT contribution which is of order \( \mathcal{O}(\varphi^2) \).
FIG. 2. **Protocol H** for several values of the coefficient of restitution $\varepsilon$ (columns, as indicated) and several packing fractions (color coded) from $\varphi = 0.48$ (yellow, bottom) to $\varphi = 0.60$ (black, top). (First row) Flow curves, shear stress $\sigma$ as a function of shear rate $\dot{\gamma}$. (Second row) Viscosity $\eta$ relative to the Boltzmann viscosity $\eta_0(T_0)$. (Third row) Stationary temperature $T$, relative to the initial temperature, $T_0$, at zero shear. The dotted line indicates $T/T_0 \equiv 2$.

**VII. RESULTS**

To obtain quantitative predictions, we numerically solved Eqs. (56, 57, 59) (see appendix B). Some of the results are presented in Ref. [24]. Here we will focus on a broader range of parameters and provide additional comparison with established kinetic theories.

**A. Rheology & Flow Curves**

1. **Protocol H**

   The phenomenology of Protocol H has been discussed in Ref. [24]. Comparing the dynamic state diagrams for different inelasticities, $\varepsilon$, in Fig. 1 confirms the broad layout of the rheological regimes. The critical density for the granular glass transition, $\varphi_c(\varepsilon)$, which increases with increasingly dissipative particles determines the boundaries of the Newtonian regime observed at low densities and small shear rates. At the highest shear rates, the power balance, Eq. (3), is dominated by shear heating and shear thickening is observed in the Bagnold regime. As the granular fluid is more susceptible to shear heating the more elastic the particles are, the onset of the Bagnold regime moves to lower shear rates for larger values
FIG. 3. Protocol T \((T \equiv T_0)\) or Protocol H \((T > T_0)\): Dynamic state diagrams in the plane spanned by Péclet number, \(Pe\), and packing fraction, \(\varphi\), for several values of the coefficient of restitution, \(\varepsilon\), as indicated. The effective exponent \(R\) quantifying the shear rate dependence of the viscosity, \(\eta(\text{Pe}) \sim \text{Pe}^R\), is color coded on the same scale as in Fig. 1. The inaccessible regime \(Pe > Pe_\infty\) is left blank. The jagged boundary is due to discretization.

of \(\varepsilon\).

Flow curves, \(\sigma(\dot{\gamma})\), corresponding to Protocol H are shown in Fig. 2 (see also Figs. 2 and 3 in Ref. [24]). Note that the precise value of the coefficient of restitution may have a huge influence on the flow behavior. For the same flow conditions, \(i.e.,\) packing fraction, \(\varphi\), and shear rate, \(\dot{\gamma}\), rather elastic particles may place the granular fluid in the flat part of the flow curve, requiring rather large stresses, \(\sigma/nT_0 \sim 10\), while for more inelastic particles the flow would still be in the Newtonian regime, requiring only negligible shear stress, \(\sigma/nT_0 \ll 1\). This is also reflected in the viscosity (Fig. 2) which may vary over many orders of magnitude for a fixed packing fraction, \(\varphi\), depending on both shear rate and coefficient of restitution. Considering the stationary temperature, \(T\), resulting from the power balance, Eq. (3), we observe that, as expected, significant shear rates are needed to make shear heating relevant and increase the stationary temperature \(T\) with respect to the temperature \(T_0\) of the unsheared fluid (Fig. 2). In Ref. [24] we defined the critical Péclet number, \(Pe^*\), for the onset of shear thickening, as the point where \(T = 2T_0\). Comparing the temperature curves in Fig. 2 with the viscosity curves, \(\eta(\dot{\gamma})\), confirms the utility of this definition.

If we normalize the shear stress, \(\sigma/nT\), with the stationary temperature, \(T\), instead of the initial temperature, \(T_0\), and express the shear rate, \(\dot{\gamma}\), in terms of the Péclet number, \(Pe\), we arrive at a description of the rheology in terms of intrinsic quantities that make the temperature independence of the (inelastic) hard sphere fluid manifest (Figs. 3,4). In this form, the predictions for Protocol H are identical to the ones for Protocol T as they only differ in the temperature control (cf. Sec. II A).
FIG. 4. **Protocol T** ($T \equiv T_0$) or **Protocol H** ($T > T_0$): Flow curves, shear stress $\sigma$ as a function of Péclet number $Pe$ (first row), and viscosity $\eta$ relative to the Boltzmann viscosity $\eta \equiv \eta_0(T)$ (second row) for several values of the coefficient of restitution $\varepsilon$ (columns, as indicated) and several packing fractions (color coded) from $\varphi = 0.48$ (yellow, bottom) to $\varphi = 0.60$ (black, top). The filled circles mark the maximum Péclet number $Pe_\infty$, i.e., the end of the flow curves for the respective densities.

FIG. 5. **Protocol T** ($T \equiv T_0$) or **Protocol H** ($T > T_0$): Flow curves, $\sigma(\text{Pe})$, for several values of the coefficient of restitution $\varepsilon$ (as indicated) and several packing fractions (color coded) from $\varphi = 0.54$ (yellow, bottom) to $\varphi = 0.60$ (black, top) close to and above the glass transition density. Note the linear scale for the shear stress.

2. **Protocol T**

Employing Protocol $T$ makes it straightforward to obtain the intrinsic quantities, $\sigma/nT$, and $Pe = \dot{\gamma}/\omega_c(\varphi, T)$, as the temperature is held constant, $T \equiv T_0$, throughout. In terms of the packing fraction, $\varphi$, and the Péclet number, $Pe$, the dynamic state diagram is shown in Fig. 3 for different inelasticities $\varepsilon$. We readily observe that the shear thickening regime vanishes altogether compared to the diagrams for Protocol $H$ (Fig. 1). The apparent shear thickening observed in Protocol $H$ is due to shear heating only which is absent in Protocol $T$. As the Péclet number is restricted to be smaller than the maximal value, $Pe \leq Pe_\infty$ [21], the
dynamic state diagram includes unreachable regions of large Péclat number, $\text{Pe} > \text{Pe}_\infty(\varphi, \varepsilon)$ that cannot be realized in a granular fluid. The Bagnold regime of Protocol $H$ (cf. Fig. 1) shrinks to the line $\text{Pe} = \text{Pe}_\infty(\varphi, \varepsilon)$ for Protocol $T$. At low Péclat number or shear rate, where shear heating is negligible, the dynamic state diagrams become indistinguishable between Protocols $H$ and $T$ (cf. Figs. 1 and 3). Shear thinning behavior, which is caused by the slow relaxation in the fluid [24, 31] is independent of temperature control and this therefor also observed in Protocol $T$.

The flow curves, $\sigma(\text{Pe})$, for Protocol $T$ shown in Fig. 4 (see also Fig. 2 in Ref. [24]) also reflect the finite admissible range of Péclat numbers as they end at $\text{Pe} = \text{Pe}_\infty$. The viscosity curves (Fig. 4) confirm that no shear thickening is observed in Protocol $T$ and the Newtonian regime at low densities and small shear rates is complemented by a shear thinning regime only. For packing fractions, $\varphi > \phi_c(\varepsilon)$, above the glass transition, the variation of the shear stress, $\sigma$, with Péclat number, $\text{Pe}$, is remarkably small throughout the whole range of admissible Péclat numbers (Fig. 5). Once the yield stress, $\sigma_y = \sigma(\text{Pe} \rightarrow 0)$, is exceeded, no more than roughly a doubling of the shear stress will be needed to achieve arbitrary shear rates.

**B. Transport Coefficients & Yield Stress**

Irrespective of the possibility to handle arbitrary shear rates, gITT (and more generally ITT) can also be used to calculate the viscosity, $\eta$, in the linear response regime, $\dot{\gamma} \rightarrow 0$. Recall that in this limit Protocol $T$ and $H$ become indistinguishable as there is no shear heating. Employed in this way, gITT extends the low density Enskog predictions [13], to higher densities (Fig. 6). In particular it captures the strong increase (and eventual divergence) of the viscosity as the glass transition is approached [52]. This divergence can, of course, not be recovered by the low density, Enskog predictions. The variations in the glass transition, $\phi_c(\varepsilon)$, with the coefficient of restitution, $\varepsilon$, leads to a correspondingly large variation of the viscosity, $\eta(\varepsilon)$, which far exceeds the variations predicted by Enskog theory.

The large shear rate behavior, $\dot{\gamma} \rightarrow \infty$, or $\text{Pe} \rightarrow \text{Pe}_\infty$, respectively, is characterized by the Bagnold coefficient $B$, Fig. 7a. As shear heating is more effective for more elastic particles (in Protocol $H$), the Bagnold coefficient increases with $\varepsilon$. As the glass is already shear-molten in the Bagnold regime, unlike the viscosity $\eta$, the Bagnold coefficient does not diverge at the glass transition density, $\phi_c(\varepsilon)$. However, the increasing sluggishness of the fluid at high densities is also reflected in the Bagnold coefficient which increases rapidly with density. Such a quick rise is naturally not recovered by the existing Enskog predictions. The theories by Mitarai and Nakanishi [53], and Kumaran [54] both come close to the results from gITT for lower densities but deviate by orders of magnitude above the glass transition density. The phenomenally simple prediction by Savage and Jeffrey [55], $B_{SJ} \cdot d = 32 \varphi \chi(\varphi)/35\pi$, where $\chi(\varphi)$ is the value of the pair correlation function at contact is independent of the coefficient of restitution but also yields the right order of magnitude at low densities.

Above the glass transition density, $\phi_c(\varepsilon)$, a finite (dynamic) yield stress, $\sigma_y$, has to be exceeded to keep the system flowing and to prevent it from freezing into an amorphous glass. The critical yield stress, $\sigma_y^c(\varepsilon)$ (cf. Fig. 3 in Ref. [24]) right at the glass transition is on the order of $2nT$. For larger densities, $\varphi > \phi_c(\varepsilon)$, the yield stress quickly rises before settling to a narrow band around $4-5nT$ (Fig. 7b) which is only exceeded at the highest densities [56].
FIG. 6. Viscosity $\eta$, normalized by the Boltzmann viscosity $\eta_0$ at small shear rate, $\dot{\gamma} \to 0$. (a) As a function of the coefficient of restitution $\varepsilon$ for a number of packing fractions from $\varphi = 0.47$ (yellow, bottom) to $\varphi = 0.51$ (black, top). (b) As a function of packing fraction, $\varphi$, for a number of values of the coefficient of restitution, $\varepsilon$, from $\varepsilon = 0.1$ (cyan, bottom) to $\varepsilon = 0.9$ (magenta, top). Solid lines denote gITT predictions while dashed lines indicate the Enskog low density expansion by Garzó and Montanero [13]. The arrows indicate the glass transition density, $\varphi_c(\varepsilon)$.

FIG. 7. (a) Bagnold coefficient $B$ as a function of packing fraction $\varphi$. Solid lines are gITT predictions for several values of the coefficient of restitution $\varepsilon = 0, 0.3, 0.6, 0.9$ from bottom to top. The dashed lines denote Enskog predictions from Savage and Jeffrey [55] (blue), Kumaran [54] (orange), and Mitarai and Nakanishi [53] (green). The last two are for $\varepsilon = 0.9$. The arrows indicate the glass transition density, $\varphi_c(\varepsilon)$. (b) Yield stress, $\sigma_y$, as a function of volume fraction, $\varphi$, for a number of values of the coefficient of restitution, $\varepsilon$, from $\varepsilon = 0.9$ (magenta, left) to $\varepsilon = 0.1$ (cyan, right). Points are calculated and lines are spline fits. The dotted lines are guides to the eye.

VIII. CONCLUSION

In summary we have shown how to derive generalized Green-Kubo relations for sheared inelastic hard sphere fluids at finite shear rates and densities around the (granular) glass transition density. In particular, we have shown that an ITT formalism can be derived with respect to a reference system that is already out of equilibrium before the shear is applied. Employing a number of reasonable approximations, the shear stress of a granular fluid is given by a Green-Kubo relation, Eq. [29], that is formally almost identical to the one for colloidal suspensions, [cf. Eq. (37) in Ref. [26]]. The differences are: (i) the explicit dependence on the coefficient of restitution reflecting the dissipative interactions; and (ii) the
replacement $S_k \rightarrow \varphi C_k$ due to the hard-core interactions. The increase of the shear stress at high densities is driven by the slow structural relaxation of the system around the glass transition. The dependence of the glass transition on the coefficient of restitution yields a strong sensitivity of the transport coefficients and even the qualitative rheological behavior on the inelasticity of the particles. This sensitivity, together with the strong increase (and eventual divergence) of the small shear viscosity, $\eta(\dot{\gamma} \rightarrow 0)$, shows that an extrapolation of the Enskog predictions from the gaseous state of vanishing density, $\varphi \ll 1$, to significant densities, $\varphi \sim \mathcal{O}(1)$, cannot work as it completely neglects the dramatic slowing down of structural relaxation at high densities. For the Bagnold coefficient, $B$, we have argued that it is only defined for finite shear rates, $\dot{\gamma} \rightarrow \omega_c \Pe_\infty$. Except for the elastic limit, $\varepsilon \rightarrow 1$, where $\Pe_\infty \ll 1$, this makes the Bagnold coefficient inaccessible to linear response theories but places it well within the reach of gITT.

The hard sphere property that the temperature, $T$, only enters as a timescale via the collision frequency, $\omega_c \sim \sqrt{T}$, and does not control the physics is retained by gITT. In terms of the Péclet number, $\Pe$, and the dimensionless shear stress $\sigma/nT$, the theory is manifestly temperature independent. The choice of temperature control in an experiment, however, has a profound influence on the phenomenology observed. If shear heating is not compensated (Protocol $H$), the work expended on heating the system will manifest as an apparent shear thickening (Fig. 1). However, the viscosity $\eta \sim \sqrt{T}$ trivially rises with temperature and if we take this into account (Fig. 3), no shear thickening remains. Dialing down the random driving force we can keep the temperature constant (Protocol $T$), However, this only works below a maximal shear rate, $\dot{\gamma} \leq \omega_c \Pe_\infty$. For higher shear rates even switching off the random driving completely cannot compensate shear heating.

The Sllod equations enforce the shear profile down to the microscopic level. This is both physically questionable and prevents a straight forward coarse graining as we have seen above (Sec. IV B 1). Here we have chosen to drop the momentum buildup term $-c_i \cdot k$ in Eq. (6b) reasoning that it must vanish on macroscopic scales. Extrapolating this to the highest wave numbers constitutes an approximation on the same level as using the hydrodynamic transport coefficients away from the limit of small wave numbers. Chong and Kim [27], and Suzuki and Hayakawa [32] have chosen to retain that term, effectively neglecting the momentum conservation constraint, Eq. (6c) on all length scales. This results in an extra term $k \cdot H_q(t)$ in Eq. (47b). Both approaches are not completely satisfactory and more work is needed to derive microscopic equations of motion that enforce a linear shear profile macroscopically but are more amenable to systematic coarse graining. A possible starting point is given by Ref. 57.

We have focused here on derivation of gITT and only discussed the most fundamental predictions of the theory. The experience from the rheology of colloidal suspensions shows that the ITT formalism can contribute to the description of a much broader range of phenomena. We are planning to explore these in future work.

ACKNOWLEDGMENTS

We acknowledge crucial insight from discussions with Hisao Hayakawa, Koshiro Suzuki, Thomas Voigtmann, and Claus Heussinger. We thank the DFG for partial funding through FOR1394.
Appendix A: Density-Stress-Overlap for Hard Spheres

Only the interaction part contributes to the density-stress-overlap,

\[
\langle \sigma_{xy} | \rho q \rho_q \rangle = \frac{1 + \epsilon}{4} \times \frac{d}{N^2} \sum_{j<k} \sum_{\ell,m} \left\langle (\hat{r}_{jk} \cdot \mathbf{v}_{jk})^2 \hat{r}_j^\alpha \hat{r}_k^\beta \Theta(-\hat{r}_{jk} \cdot \mathbf{v}_{jk}) \delta(r_{jk} - d) e^{iq \cdot r_{\ell m}} \right\rangle.
\]

(A1)

The velocity average yields a factor \(T/2\), i.e.,

\[
\langle \sigma_{xy} | \rho q \rho_q \rangle = \frac{q_x q_y}{q^2} \times \frac{1 + \epsilon}{8} \times \frac{T d}{N^2} \sum_{j<k} \left\langle (\hat{q} \cdot \hat{r}_{jk})^2 \delta(r_{jk} - d) \left( e^{iq \cdot r_{jk}} + e^{-iq \cdot r_{jk}} \right) \right\rangle.
\]

(A2)

Moreover,

\[
\left\langle (\hat{q} \cdot \hat{r}_{jk})^2 \delta(r_{jk} - d) \cos(q \cdot r_{12}) \right\rangle = \frac{8 \pi}{V} \int_{0}^{\infty} dr \int_{0}^{\pi} d\vartheta r^2 g(r) \delta(r - d) \sin \vartheta \cos^2 \vartheta \Theta \left( r - d \right)
\]

(A3)

and therefore

\[
\left\langle (\hat{q} \cdot \hat{r}_{12})^2 \delta(r_{12} - d) \cos(q \cdot r_{12}) \right\rangle = -\frac{8 \pi n d N^2 \chi}{V} \frac{d^2}{d(qd)^2} \int_{0}^{\pi} d\vartheta \sin \vartheta e^{iqd \cos \vartheta},
\]

(A4)

i.e.,

\[
\left\langle (\hat{q} \cdot \hat{r}_{12})^2 \delta(r_{12} - d) \cos(q \cdot r_{12}) \right\rangle = -\frac{96 \varphi \chi}{Nd} j_0''(qd).
\]

(A5)

Collecting terms we arrive at Eq. (28).

Appendix B: Numerics

In order to solve Eqs. (56, 57, 59) numerically, we adapted an established code [25]. The temperature independence of the hard sphere equations is exploited and the explicit dependence on the coefficient of restitution has been added. For the structure factor, we use the Percus-Yevick [58] explicit solution for hard spheres [59] and for the value of the pair correlation function at contact, \(\chi\), we use the Woodcock equation of state WC1 [60]. The collision frequency is then given as the elastic Enskog expression, \(\omega_c(\varphi, T) \approx 24 \varphi \chi d^{-1} \sqrt{T/\pi} [47\]. For simplicity, instead of calculating \(\sigma\) directly, we determine the temperature independent quantity

\[
\tilde{\eta}(\text{Pe}, \varphi, \varepsilon) := \frac{1}{5\pi} \times \frac{1 + \varepsilon}{4} \int_{0}^{\infty} \frac{d\tau}{1 + (\text{Pe} \tau)^2/3} \times \int_{0}^{\infty} dk \kappa^2 j''_0\left( \text{Pe} \tau \right) j''_0(\kappa) \frac{2^2}{S^2_{\kappa}} \Phi^2_{\text{Pe} \tau}(\text{Pe} \tau).
\]

(B1)

From this result, the quantities of interest can be obtained as

\[
\frac{\sigma}{nT} = \frac{1}{2} \text{Pe} \varphi \chi^2 \tilde{\eta}, \quad \frac{\eta}{\eta_0(T)} = \frac{2}{5} \varphi \chi \tilde{\eta}, \quad \eta_B d = \frac{\tilde{\eta}}{192 \text{Pe}}.
\]

(B2)
As $\eta_0 \propto \sqrt{T}$, we can derive $\eta/\eta_0(T_0) = \sqrt{T/T_0} \times \eta/\eta_0(T)$ and in the same manner $\dot{\gamma}/\omega_c(T_0) = \text{Pe} \sqrt{T/T_0}$.

The Enskog term, $\nu_q$ Eq. (49), is known to drastically underestimate sound damping at high densities. To this end we replace it,

$$\nu_q \rightarrow \frac{20}{3} \times \frac{D_S q}{d^2} [1 + 3 j''_0(qd)],$$

where we chose the Enskog expression for the sound damping constant $D_S$ [13] and note that this expression has the correct hydrodynamic limit, $2D_S q^2$ for $q \to 0$.

For the wave number integrals, the wave numbers are discretized uniformly at 100 points between $k^* = 0.4$ and $k^* = 40$. The initial time step is $\Delta \tau = 10^{-5}$ and the step size is doubled every 100 time steps to bridge the time scales.

[1] Ralph A. Bagnold, “Experiments on a gravity-free dispersion of large solid spheres in a newtonian fluid under shear,” Proc. Royal Soc. A 225, 49–63 (1954).
[2] P. K. Haff, “Grain flow as a fluid-mechanical phenomenon,” J. Fluid Mech. 134, 401–430 (1983).
[3] Otis R. Walton and Robert L. Braun, “Viscosity, granular-temperature, and stress calculations for shearing assemblies of inelastic, frictional disks,” J. Rheol. 30, 949–980 (1986).
[4] Charles S. Campbell, “Rapid granular flows,” Annu. Rev. Fluid Mech. 22, 57–90 (1990).
[5] Heinrich M. Jaeger and Sidney R. Nagel, “Physics of the granular state,” Science 255, 1523 (1992).
[6] Richard M. Iverson, “The physics of debris flows,” Rev. Geophys. 35, 245–296 (1997).
[7] J. Javier Brey, James W. Dufty, Chang Sub Kim, and Andrés Santos, “Hydrodynamics for granular flow at low density,” Phys. Rev. E 58, 4638 (1998).
[8] S. B. Savage, “Analyses of slow high-concentration flows of granular materials,” J. Mech. 377, 1–26 (1998).
[9] Nikolai V. Brilliantov and Thorsten Pöschel, Kinetic theory of granular gases (Oxford University Press, 2004).
[10] Alexander Goldshtein and Michael Shapiro, “Mechanics of collisional motion of granular materials. Part 1. General hydrodynamic equations,” J. Fluid Mech. 282, 75–114 (1995).
[11] Isaac Goldhirsch, “Rapid granular flows,” Annu. Rev. Fluid Mech. 35, 267–293 (2003).
[12] Katharina Vollmayr-Lee, Timo Aspelmeier, and Annette Zippelius, “Hydrodynamic correlation functions of a driven granular fluid in steady state,” Phys. Rev. E 83, 011301 (2011).
[13] Vicente Garzó and José María Montanero, “Transport coefficients of a heated granular gas,” Physica A 313, 336–356 (2002).
[14] J. T. Jenkins and M. W. Richman, “Grad’s 13-moment system for a dense gas of inelastic spheres,” Arch. Rational Mech. Analysis 87, 355–377 (1985).
[15] Vicente Garzó, “Grad’s moment method for a granular fluid at moderate densities: Navier-stokes transport coefficients,” Phys. Fluids 25, 043301 (2013).
[16] James W. Dufty, “Fourier’s law for a granular fluid,” J. Phys. Chem. C 111, 15605–15612 (2007).
[17] Heinrich M. Jaeger, Sidney R. Nagel, and Robert P. Behringer, “Granular solids, liquids, and gases,” Rev. Mod. Phys. 68, 1259 (1996).
[18] B. P. Kokelaar, R. S. Bahia, K. H. Joy, S. Viroulet, and J. M. N. T. Gray, “Granular avalanches on the moon: Mass-wasting conditions, processes and features,” J. Geophys. Res. Planets (2017).

[19] K. Anki Reddy and V. Kumaran, “Applicability of constitutive relations from kinetic theory for dense granular flows,” Phys. Rev. E 76, 061305 (2007).

[20] V. Kumaran, “Dense shallow granular flows,” J. Fluid Mech. 756, 555–599 (2014).

[21] Kosho Suzuki and Hisao Hayakawa, “Rheology of dense sheared granular liquids,” in AIP Conference Proceedings, Vol. 1628 (AIP, 2014) pp. 457–466.

[22] W. Till Kranz and Matthias Sperl, “Kinetic theory for strong uniform shear flow of granular media at high density,” in EPJ Web of Conferences, Vol. 140 (EDP Sciences, 2017) p. 03064.

[23] James Jenkins and Diego Berzi, “Dense, collisional, shearing flows of compliant spheres,” in EPJ Web of Conferences, Vol. 140 (EDP Sciences, 2017) p. 01004.

[24] W. Till Kranz, Fabian Frahsa, Annette Zippelius, Matthias Fuchs, and Matthias Sperl, “Rheology of inelastic hard spheres at finite density and shear rate,” submitted to Phys. Rev. Lett. (2017).

[25] Matthias Fuchs and Michael E. Cates, “Theory of nonlinear rheology and yielding of dense colloidal suspensions,” Phys. Rev. Lett. 89, 248304 (2002).

[26] Matthias Fuchs and Michael E. Cates, “A mode coupling theory for brownian particles in homogeneous steady shear flow,” J. Rheol. 53, 957–1000 (2009).

[27] Song-Ho Chong and Bongsoo Kim, “Nonequilibrium mode-coupling theory for uniformly sheared systems,” Phys. Rev. E 79, 021203 (2009).

[28] Joseph M. Brader, Thomas Voigtmann, Matthias Fuchs, Ronald G. Larson, and Michael E. Cates, “Glass rheology: From mode-coupling theory to a dynamical yield criterion,” Proc. Natl. Acad. Sci. 106, 15186–15191 (2009).

[29] Alexandre Nicolas and Matthias Fuchs, “Shear-thinning in dense colloidal suspensions and its effect on elastic instabilities: From the microscopic equations of motion to an approximation of the macroscopic rheology,” J. Non-Newtonian Fluid Mech. 228, 64–78 (2016).

[30] W. van Megen, “Crystallisation and the glass transition in suspensions of hard colloidal spheres,” Transp. Theory Stat. Phys. 24, 1017–1051 (1995).

[31] W. Till Kranz, Matthias Sperl, and Annette Zippelius, “Glass transition for driven granular fluids,” Phys. Rev. Lett. 104, 225701 (2010).

[32] Kosho Suzuki and Hisao Hayakawa, “Nonequilibrium mode-coupling theory for uniformly sheared underdamped systems,” Phys. Rev. E 87, 012304 (2013).

[33] Denis J. Evans and Gary P. Morriss, Statistical Mechanics of Nonequilibrium Liquids (ANU Press, 2007).

[34] Timo Aspelmeier, Martin Huthmann, and Annette Zippelius, “Free cooling of particles with rotational degrees of freedom,” in Granular Gases, edited by T. Pöschel and S. Luding (Springer, 2001) pp. 31–58.

[35] D. R. M. Williams and F. C. MacKintosh, “Driven granular media in one dimension: Correlations and equation of state,” Phys. Rev. E 54, R9 (1996).

[36] C. Bizon, M. D. Shattuck, J. B. Swift, and Harry L Swinney, “Transport coefficients for granular media from molecular dynamics simulations,” Phys. Rev. E 60, 4340 (1999).

[37] Adam Ross Abate and Douglas J. Durian, “Approach to jamming in an air-fluidized granular bed,” Phys. Rev. E 74, 031308 (2006).

[38] Matthias Sperl, W. Till Kranz, and Annette Zippelius, “Single-particle dynamics in dense granular fluids under driving,” Europhys. Lett. 98, 28001 (2012).
[39] W. Till Kranz, Matthias Sperl, and Annette Zippelius, “Glass transition in driven granular fluids: A mode-coupling approach,” Phys. Rev. E 87, 022207 (2013).

[40] Sydney Chapman and Thomas George Cowling, The mathematical theory of non-uniform gases: An account of the kinetic theory of viscosity, thermal conduction and diffusion in gases (Cambridge University Press, 1970).

[41] B. J. Edwards, Chunggi Baig, and D. J. Keffer, “A validation of the p-SLLOD equations of motion for homogeneous steady-state flows,” J. Chem. Phys. 124, 194104 (2006).

[42] Aparna Baskaran, James W. Dufty, and J. Javier Brey, “Transport coefficients for the hard-sphere granular fluid,” Phys. Rev. E 77, 031311 (2008).

[43] James W. Dufty, “Stress tensor and elastic properties for hard and soft spheres,” Granular Matter 14, 271–275 (2012).

[44] We use the convention $\mathcal{F}[f](q) = \int f(r) e^{-iqr} d^3r$.

[45] The Knudsen number $Kn = \ell_0 / L$ is the dimensionless ratio of the mean free path, $\ell_0$, to a characteristic length-scale for gradients, $L$. Defining $L$ as the length over which the shear speed becomes comparable to the thermal velocity, $\dot{\gamma} L \sim \sqrt{T} \sim \omega_c \ell_0$, we have $Kn \sim Pe$.

[46] Martin Huthmann and Annette Zippelius, “Dynamics of inelastically colliding rough spheres: Relaxation of translational and rotational energy,” Phys. Rev. E 56, R6275 (1997).

[47] Jean-Pierre Hansen and Ian R. McDonald, Theory of simple liquids (Elsevier, 1990).

[48] Alan Jeffrey and Daniel Zwillinger, eds., Gradshteyn and Ryzhik’s Table of Integrals, Series, and Products, 6th ed. (Academic Press, 2000).

[49] W. Till Kranz, “A classical long-time tail in a driven granular fluid,” J. Stat. Mech. 2014, P02010 (2014).

[50] Here we use that $[q(t) - q] \cdot k = -q \cdot k \cdot kt = 0$ for simple shear.

[51] For small wave numbers $q \rightarrow 0$, and small densities, $n$, the Enskog term converges to $\nu_q \simeq 9\zeta_E q^2 / 5n$, where $\zeta_E$ is the Enskog expression for the bulk viscosity [13].

[52] Pablo G. Debenedetti and Frank H. Stillinger, “Supercooled liquids and the glass transition,” Nature 410, 259 (2001).

[53] Namiko Mitarai and Hiizu Nakanishi, “Bagnold scaling, density plateau, and kinetic theory analysis of dense granular flow,” Phys. Rev. Lett. 94, 128001 (2005).

[54] V. Kumaran, “The constitutive relation for the granular flow of rough particles, and its application to the flow down an inclined plane,” J. Fluid Mech. 561, 1–42 (2006).

[55] S. B. Savage and D. J. Jeffrey, “The stress tensor in a granular flow at high shear rates,” J. Fluid Mech. 110, 255–272 (1981).

[56] To calculate $\sigma_y$, a Herschel-Bulkley law, $\sigma(Pe) = \sigma_y + \alpha Pe^n$ [61], is fitted to the numerically determined flow curves for $Pe \leq 10^{-6}$.

[57] E. R. Smith, D. M. Heyes, D. Dini, and T. A. Zaki, “A localized momentum constraint for non-equilibrium molecular dynamics simulations,” J. Chem. Phys. 142, 074110 (2015).

[58] Jerome K. Percus and George J. Yevick, “Analysis of classical statistical mechanics by means of collective coordinates,” Phys. Rev. 110, 1 (1958).

[59] Neil W. Ashcroft and J. Lekner, “Structure and resistivity of liquid metals,” Phys. Rev. 145, 83 (1966).

[60] Marcus N. Bannerman, Leo Lue, and Leslie V. Woodcock, “Thermodynamic pressures for hard spheres and closed-virial equation-of-state,” J. Chem. Phys. 132, 084507 (2010).

[61] Winslow H. Herschel and Ronald Bulkley, “Konsistenzmessungen von Gummi-Benzollössungen,” Kolloid Z. 39, 291–300 (1926).