Kinetic theory of discontinuous shear thickening of a moderately dense inertial suspension of frictionless soft particles

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(Dated: August 1, 2022)

We demonstrate that discontinuous shear thickening (DST) can take place even in a dilute or a moderately dense inertial suspension consisting of frictionless soft particles. DST can be regarded as an ignited-quenched transition in inertial suspensions. An approximate kinetic theory agrees well with the results of the Langevin simulation results over a wide range of the volume fraction without any fitting parameters.

I. INTRODUCTION

When shear is applied to dense suspensions, there is a discontinuous jump in viscosity at a certain shear rate. This discontinuous change in viscosity is known as discontinuous shear thickening (DST) [1–4]. DST also causes a discontinuous change in the normal stress difference [5, 6]. DST can be observed even in frictional dry granular materials [7]. Although DST is analogous to the first order phase transition at equilibrium in which there exists a hysteresis, DST takes place only in nonequilibrium situations. DST is closely related to shear jamming [8–12]. Thus, DST is important for studying the physics of densely packed particles.

The origin of DST has been debated. Frictional contacts between particles are believed to be the main origin of DST [4, 7, 13, 14]. Other DST mechanisms such as order–disorder transitions [15–17] and hydrodynamic clusters [1, 18–23] have also been proposed. One of the natural questions is whether a DST-like process can take place, even if we are interested in suspensions consisting of frictionless particles.

A DST-like phenomenon can be observed in inertial suspensions, a model of aerosols [24–26], where collisions between particles play important roles. There are several theoretical studies on inertial suspensions consisting of hard-core frictionless particles based on the kinetic theory under the influence of Stokes’ drag [27–37]. The theoretical prediction quantitatively reproduces the simulation results over a wide range of volume fractions ($\varphi \lesssim 0.50$) [36, 37]. Note that the DST-like behavior, caused by an ignited–quenched transition of kinetic temperature, can be observed only in dilute inertial suspensions of hard-core particles. In particular, DST transforms into continuous shear thickening (CST) if the volume fraction $\varphi$ is greater than a few percentage [29, 33, 36, 37]. This behavior completely differs from DST commonly observed in colloidal suspensions in which DST can be observed only in dense suspensions.

Recently, Sugimoto and Takada have developed the kinetic theory of a dilute inertial suspension consisting of frictionless soft particles [38] and have found that discontinuous changes in the kinetic temperature and viscosity can take place twice. Their theoretical results agree with the results of simulations without any fitting parameters. This is a remarkable result even though the second discontinuous change can be barely observed in real experiments because the kinetic temperature in the ignited phase becomes approximately $10^6$ times higher than that in the quenched phase.

In this paper, we extend the analysis of the dilute suspension in Ref. [38] to denser situations based on the Enskog theory [36, 37, 39–44]. The relevancy of the kinetic theory in realistic systems in which hydrodynamic interactions between particles exist is discussed in a companion paper in detail [45].

The organization of this paper is as follows. In the next section, we briefly explain the Langevin equation of inertial suspensions. In Sect. III, we develop the kinetic theory of inertial suspensions under the influence of Stokes’ drag in

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a simple shear flow, and derive a set of dynamic equations describing the rheology of this system. In Sect. IV, we present the results of steady state rheology obtained from both the kinetic theory and Langevin simulation, where we verify the existence of DST-like processes over a wide range of parameters. In Sect. V, we conclude and discuss our results. Appendix A contains an explanation of the framework of the kinetic theory and the derivation of the kinetic equation. In Appendix B, we present detailed expressions of the scattering angle $\chi$ and the minimum distance $r_{\text{min}}$ for a contact. In Appendix C, we discuss the convergence of the expression of the stress tensor in terms of a series expansion of the dimensionless shear rate.

II. LANGEVIN MODEL

We consider $N$ monodisperse frictionless soft particles (mass $m$ and diameter $d$ of each particle), which are suspended in a fluid (the viscosity $\eta_0$) and are confined in a three-dimensional cubic box with the linear size $L$ as shown in Fig. 1. We assume that the contact force between particles is described by the harmonic potential

$$U(r) = \frac{\varepsilon}{2} \left(1 - \frac{r}{d}\right)^2 \Theta \left(1 - \frac{r}{d}\right)$$

for $r > r_{\text{min}}$, where $r$ represents the inter-particle distance and $\varepsilon$ represents the energy scale to characterize the repulsive interaction, $\Theta(x)$ defined as $\Theta(x) = 1$ ($x \geq 0$) and $0$ ($x < 0$) is the step function. We also assume the existence of an inner-hard core at $r = r_{\text{min}}$ for the theoretical analysis; however, we do not take into account the inner-hard-core for the Langevin simulation. Although clustering effects caused by attractive interactions between particles cannot be ignored in realistic situations, such effects are suppressed if the particles are charged [46–48]. In addition, particles are prevented from clustering if the temperature is sufficiently high [27, 49–51].

FIG. 1. A snapshot of our system. Particles are initially distributed at random. The arrows indicate the shear direction.

The equation of motion of the suspended particle $i$ (its position $\mathbf{r}_i$ and peculiar momentum $\mathbf{p}_i$) under a simple shear with the shear rate $\dot{\gamma}$ is given by

$$\frac{d\mathbf{p}_i}{dt} = \sum_{j \neq i} \mathbf{F}_{ij} - \zeta \mathbf{p}_i + \mathbf{\xi}_i,$$  \hspace{1cm} (2)

where $\mathbf{p}_i \equiv m \mathbf{V}_i$ with $\mathbf{V}_i \equiv \mathbf{v}_i - \dot{\gamma} y_i \hat{e}_x$ with the unit vector $\hat{e}_x$ parallel to the $x$ direction and the velocity $\mathbf{v}_i$ of $i$–th particle, $\mathbf{F}_{ij} \equiv -\partial U(r_{ij})/\partial \mathbf{r}_{ij}$ is the inter-particle force between $i$–th and $j$–th particles with $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$ and $r_{ij} \equiv |\mathbf{r}_{ij}|$. Note that the drag coefficient $\zeta$ is expressed as $\zeta = 3\pi \eta_0 d/m$. The noise $\mathbf{\xi}_i(t) = \xi_{i,\alpha}(t) \hat{e}_\alpha$ satisfies the fluctuation–dissipation relation:

$$\langle \mathbf{\xi}_i(t) \rangle = 0, \quad \langle \xi_{i,\alpha}(t) \xi_{j,\beta}(t') \rangle = 2mT_{\text{env}} \zeta \delta_{ij} \delta_{\alpha\beta} \delta(t - t'),$$  \hspace{1cm} (3)

where $\langle \cdot \rangle$ denotes the average over the noise and $T_{\text{env}}$ is the environmental (solvent) temperature.

The assumptions behind Eqs. (2) and (3) are summarized as follows. (i) Particles are suspended by a fluid in which the motion of particles is agitated by the white Gaussian noise as in Eq. (3), (ii) the hydrodynamic interaction between
particles is negligible, (iii) the environmental temperature $T_{\text{env}}$ is independent of the motion of suspended particles, and (iv) the effects of gravity can be ignored. Although gravitational sedimentation affects aerosols, the effect is negligible within the observation time for small suspended particles [25, 26]. In addition, an inertial suspension can be regarded as a model of a colloidal suspension, where the sedimentation effect is negligible. Note that the role of hydrodynamic interactions among particles in inertial suspensions is analyzed in the complementary paper [45].

We adopt the SLLOD dynamics [52, 53] to simulate the shear flow under the Lees-Edwards boundary condition [54] (see Fig. 1). To the best of our knowledge, the uniform flow is stable once the system reaches a steady state.

III. KINETIC THEORY OF INERTIAL SUSPENSIONS

In this section, we develop the kinetic theory of inertial suspensions consisting of frictionless soft particles. In the first subsection, we present the kinetic equation for a one-body distribution (Enskog equation) for inertial suspensions. In the next subsection, we present moment equations for the stress tensor. In the third subsection, we employ Grad’s approximation to obtain a set of closure equations.

A. Enskog equation for inertial suspensions

The kinetic theory is a powerful tool for describing the behavior of inertial suspensions quantitatively. The basic assumption of the kinetic theory is that both the random noise and collisions between particles are important even though collisions have previously been ignored in colloidal suspension analysis.

As shown in Appendices A1 and A2, the kinetic equation for the one-body distribution function $f(r_1, V_1; t)$ can be written as

$$\left[\frac{\partial}{\partial t} + (V_1 + \gamma y_1 \hat{e}_x) \cdot \frac{\partial}{\partial r_1} - \gamma V_{1,y} \frac{\partial}{\partial V_{1,z}}\right] f(1) \approx \zeta \frac{\partial}{\partial V_1} \cdot \left[ \left(V_1 + \frac{T_{\text{env}}}{m} \frac{\partial}{\partial V_1}\right) f(1) \right] + J[V|f^{(2)}(1, 2)],$$

where (1) is the abbreviation of $(r_1, V_1; t)$. Here, we have introduced $f^{(2)}(1, 2) \equiv f^{(2)}(r_1, V_1, r_2, V_2; t)$ as the two-body distribution function. Since it is difficult to handle hydrodynamic interactions between particles within the framework of the kinetic theory, we ignore such hydrodynamic interactions.

If the system is assumed to be spatially uniform, Eq. (4) is reduced to [29, 30, 32, 37, 39–44]

$$\left(\frac{\partial}{\partial t} - \gamma V_{1,y} \frac{\partial}{\partial V_{1,z}}\right) f(V_1, t) = \zeta \frac{\partial}{\partial V_1} \cdot \left[ \left(V_1 + \frac{T_{\text{env}}}{m} \frac{\partial}{\partial V_1}\right) f(V_1, t) \right] + J[V|f^{(2)}(1, 2)].$$

If the interaction is short-ranged, $J[V|f^{(2)}(1, 2)]$ is given by [39]

$$J[V|f^{(2)}(1, 2)] = \int dV_2 \int d\Omega S(\chi, V_{12}) V_{12} \left[f^{(2)}(1'', 2'') - f^{(2)}(1, 2)\right],$$

where $V_{12} \equiv |V_1 - V_2|$, $(1'', 2'')$ denotes a set of pre-collisional positions and velocities of $(1, 2)$, $\chi$ represents the scattering angle, $d\Omega = \sin \chi d\chi d\phi$, and $S(\chi, V)$ is the differential collision cross-section (see also Fig. 2). The explicit expression of $\chi$ is presented in Appendix B.

So far, the kinetic equation (5) for the one-body distribution $f(V, t)$ cannot be solved because it contains the two-body distribution $f^{(2)}(1, 2)$. Let us adopt four assumptions to obtain the closure of the one-body distribution. First, we assume that $J[V|f^{(2)}(1, 2)]$ can be approximated as [39]

$$J[V|f^{(2)}(1, 2)] \approx \int dV_2 \int d\Omega S(\chi, V_{12}) V_{12} \left[f^{(2)}(r, V_1''', r + r_{\text{min}} \hat{k}_{12}, V_2'''; t) - f^{(2)}(r, V_1, r - r_{\text{min}} \hat{k}_{12}, V_2; t)\right],$$

where $\hat{k}_{12} \equiv (r_2 - r_1)/r_2 - r_1$, and the minimum relative distance between the contacted particles $r_{\text{min}}$ for the inner-hard-core is given by Eq. (B1b). Second, we assume that the relationships between pre-collisional velocities $(V_1''', V_2''')$ and post-collisional ones $(V_1, V_2)$ at $r = r_{\text{min}}$ are given by

$$\begin{cases} V_1''' \simeq V_1 - (V_{12} \cdot \hat{k}_{12}) \hat{k}_{12} \\ V_2''' \simeq V_2 + (V_{12} \cdot \hat{k}_{12}) \hat{k}_{12} \end{cases},$$

where there is no energy dissipation during a collision. We also adopt the decoupling approximation of the two-body distribution function in which the function can be expressed as a product of one-body distribution functions multiplied
FIG. 2. A schematic of a scattering process between two colliding particles with the impact parameter $b$ and the relative speed $v$, where the scattering angle $\chi$ and the closest distance $r_{\text{min}}$ are given by Eqs. (B1).

by the correlation function. Such a procedure is used in the Boltzmann equation for dilute gases and its counterpart the Enskog equation for moderately dense gases [29, 30, 32, 37, 39–44]. Because there exists the inner-hard core at $r = r_{\text{min}}$, we may use the decoupling approximation for hard-core particles as

$$f^{(2)}(1, 2) \approx g_0 f(1) f(2),$$

where $g_0 = (1 - \varphi/2)/(1 - \varphi)^3$ with the volume fraction $\varphi \equiv \pi N d^3/(6L^3)$ is the dimensionless geometric factor to express the effect of the finite density [55]. Note that the volume fraction is not measured by the inner-core but by the outer boundary of the potential force. The last assumption we use is

$$f \left( r \mp \frac{r_{\text{min}}}{2} k_{12}, v_1, t \right) \approx f \left( V_1 \pm \frac{1}{2} \dot{\gamma} r_{\text{min}} k_{12} e_x, t \right),$$

because we are interested in spatially uniform cases. The validity of the above crude approximations can be verified by comparing the theoretical results with the numerical results.

Thus, we obtain the Enskog equation for the inertial suspension of soft frictionless particles as

$$\left( \frac{\partial}{\partial t} - \dot{\gamma} V_{1,y} \frac{\partial}{\partial V_{1,x}} \right) f(V_1, t) = \zeta \frac{\partial}{\partial V_1} \left[ \left( V_1 + \frac{T_{\text{env}}}{m} \frac{\partial}{\partial V_1} \right) f(V_1, t) \right]$$

$$+ g_0 \int dV_2 \int d\Omega S(\chi, V_{12}) V_{12} \left[ f \left( V_1'' - \frac{1}{2} \dot{\gamma} r_{\text{min}} k_{12} e_x, t \right) f \left( V_2'' + \frac{1}{2} \dot{\gamma} r_{\text{min}} k_{12} e_x, t \right) \right]$$

$$- f \left( V_1 + \frac{1}{2} \dot{\gamma} r_{\text{min}} k_{12} e_x, t \right) f \left( V_2 - \frac{1}{2} \dot{\gamma} r_{\text{min}} k_{12} e_x, t \right).$$

B. Moment equations of the stress tensor

This study focuses on viscosity, kinetic temperature, and normal stress differences. Thus, let us define the kinetic temperature $T$

$$T \equiv \frac{1}{N} \sum_i \left\langle \frac{p_i^2}{3m} \right\rangle,$$

and the viscosity $\eta$

$$\eta \equiv \frac{\sigma_{xy}}{\dot{\gamma}}.$$

Here, the stress tensor $\sigma_{\alpha\beta}$ consists of two parts:

$$\sigma_{\alpha\beta} = \sigma_{\alpha\beta}^k + \sigma_{\alpha\beta}^c,$$
respectively, with the dimensionless shear rate \( \dot{\gamma} \) where the former and latter characterize the softness of particles \[38\] and the strength of noise \[27, 36, 38\], respectively.

Let us introduce two dimensionless parameters for later convenience:

\[
\varepsilon^* \equiv -\frac{\varepsilon}{md^2\zeta_T}, \quad \xi_{\text{env}} \equiv \frac{1}{m} \frac{1}{d\varepsilon},
\]

where the former and latter characterize the softness of particles \[38\] and the strength of noise \[27, 36, 38\], respectively. We note that \( \varepsilon^* \) and \( \xi_{\text{env}} \) diverge as \( m \) approaches zero. In particular, \( \varepsilon^* \rightarrow \infty \) and \( \xi_{\text{env}} \rightarrow \infty \) correspond to the over-damp limit.

Once we adopt the above-mentioned approximations, the contact stress tensor is written as

\[
\sigma_{\alpha\beta}^c \simeq \frac{m}{2} g_0 \int dV_1 \int dV_2 \int d\Omega S(\chi, V_{12}) V_{12}^2 r_{\text{min}}(V_{12} : \mathbf{k}_{12}) \mathbf{k}_{12,\alpha} \mathbf{k}_{12,\beta} \times f \left( V_1 + \frac{1}{2} \dot{\gamma} r_{\text{min}} \hat{\mathbf{k}}_{12,y} \hat{\mathbf{e}}_x, t \right) f \left( V_2 - \frac{1}{2} \dot{\gamma} r_{\text{min}} \hat{\mathbf{k}}_{12,y} \hat{\mathbf{e}}_x, t \right).
\]

Multiplying Eq. (5) by \( mV_\alpha V_\beta \) we obtain the evolution equations for the kinetic stress \( \sigma_{\alpha\beta}^k \) as

\[
\frac{d}{dt} \sigma_{\alpha\beta}^k + \dot{\gamma} \left( \delta_{\alpha x} \sigma_{y\beta}^k + \delta_{\beta x} \sigma_{y\alpha}^k \right) = -2\zeta \left( \sigma_{\alpha\beta}^k + nT_{\text{env}} \delta_{\alpha\beta} \right) + \Lambda_{\alpha\beta},
\]

where

\[
\Lambda_{\alpha\beta} \equiv -m \int dV V_\alpha V_\beta J[V|f, f].
\]

The collisional moment \( \Lambda_{\alpha\beta} \) in Eq. (19) can be expressed as

\[
\Lambda_{\alpha\beta} \simeq \frac{m}{2} g_0 \int dV_1 \int dV_2 \int d\Omega S(\chi, V_{12}) V_{12}(V_{12} : \mathbf{k}_{12}) \times \left[ V_{12,\alpha} \hat{\mathbf{k}}_{12,\beta} + V_{12,\beta} \hat{\mathbf{k}}_{12,\alpha} - 2(V_{12} : \mathbf{k}_{12}) \hat{\mathbf{k}}_{12,\alpha} \hat{\mathbf{k}}_{12,\beta} \right] f \left( V_1 + \frac{1}{2} \dot{\gamma} r_{\text{min}} \hat{\mathbf{k}}_{12,y} \hat{\mathbf{e}}_x, t \right) f \left( V_2 - \frac{1}{2} \dot{\gamma} r_{\text{min}} \hat{\mathbf{k}}_{12,y} \hat{\mathbf{e}}_x, t \right)
\]

\[
- \dot{\gamma} \left( \delta_{\alpha x} \sigma_{y\beta}^c + \delta_{\beta x} \sigma_{y\alpha}^c \right).
\]

Then, we obtain

\[
\frac{d\theta}{dt} = -\frac{2}{3} \dot{\gamma}^* \Pi_{xy} + 2(1 - \theta) - \frac{1}{3} \Lambda_{\alpha\alpha}^*,
\]

\[
\frac{d\Delta \theta}{dt} = -2\dot{\gamma}^* \Pi_{xy} - 2\Delta \theta - \Delta \Lambda_{xx}^* + \Delta \Lambda_{yy}^*,
\]

\[
\frac{d\delta \theta}{dt} = -2\dot{\gamma}^* \Pi_{xy} - 2\delta \theta - 2\delta \Lambda_{xx}^* - \delta \Lambda_{yy}^*,
\]

\[
\frac{d\Pi_{xy}}{dt} = -\dot{\gamma}^* (\theta + \Pi_{yy}) - 2\Pi_{xy} - \Lambda_{xy}^*,
\]

where we have introduced the dimensionless temperature \( \theta \), anisotropic temperatures \( \Delta \theta \) and \( \delta \theta \), and dimensionless kinetic deviatoric stress \( \Pi_{xy} \) as

\[
\theta \equiv \frac{T}{T_{\text{env}}}, \quad \Delta \theta \equiv \frac{\sigma_{xy}^k - \sigma_{xx}^k}{nT_{\text{env}}}, \quad \delta \theta \equiv \frac{\sigma_{zz}^k - \sigma_{xx}^k}{nT_{\text{env}}}, \quad \Pi_{\alpha\beta} \equiv \frac{\sigma_{\alpha\beta}^k}{nT_{\text{env}}} + \theta \delta_{\alpha\beta},
\]

respectively, with the dimensionless shear rate \( \dot{\gamma}^* \equiv \dot{\gamma}/\zeta \) and the dimensionless time \( \tau \equiv \zeta t \). We have also introduced the scaled collisional moment \( \Lambda_{\alpha\beta}^* \equiv \Lambda_{\alpha\beta}/(n\zeta T_{\text{env}}) \) with

\[
\delta \Lambda_{xx}^* \equiv \Lambda_{xx}^* - \frac{1}{3} \Lambda_{\alpha\alpha}^*, \quad \delta \Lambda_{yy}^* \equiv \Lambda_{yy}^* - \frac{1}{3} \Lambda_{\alpha\alpha}^*.
\]

In this paper, we adopt Einstein’s convention in which double Greek characters take summation over \( x, y, \) and \( z \), i.e., \( \Lambda_{\alpha\alpha}^* = \Lambda_{xx}^* + \Lambda_{yy}^* + \Lambda_{zz}^* \).
C. Grad’s approximation

Although we have adopted four assumptions to simplify our calculation, it is still difficult to solve a set of equations (21) because the collision moment $\Lambda^*_\alpha\beta$ is an integral of the nonlinear function of $f(\mathbf{V}, t)$. It is known that Grad’s approximation [44, 56, 57]

$$f(\mathbf{V}, t) \simeq n v_T^{-3} f_M(c, t) \left(1 - \frac{\Pi_{\alpha\beta}}{\theta} c_\alpha c_\beta\right)$$  \hspace{1cm} (24)

with

$$c \equiv \frac{\mathbf{V}}{v_T}, \quad v_T \equiv \sqrt{\frac{2T}{m}},$$  \hspace{1cm} (25)

and the Maxwell distribution

$$f_M(c, t) = \pi^{-3/2} \exp \left(-c^2 \right),$$  \hspace{1cm} (26)

yields good approximations of $\Lambda^*_\alpha\beta$ for hard-core [27, 36, 37, 42, 44, 58–66] and dilute soft-core [38, 67] systems. An extended Grad’s approximation is also used for non-Brownian suspensions, where $\Pi_{\alpha\beta}$ is replaced with the counterpart of the contact stress [68]. We adopt Grad’s approximation for moderately dense inertial suspensions consisting of soft-core particles in this paper.

When analyzing collision processes of soft particles, we need to consider the time dependence of differential cross section $S(\chi, V_{12})$, which is very complicated to handle precisely. Instead, we adopt the replacement in Eq. (17) with

$$\int d\Omega S(\chi, V_{12}) V_{12} F(\hat{\mathbf{k}}, r_{\min}) \rightarrow \Omega^*_{2,2} d^2 \int d\hat{\mathbf{k}} \Theta(V_{12} \cdot \hat{\mathbf{k}})(V_{12} \cdot \hat{\mathbf{k}}) F(\hat{\mathbf{k}}, d)$$  \hspace{1cm} (27)

for an arbitrary function $F(\hat{\mathbf{k}}, r_{\min})$ of $\hat{\mathbf{k}}$ and $r_{\min}$, where $\Omega^*_{2,2}$ is defined as [38, 69, 70]

$$\Omega^*_{k,\ell}(T^*) \equiv \int_0^\infty dy y^{2\ell+3} e^{-y^2} \int_0^1 db^* b^* \left[1 - \sin^k \left(b^*, 2y\sqrt{T^*}\right)\right]$$  \hspace{1cm} (28)

with $k = \ell = 2$. The replacement (27) means that the collision cylinder per unit time of soft-core particles $S(\chi, V_{12}) V_{12}$ is approximated by that of hard-core particles $d^2(V_{12} \cdot \hat{\mathbf{k}})$ with the effect of softness $\Omega^*_{2,2}$. The temperature dependence of $\Omega^*_{2,2}$ is plotted in Fig. 3. The integral $\Omega^*_{2,2}$ behaves as $\Omega^*_{2,2} \sim T^{-2}$ and $1 - \Omega^*_{2,2} \sim T^{1/2}$ in the high and low temperature regimes, respectively [38]. We also find that the temperature dependence of $\Omega^*_{2,2}$ can be well fitted by:

$$\Omega^*_{2,2}(T^*) = \frac{1}{1 + a_0 \sqrt{T^*} + a_1 T^* + a_2 T^{*2}},$$  \hspace{1cm} (29)
with $T^* = T/\varepsilon$ and

$$a_0 \simeq 2.6206, \quad a_1 \simeq 0.39208, \quad a_2 \simeq 154.37.$$  \hfill (30)

The relative error $|\Omega^*_{2,2} - \Omega_{2,2}|/\Omega^*_{2,2}$ is smaller than $2 \times 10^{-2}$ as shown in the inset of Fig. 3. Thus, it is sufficient to use Eq. (29) for the practical application of $\Omega^*_{2,2}$.

After we introduce the approximation Eq. (27), softness only appears through $\Omega^*_{2,2}$. Now, it is useful to introduce the collision frequency of soft-core particles as

$$\nu_{\text{soft}} \equiv \Omega^*_{2,2}\nu_{\text{HC}},$$  \hfill (31)

with the collision frequency for hard-core gases

$$\nu_{\text{HC}} \equiv \frac{96}{5\sqrt{\pi}}g_0\varphi_{\text{env}}\sqrt{\zeta},$$  \hfill (32)

Based on Eqs. (24) and (27), we can rewrite Eqs. (17) and (20) as

$$\tau_{\alpha\beta} \simeq -\gamma \left( \delta_{\alpha x}\sigma_{x\beta} + \delta_{\beta x}\sigma_{x\alpha} \right) + \frac{m}{2}d^2\gamma_0\Omega^*_{2,2} \int dV_1 \int dV_2 \int d\hat{k}\Theta(V_{12}\cdot\hat{k})(V_{12}\cdot\hat{k})^2$$

$$\times \left[ V_{12,\alpha}\hat{k}_\beta + V_{12,\beta}\hat{k}_\alpha - 2(V_{12}\cdot\hat{k})\hat{k}_\alpha\hat{k}_\beta \right] f(V_1 + \gamma d\hat{k}_y\hat{e}_x, t)f(V_2, t),$$  \hfill (33a)

$$\sigma_{\alpha\beta} \simeq -\frac{m}{2}d^3\gamma_0\Omega^*_{2,2} \int dV_1 \int dV_2 \int d\hat{k}\Theta(V_{12}\cdot\hat{k})(V_{12}\cdot\hat{k})^2\hat{k}_\alpha\hat{k}_\beta f \left( V_1 + \frac{1}{2}\gamma d\hat{k}_y\hat{e}_x, t \right)f \left( V_1 - \frac{1}{2}\gamma d\hat{k}_y\hat{e}_x, t \right),$$  \hfill (33b)

respectively. We follow a procedure parallel to those used in Refs. [37, 71, 72], where the collisional moment and contact stress are written in series of the shear rate. Thus, the corresponding terms in Eq. (23) are, respectively, given by

$$\Lambda^*_{\alpha\beta} \simeq \varphi_0\varphi_{\text{env}}\theta^{3/2}\Omega^*_{2,2} \sum_{i=0}^{\infty} C^{(i)}_{1} \tilde{\gamma}^i,$$  \hfill (34a)

$$\Lambda^*_{xy} \simeq \varphi_0\varphi_{\text{env}}\theta^{3/2}\Omega^*_{2,2} \sum_{i=0}^{\infty} C^{(i)}_{2} \tilde{\gamma}^i,$$  \hfill (34b)

$$\delta\Lambda^*_{xx} \simeq \varphi_0\varphi_{\text{env}}\theta^{3/2}\Omega^*_{2,2} \sum_{i=0}^{\infty} C^{(i)}_{3} \tilde{\gamma}^i,$$  \hfill (34c)

$$\delta\Lambda^*_{yy} \simeq \varphi_0\varphi_{\text{env}}\theta^{3/2}\Omega^*_{2,2} \sum_{i=0}^{\infty} C^{(i)}_{4} \tilde{\gamma}^i,$$  \hfill (34d)

$$\Pi^*_{xy} \simeq \varphi_0\theta\Omega^*_{2,2} \sum_{i=0}^{\infty} C^{(i)}_{5} \tilde{\gamma}^i,$$  \hfill (34e)

where we have introduced the dimensionless contact stress

$$\Pi^*_{\alpha\beta} \equiv \frac{\sigma^*_\alpha\beta}{nT_{\text{env}}} + \theta\delta_{\alpha\beta},$$  \hfill (35)

and the expansion parameter $\tilde{\gamma}$ as

$$\tilde{\gamma} \equiv \frac{\tilde{\gamma}^*}{\sqrt{\varphi_{\text{env}}}}.$$  \hfill (36)

Note that the expressions of the coefficients $C^{(i)}_1$, $C^{(i)}_2$, $C^{(i)}_3$, $C^{(i)}_4$, and $C^{(i)}_5$ are equivalent to $\Lambda^{(i)}_{0\alpha}$, $\Lambda^{(i)}_{xy}$, $\delta\Lambda^{(i)}_{xx}$, $\delta\Lambda^{(i)}_{yy}$, and $\Pi^{(i)}_{xy}$ in Ref. [37], respectively. We also note that $\tilde{\gamma}$ approaches zero in both the low and high shear limits as reported in Ref. [37]. In particular, the expansions in the set of equations (34) become crucial only for the intermediate shear rate.
IV. STEADY RHEOLOGY IN THE SCALAR DRAG MODEL

In this section, we present rheology based on our model by solving a set of dynamic equations (21). However, it is impossible to obtain the analytic expressions of the set of equations (34). Nonetheless, we use numerical expansions of Eqs. (34) with the truncation by $N_c$ terms. We have verified that $N_c = 2$ is sufficient to obtain convergent results as shown in Appendix C. Although the results of the linear theory with $N_c = 1$ slightly deviate from those of $N_c \geq 2$, there are some analytic expressions in the linear theory, as presented in Appendix C. Substituting them into Eqs. (21), we obtain a steady solution of Eq. (21). Once we obtain the steady solution, the expression of the viscosity becomes

$$\eta^* \equiv \frac{\Pi_{xy} + \Pi_{cxy}}{\dot{\gamma}^*},$$

(37)

To reach a steady state, we gradually increase and decrease the dimensionless shear rate as $\dot{\gamma}^* = a_n \dot{\gamma}^*_0$ with $a_n = 10^{-0.01} = 1.023$ and $a = 10^{-0.01} = 0.9772$, where we have chosen $\dot{\gamma}^*_0 = 1.0$ and 100, respectively.

![Fig. 4](https://example.com/fig4.png)

**Fig. 4.** Plots of the theoretical (a) $\eta^*$ and (b) $\theta$ against $\dot{\gamma}^*$ for $\phi = 0.10$ (dotted line), 0.20 (dashed line), and 0.30 (solid line) with fixing $\xi_{mov} = 1.0$, $\varepsilon^* = 10^4$, and $N_c = 2$, where the theoretical curves are obtained by Eqs. (21), (34), and (37). The left and right vertical dotted lines indicate discontinuous changes in $\eta^*$ and $\theta$ from the ignited and quenched phases, respectively. The circle ($\phi = 0.3$), square ($\phi = 0.2$), and triangle ($\phi = 0.1$) symbols correspond to the simulation results.

![Fig. 5](https://example.com/fig5.png)

**Fig. 5.** Plots of the theoretical (a) $\eta^*$ and (b) $\theta$ against $\dot{\gamma}^*$ for $\phi = 0.40$ (dotted line) and 0.50 (dashed line) with fixing $\xi_{mov} = 1.0$ and $\varepsilon^* = 10^4$, where the theoretical curves are obtained by Eqs. (21), (34), and (37). The left and right vertical dotted lines indicate discontinuous changes in $\eta^*$ from the ignited and quenched phases, respectively. The circle ($\phi = 0.50$) and square ($\phi = 0.40$) symbols correspond to the simulation results.

Figures 4 and 5 compare the theory of $N_c = 2$ for $\eta^*$ and $\theta$ versus $\dot{\gamma}^*$ with the simulation results for $\phi = 0.10$, 0.20, and 0.30 in Fig. 4, and 0.40 and 0.50 in Fig. 5, respectively, with fixing $\varepsilon^* = 10^4$, and $\xi_{mov} = 1.0$. The theoretical values of $\eta^*$ and $\theta$ are obtained by solving the set of Eqs. (21) with the aid of Eqs. (34) and (37). We have numerically solved the set of equations (21) under the initial kinetic temperature $\theta = 1$ at $t = 0$. As shown in these figures, the theory agrees well with the simulation results, even for $\phi = 0.50$, even though the agreement between the theory and
simulation results for large $\varphi$ is slightly worse than that in the dilute case. Note that all theoretical flow curves with DST and ignited–quenched transitions are associated with hysteresis. Thus, DST and ignited–quenched transitions are similar to the first-order phase transition in equilibrium thermodynamics.

Remarkably, DST can be observed over a wide range of $\varphi$ from the dilute limit [38] to $\varphi = 0.50$, as shown in Figs. 4 and 5. These results differ from the conventional DST, which can be observed only in dense colloidal suspensions [1–4, 51]. These discontinuous changes in $\eta^*$ and $\theta$ in the wide range of $\varphi$ are also different from those of hard-core inertial suspensions, where DST transforms into the CST above a critical fraction which is a few percentage [27, 29, 33, 36, 37]. Our results indicate that the DST observed here is induced by the softness and the inertial effect of particles.

Interestingly, the contact stress $\sigma_{xy}^c$ decreases as $\dot{\gamma}^*$ increases for $\dot{\gamma} > \dot{\gamma}_c^*$, whereas the kinetic stress abruptly increases around $\dot{\gamma} = \dot{\gamma}_c$ as shown in Fig. 6. These are because the duration time becomes negligibly small when the kinetic temperature becomes sufficiently high. Thus, DST can be observed only when we consider the kinetic stress. Our result is consistent with that of Kawasaki et al. [49] who presented only the contact stress.

Figures 7 and 8 also show how the DST-like transitions of $\eta^*$ and $\theta$ depend on $\varphi$ and $\dot{\gamma}^*$ for $\xi_{av} = 1.0$ and $\varepsilon^* = 10^4$, respectively, with fixing $\xi_{av} = 1.0$ based on the kinetic theory with $N_c = 2$. As indicated by Ref. [38], there are two-step DST-like changes in $\eta^*$ and $\theta$ at $\dot{\gamma}_c^*$ and $\dot{\gamma}_c^*$ for dilute inertial suspensions. The DST-like change at $\dot{\gamma}_c^*$ disappears for $\varphi > \varphi_{c1} \approx 0.01$, corresponding to the disappearance of DST in hard-core systems. On the other hand, the DST-like changes in $\eta^*$ and $\theta$ at $\dot{\gamma}_c^*$ survive in the wide range of $\varphi$ for larger $\varepsilon^*$ (see Fig. 8).

These results are counter-intuitive, but as shown in Fig. 9, $\eta^*$ can be scaled by $\varepsilon^*^{4/3}$ in the vicinity of $\dot{\gamma}_c^*$ except for the case of $\varepsilon^* = 1.0$. This means that viscosity in the ignited phase diverges in the hard-core limit. Thus, we can only observe CST in moderately dense inertial suspensions consisting of hard-core particles. Note that $\eta^*$ is almost
FIG. 8. The theoretical flow curves ((a) \( \eta^* \) and (b) \( \theta \)) against \( \varphi \) and \( \dot{\gamma}^* \) for \( \xi_{\text{env}} = 1.0 \) and \( \varepsilon^* = 10^8 \), where the theoretical curves are obtained by Eqs. (21), (34), and (37). Here, the red and blue lines indicate the flow curves in the ignited and quenched phases, respectively, whereas the purple lines represent the intermediate thickening phase that appears only for \( \varphi < 1.8 \times 10^{-2} \).

FIG. 9. Plots of \( \eta^*/\varepsilon^{4/3} \) against \( \dot{\gamma}^* \) for various \( \varepsilon^* \) with fixing \( \varphi = 0.40 \) and \( \xi_{\text{env}} = 1.0 \). The theoretical results are expressed as lines (red solid lines for \( \varepsilon^* = 10^8 \), blue dashed line for \( \varepsilon^* = 10^4 \), purple dotted line for \( \varepsilon^* = 10^2 \) and black chain line for \( \varepsilon^* = 1 \)), where the theoretical curves are obtained by Eqs. (21), (34), and (37). The symbols (circles for \( \varepsilon^* = 10^8 \), squares for \( \varepsilon^* = 10^4 \), purple upper triangles for \( \varepsilon^* = 10^2 \) and black lower triangles for \( \varepsilon^* = 1 \)) are obtained by simulations. The left and right vertical dotted lines represent discontinuous changes in \( \eta^* \) from the ignited and quenched phases, respectively.

independent of \( \dot{\gamma}^* \) for \( \varepsilon^* = 1.0 \). This suggests that the rheology of the inertial suspension of very soft particles is different from that of moderately hard particles.

We also check how rheology depends on the softness parameter \( \varepsilon^* \). Figure 10 compares the theoretical results with the simulation results for \( \varepsilon^* = 10^0, 10^2, 10^4, \) and \( 10^6 \) with fixed \( \varphi = 0.40 \) and \( \xi_{\text{env}} = 1.0 \). As shown in Fig. 10, the theory agrees well with the simulation results. Figure 10 also indicates that the DST-like discontinuous changes in \( \eta^* \) and \( \theta \) of moderately dense inertial suspensions disappear, at least, for \( \varepsilon^* \leq 10 \).

Next, let us investigate the \( \xi_{\text{env}} \) dependence of the flow curves. Figure 11 shows that the theory works well over the wide range of \( \xi_{\text{env}} \) when we fix \( \varphi = 0.30 \) and \( \varepsilon^* = 10^3 \). The DST-like changes in \( \eta^* \) and \( \theta \) disappear if \( \xi_{\text{env}} \) is sufficiently large such as \( \xi_{\text{env}} = 10^5 \). To clarify the critical \( \xi_{\text{env}} \), we control \( \xi_{\text{env}} \) in the range \( 60 \leq \xi_{\text{env}} \leq 70 \) with fixing \( \varphi = 0.30 \) and \( \varepsilon^* = 10^3 \). As shown in Fig. 12, the divergence of the slope \( d\eta^*/d\dot{\gamma}^* \) disappears at around \( \xi_{\text{env}} \approx 66 \). This means that there is a transition from DST to CST at this point.

Figures 13 presents the simulation results to show how \( \eta^* \) and \( \theta \) depend on \( \varepsilon^* \) and \( \dot{\gamma}^* \) for \( \varphi = 0.4 \) and \( \xi_{\text{env}} = 1.0 \). These figures indicate that both \( \eta^* \) and \( \theta \) are continuous for small \( \varepsilon^* \) but become discontinuous if \( \varepsilon^* \) is greater than a critical value. Similarly, Fig. 14 illustrates how \( \eta^* \) and \( \theta \) depend on \( \dot{\gamma}^* \) and \( \xi_{\text{env}} \) for \( \varphi = 0.40 \) and \( \varepsilon^* = 10^4 \). These figures indicate that the discontinuous changes in \( \eta^* \) and \( \theta \) become continuous if \( \xi_{\text{env}} \) is greater than a critical value.

V. CONCLUDING REMARKS

In this paper, we have successfully demonstrated the existence of DST-like changes in the viscosity and kinetic temperature for moderately dense inertial suspensions composed of frictionless soft particles through Langevin simu-
FIG. 10. Plots of (a) $\eta^*$ and (b) $\theta$ against $\dot{\gamma}^*$ for $\varepsilon^* = 1, 10^2, 10^4$, and $10^6$ with fixed $\varphi = 0.40$ and $\xi_{env} = 1.0$. Here, the lines express the theoretical flow curves with $N_c = 2$ obtained by Eqs. (21), (34), and (37). The corresponding symbols are obtained by simulations. The left and right vertical dotted lines represent discontinuous changes in $\eta^*$ from the ignited and quenched phases, respectively.

FIG. 11. Plots of (a) $\eta^*$ and (b) $\theta$ against $\dot{\gamma}^*$ for $\xi_{env} = 10^{-1}, 10^0, 10^1$, and $10^2$ when we fix $\varphi = 0.30$ and $\varepsilon^* = 10^4$. Here, the lines express the theoretical expressions, where the theory is given by Eqs. (21), (34), and (37). The corresponding symbols are obtained by simulations. The left and right vertical dotted lines represent discontinuous changes in $\eta^*$ from the ignited and quenched phases, respectively.

FIG. 12. Plots of $d\eta^*/d\dot{\gamma}^*$ against $\dot{\gamma}^*$ obtained from the theory for $\xi_{env} = 60, 66,$ and $70$ when we fix $\varphi = 0.30$ and $\varepsilon^* = 10^4$. 
FIG. 13. Plots of the theoretical (a) $\eta^*$ and (b) $\theta$ against $\dot{\gamma}^*$ and $\varepsilon^*$ when we fix $\varphi = 0.30$ and $\xi_{env} = 1.0$, where the theoretical curves are drawn using Eqs. (21), (34), and (37). The red and blue lines indicate the flow curves in the ignited and quenched phases, respectively, whereas the purple lines represent the flow curves for CST.

FIG. 14. Plots of the theoretical (a) $\eta^*$ and (b) $\theta$ against $\dot{\gamma}^*$ and $\xi_{env}$ when we fix $\varphi = 0.30$ and $\varepsilon^* = 10^4$, where the theoretical curves are drawn using Eqs. (21), (34), and (37). The red and blue lines represent the flow curves in the ignited and quenched phases, respectively, whereas the purple lines represent the flow curves for the continuous shear thickening.

lations. The kinetic theory adequately describes the discontinuous behaviors of both viscosity and kinetic temperature over a wide range of parameters if hydrodynamic interactions among particles are ignored. We have confirmed that such discontinuous changes still take place even if hydrodynamic interactions between particles are considered, as described in Ref. [45]. Our results reveal a new mechanism of DST caused by the ignited–quenched transition for frictionless soft particles.

It is difficult to observe the significant discontinuous changes in $\eta^*$ and $\theta$ obtained in our model if the solvent is a liquid. Indeed, if the kinetic temperature in the ignited phase becomes $10^6$ times higher than that in the quenched phase, the liquid in the ignited phase may evaporate because of the strong stirred effect of suspended particles even though our model does not include such effects. Even if we consider particles suspended in a gas, it may be difficult to avoid the melting of solid particles. Nevertheless, the indication of the existence of DST-like changes in $\eta^*$ and $\theta$ for frictionless soft particles, even for relatively dense suspensions, is important.

Let us discuss the possibility of experimental observation when we consider aerosols. Here, let us assume that the diameter, mass density, and Young’s modulus $Y$ of aerosol particles are roughly given by $d \sim 10^{-6}$ m, $\rho \sim 10^3$ kg/m$^3$, and $Y \sim 10$ GPa, respectively, and thus, the mass becomes $m \sim 10^{-14}$ kg. When we consider a case when the solvent is air, whose viscosity is approximately $\eta_0 \sim 10^{-5}$ Pa·s, the corresponding drag coefficient becomes $\zeta = 3\pi \eta_0 d/m \sim 10^4$ 1/s. Because DST takes place at around $\dot{\gamma} \sim \zeta \sim 10^4$ 1/s, this corresponds to the shear rate $\dot{\gamma} \sim 10^4$ 1/s.

As indicated in Ref. [45] the used value of $\xi_{env}$ is too large, if we compare them with the typical value $\sim 10^{-4}$ for colloidal suspensions. However, the kinetic theory predicts the existence of the DST for $\xi_{env} = 10^{-4}$ as shown in Fig. 15 because this value is smaller than the critical value above which the DST disappears as shown in Fig. 12. This means that we can expect the experimental observation of the DST using this setup.

It is important to analyze suspensions of frictional grains corresponding to the typical experimental setup for colloidal suspensions. This subject would be our future task.

ACKNOWLEDGEMENTS

The authors thank Takeshi Kawasaki, Takashi Uneyama, Michio Otsuki, and Pradipto for their helpful comments. This research was partially supported by the Grant-in-Aid of MEXT for Scientific Research (Grant Nos. JP20K14428
Appendix A: The basis of the kinetic theory of inertial suspension of soft particles

In this appendix, we explain the basis of the kinetic theory. The appendix comprises two subsections. In the first subsection, we explain the framework of the kinetic theory. In the second subsection, we derive the kinetic equation of the inertial suspension of soft particles.

1. Framework of kinetic model

Let us consider an $N$-body distribution function $f^{(N)}(\{r_i\}, \{p_i\}, t)$. We adopt the abbreviation $f^{(N)} ≡ f^{(N)}(\{r_i\}, \{p_i\}, t)$ to simplify the notation. From the conservation of probability, the following is obtained [39, 52, 73, 74] for soft particles. Substituting Eq. (2) into Eq. (A1), we obtain the stochastic-Liouville equation

\[
\frac{\partial f^{(N)}}{\partial t} + \sum_i \frac{\partial}{\partial r_i} \cdot \left( \frac{dr_i}{dt} f^{(N)} \right) + \sum_i \frac{\partial}{\partial p_i} \cdot \left( \frac{dp_i}{dt} f^{(N)} \right) = 0
\]

for soft particles. Substituting Eq. (2) into Eq. (A1), we obtain the stochastic-Liouville equation

\[
\frac{\partial f^{(N)}}{\partial t} + \sum_i \frac{\partial}{\partial r_i} \cdot \left( \left( \frac{p_i}{m} + \gamma y_i \hat{e}_x \right) f^{(N)} \right) + \sum_i \frac{\partial}{\partial p_i} \cdot \left[ \left( \sum_{j \neq i} F_{ij} - \gamma p_{i,y} \hat{e}_x - \zeta p_i + \xi_i \right) f^{(N)} \right] = 0.
\]

(A2)

with the aid of the noise average, Eq. (A2) can be rewritten as

\[
\left[ \frac{\partial}{\partial t} + \sum_i \left( V_i + \gamma y_i \hat{e}_x \right) \cdot \frac{\partial}{\partial r_i} - \gamma V_{i,y} \frac{\partial}{\partial V_{i,x}} \right] \langle f^{(N)} \rangle = \sum_i \frac{\partial}{\partial V_i} \left[ \zeta \left( V_i + \frac{T_{\text{env}}}{m} \frac{\partial}{\partial V_i} \right) \langle f^{(N)} \rangle \right] - \sum_{i,j} \frac{\partial}{\partial V_i} \left( \frac{F_{ij}}{m} \langle f^{(N)} \rangle \right),
\]

(A3)

where $\langle f^{(N)} \rangle$ is the noise-averaged distribution function and we have introduced $V_i ≡ p_i/m$. Integrating Eq. (A3) over $r_i$ and $V_i$ for $i = 2, 3, \cdots, N$, we obtain

\[
\left[ \frac{\partial}{\partial t} + \left( V_1 + \gamma y_1 \hat{e}_x \right) \cdot \frac{\partial}{\partial r_1} - \gamma V_{1,y} \frac{\partial}{\partial V_{1,x}} \right] f(X_1; t) = \frac{\partial}{\partial V_1} \left[ \zeta \left( V_1 + \frac{T_{\text{env}}}{m} \frac{\partial}{\partial V_1} \right) f(X_1; t) \right] - \sum_j \frac{\partial}{\partial V_1} \left( \frac{F_{1j}}{m} f^{(2)}(X_1, X_2; t) \right),
\]

(A4)

where we have introduced one- and two-body distribution functions as

\[
f(X_1; t) = \frac{1}{(L^3)^{N-1}} \int \prod_{j=2}^N dX_j \langle f^{(N)} \rangle,
\]

(A5a)

\[
f^{(2)}(X_1, X_2; t) = \frac{1}{(L^3)^{N-2}} \int \prod_{j=3}^N dX_j \langle f^{(N)} \rangle.
\]

(A5b)
with \( dX_j = dr_j dp_j \), and \( X_j = (r_j, p_j) \). Without loss of generality, we put \( j = 2 \) and attach the \( N - 1 \) factor to the second and third terms on the right hand side (RHS) of Eq. (A4). As shown in Appendix A2, the last term on the RHS of Eq. (A4) can be written as the collision integral \( J[\mathcal{V}_1 f^{(2)}(1, 2)] \), at least, in the low density limit. Thus, we obtain Eq. (4).

2. Derivation of the equation of one-body distribution function

In this subsection, we derive the collision operator for a dilute gas without solvents based on Ref. [73]. The stochastic Liouville equation can be rewritten as

\[
\frac{\partial f^{(N)}(t)}{\partial t} = (\mathcal{L}^{(N)} + \mathcal{L}_\gamma + \mathcal{L}_{\text{hyd}}) f^{(N)}(t) \tag{A6}
\]

where we have introduced three parts of Liouvillian acting on a variable A as

\[
\mathcal{L}^{(N)} A \equiv \{ \mathcal{L}^{(N)}, H^{(N)} \} \tag{A7}
\]

\[
\mathcal{L}_\gamma A \equiv -\gamma \sum_{i=1}^{N} \left\{ \frac{\partial}{\partial x_i} (yA) - \frac{\partial}{\partial p_{i,x}} (p_{i,y} A) \right\} \tag{A8}
\]

\[
\mathcal{L}_{\text{hyd}} A \equiv \sum_{i=1}^{N} \frac{\partial}{\partial p_i} \cdot \left[ (\zeta_i p_j + \xi_i) A \right] \tag{A9}
\]

with Poisson’s bracket \( \{ A, B \} \):

\[
\{ A, B \} \equiv \sum_{i=1}^{N} \left( \frac{\partial A}{\partial r_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial r_i} \frac{\partial A}{\partial p_i} \right) \tag{A10}
\]

and the total Hamiltonian \( H^{(N)} \):

\[
H^{(N)} \equiv \sum_{i=1}^{N} \left\{ \frac{p_i^2}{2m} + \frac{1}{2} \sum_{j=1}^{N} U(r_{ij}) \right\} \tag{A11}
\]

Because Eq. (A6) is a linear equation for \( f^{(N)} \), the linear combination of the solution of each Liouville equation

\[
\frac{\partial f^{(N)}_0}{\partial t} = \mathcal{L}^{(N)} f^{(N)}_0 \tag{A12}
\]

\[
\frac{\partial f^{(N)}_\gamma}{\partial t} = \mathcal{L}_\gamma f^{(N)}_\gamma \tag{A13}
\]

\[
\frac{\partial f^{(N)}_{\text{hyd}}}{\partial t} = \mathcal{L}_{\text{hyd}} f^{(N)}_{\text{hyd}} \tag{A14}
\]

i.e., \( f^{(N)} = c_1 f^{(N)}_0 + c_2 f^{(N)}_\gamma + c_3 f^{(N)}_{\text{hyd}} \) with constants \( c_1, c_2, \) and \( c_3 \) is a solution to Eq. (A6).

Now, let us rewrite Eq. (A12). Here, the one-particle distribution \( f^{(1)}_0(1) \) with \( 1 \equiv (r_1, p_1; t) \) satisfies

\[
\frac{\partial f^{(1)}_0(1)}{\partial t} + \{ f^{(1)}_0(1), H^{(1)}(1) \} = L^{(N-1)} \int \prod_{j=2}^{N} dX_j \{ H^{(N)} - H^{(1)}(1), f^{(N)}_0 \}, \tag{A15}
\]

where \( H^{(1)}(1) \) is the one-particle Hamiltonian and \( dX_j \equiv dr_j dp_j \). The kinetic Hamiltonian is commutable with \( f^{(N)} \) because \( \int dp_j p_j \cdot \partial f^{(N)}/\partial p_j \) disappears at the boundary. Thus, the Liouville equation for the one-particle can be expressed as

\[
\frac{\partial f^{(1)}_0(1)}{\partial t} + \{ f^{(1)}_0(1), H^{(1)}(1) \} = n \int dX_2 \{ U^{(N-1)} f^{(2)}_0(1, 2) \}. \tag{A16}
\]
Poisson’s bracket with $H^{(1)}(1)$ is \{f^{(1)}(1), H^{(1)}(1)\} = v \cdot \nabla f^{(1)}(1)$ with $v = p/m$. Thus, the one-body distribution satisfies

$$\left( \frac{\partial}{\partial t} + v \cdot \nabla \right) f^{(1)}_0(1) = n J(1), \tag{A17}$$

where

$$J(1) \equiv \int dX_2 \left\{ U(r_1, r_2), j^{(2)}_0(1, 2) \right\}. \tag{A18}$$

Note that Eqs. (A17) and (A18) with the assumption of naive molecular chaos $j^{(2)}_0(1, 2) = f^{(1)}_0(1)f^{(1)}_0(2)$ do not result in the Boltzmann equation but the Vlasov equation

$$\left( \frac{\partial}{\partial t} + v \cdot \nabla \right) f^{(1)}_0(1) = \nabla_p \cdot F^{(1)} f^{(1)}_0(1), \tag{A19}$$

where $\nabla_p$ denotes the divergence in momentum space and

$$F^{(1)} \equiv -n \frac{\partial}{\partial r_1} \int dX_2 f^{(1)}_0(2) U(r_1, r_2). \tag{A20}$$

Thus, the derivation of the Boltzmann equation is non-trivial.

If the density is sufficiently low, we may neglect the contribution of the collision integral in the equation for $f^{(2)}(1, 2)$. Under this assumption, we can write the equation

$$\frac{\partial}{\partial t} f^{(2)}_0(1, 2) + \{f^{(2)}_0(1, 2), H^{(2)}(1, 2)\} = 0. \tag{A21}$$

Now, we write

$$f^{(2)}_0(1, 2) = \Omega f^{(1)}_0(1)f^{(1)}_0(2). \tag{A22}$$

with an operator

$$\Omega \equiv \lim_{\tau \to \infty} S^{(2)}(\tau) S^{(0)}(-\tau). \tag{A23}$$

Here, $S^{(s)}(t)$ is a streaming operator satisfying

$$\frac{\partial}{\partial t} S^{(s)}(t) A = \left\{ S^{(s)}(t) A, H^{(s)} \right\}. \tag{A24}$$

This operator also satisfies

$$S^{(s)}(0) = 1, \quad S^{(s)}(t) S^{(s)}(u) = S^{(s)}(t + u), \quad S^{(s)}(t)^{-1} = S^{(s)}(-t). \tag{A25}$$

Substituting Eq. (A22) into the collision operator in Eq. (A18), we obtain

$$J(1) \simeq J_2(1); \quad J_2(1) \equiv \int dX_2 \{ U(r_1, r_2), \Omega f^{(1)}_0(1)f^{(1)}_0(2) \}. \tag{A26}$$

Let us introduce a new operator $\vartheta$ defined as

$$\vartheta A(1, 2) \equiv \left\{ U(r_1, r_2), A(1, 2) \right\} = \frac{\partial U(r_1, r_2)}{\partial r_1} \cdot \left( \frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2} \right) A(1, 2). \tag{A27}$$

Because the total momentum is conserved, $\Omega$ does not affect the mass-center position or velocity, and the following can be written

$$\vartheta \Omega = v_{12} \cdot \nabla_r \Omega - \Omega v_{12} \cdot \nabla_r. \tag{A28}$$
The resulting form of $J_2(1)$ can be written as

$$J_2(1) = \int dX_2 [v_{12} \cdot \nabla_r \Omega - \Omega v_{12} \cdot \nabla_r] f_0^{(1)}(1) f_0^{(1)}(2). \quad (A29)$$

When the system is almost spatial homogeneous, $J_2(1)$ can be approximated as

$$J_2(1) = \int dX_2 v_{12} \cdot \nabla_r \Omega f_0^{(1)}(p_1; t) f_0^{(1)}(p_2; t). \quad (A30)$$

To evaluate the integral, we use the cylindrical coordinate where the $z$-axis is parallel to $v_{12}$. Then, $J_2$ can be rewritten as

$$J_2(1) = \int d^3 p_2 \int bb db \int_{-\infty}^{\infty} dz v_{12} \frac{d}{dz} \Omega f_0^{(1)}(p_1; t) f_0^{(1)}(p_2; t)$$

$$= \int d^3 p_2 \int v_{12} bb db \Omega f_0^{(1)}(p_1; t) f_0^{(1)}(p_2; t)_{|z=\infty} - \Omega f_0^{(1)}(p_1; t) f_0^{(1)}(p_2; t)_{|z=-\infty}, \quad (A31)$$

where $b$ represents the impact parameter. In this case, $S^{(0)}$ does not play any role. Then, $\Omega$ is equivalent to $\lim_{\tau \to \infty} S^{(2)}(-\tau)$. Here, there is no interaction between two particles for $|z| > 1$ in the region of $z < 0$, meaning that the second term in the bracket of Eq. (A31) is $f_0^{(1)}(p_1; t) f_0^{(1)}(p_2; t)$. In the first term, $S^{(2)}(-\tau)$ takes the particles back through a collision and converts $p_1, p_2$ to the pre-collisional momenta $p_1', p_2'$. Thus, $J_2(1)$ is reduced to Boltzmann’s collision operator.

It is straightforward to rewrite Eq. (A13) as

$$\frac{\partial f_0^{(1)}(1)}{\partial t} + \gamma \left( y \frac{\partial}{\partial x} - V_y \frac{\partial}{\partial V_y} \right) f_0^{(1)}(1) = 0 \quad (A32)$$

for the one-body distribution function.

Equation (A14) can be rewritten as

$$\frac{\partial (f_{\text{hydr}}^{(1)}(1))}{\partial t} = \frac{\partial}{\partial V_1} \cdot \left[ \zeta \left( V_1 + \frac{T_{\text{env}}}{m} \frac{\partial}{\partial V_1} \right) \right] (f_{\text{hydr}}^{(1)}(1)). \quad (A33)$$

Based on the argument of this Appendix, we can use the additive approximation of three contributions for the equation of the one-body distribution function. Based on the results of the arguments in this Appendix, we obtain Eq. (4).

**Appendix B: Detailed expressions of $\chi$ and $r_{\text{min}}$**

In this Appendix, we present the explicit expressions of the scattering angle $\chi$ and the closest distance $r_{\text{min}}$. Because their derivations have been given in Ref. [38], we only show the final results:

$$\chi = \pi - 2 \sin^{-1} \left( \frac{b}{d} \right)$$

$$r_{\text{min}} = 2 \left( \sqrt{\beta + \sqrt{-\beta - 2p - \frac{2q}{\sqrt{\beta}}} - 1} \right) \frac{1}{d}, \quad (B1a)$$

$$\left\{ \begin{array}{ll}
4 \sqrt{\frac{A_1 A_2}{(D_1 D_2)^{1/4}}} \left\{ \frac{\alpha_2}{A_2} \left[ F \left( \frac{\pi}{2}, \frac{A_2^2}{A_1^2} \right) - F \left( \sin^{-1} \left( \frac{w_0}{A_1} ; \frac{A_2^2}{A_1^2} \right) \right) \right] \\
+ \frac{\alpha_1 - \alpha_2}{A_1} \left[ \Pi \left( \frac{A_2^2}{2}, \frac{\pi}{2}, \frac{A_2^2}{A_1^2} \right) - \Pi \left( \frac{A_2^2}{2}, \sin^{-1} \left( \frac{w_0}{A_1} ; \frac{A_2^2}{A_1^2} \right) \right) \right] \right\} \\
+ \frac{\alpha_1 - \alpha_2}{\sqrt{(A_1^2 - 1)(1 - A_2^2)}} \tan^{-1} \left( \frac{(A_1^2 - 1)(A_2^2 - w_0^2)}{(1 - A_1^2)(A_2^2 - w_0^2)} \right) \\
4 \sqrt{\frac{A_1 A_2}{(-D_1 D_2)^{1/4}}} \left\{ \frac{\alpha_2}{A_2} F \left( \cos^{-1} \left( \frac{w_0}{A_1} ; \frac{A_2^2}{A_1^2} \right) \right) \\
+ \frac{\alpha_1 - \alpha_2}{(1 - A_2^2) \sqrt{A_1^2 + A_2^2}} \Pi \left( \frac{A_2^2}{1 - A_2^2}, \cos^{-1} \left( \frac{w_0}{A_1} ; \frac{A_2^2}{A_1^2} \right) \right) \\
+ \frac{\alpha_1 - \alpha_2}{\sqrt{(A_1^2 + 1)(1 - A_2^2)}} \tan^{-1} \left( \frac{(A_1^2 + 1)(A_2^2 - w_0^2)}{(1 - A_1^2)(A_2^2 + w_0^2)} \right) \right\} \\
\end{array} \right.$$

where $D_1 \geq 0$ and $D_1 < 0$.
where \( b^* \equiv b/d, \quad v^* \equiv v/(d\sqrt{k/m}) \), \( p \equiv (2 - v^2)/(b^2v^2) \), \( q \equiv -4/(b^2v^2) \), \( r \equiv -q/2, \quad P \equiv -(p^2/3 + 4r) \), \( Q \equiv -(2/27)p^3 - q^2 + (8/3)pr \), \( \Delta \equiv (Q/2)^2 + (P/3)^3 \),

\[
\beta \equiv \begin{cases} 
-\frac{2p}{3} + \left( -\frac{Q}{2} + \sqrt{\Delta} \right)^{1/3} + \left( -\frac{Q}{2} - \sqrt{\Delta} \right)^{1/3} & (\Delta \geq 0) \\
-\frac{2p}{3} + 3\sqrt{-\frac{P}{3}} \cos \left( \frac{1}{3} \cos^{-1} \left[ -\frac{Q}{2} \left( -\frac{3}{P} \right)^{3/2} \right] \right) & (\Delta < 0) 
\end{cases}
\]  

(B2)

and

\[
D_{1,2} \equiv -\beta - 2p \pm \frac{2q}{\sqrt{\beta}},
\]

(B3a)

\[
w_0 \equiv -\frac{\sqrt{q^2 + 2\beta^2(p + \beta) + q - 2\beta}}{\sqrt{q^2 + 2\beta^2(p + \beta) - q + 2\beta}},
\]

(B3b)

\[
\alpha_{1,2} \equiv \frac{q \pm \sqrt{q^2 + 2\beta^2(p + \beta)}}{2\beta},
\]

(B3c)

\[
A_1 \equiv \sqrt{\frac{\beta^2 D_1}{\sqrt{q^2 + 2\beta^2(p + \beta) - q - \beta^3/2}}}, \quad \frac{\beta^2 D_1}{\sqrt{q^2 + 2\beta^2(p + \beta) - q - \beta^3/2}} = \sqrt{q + \beta^3/2 + \sqrt{q^2 + 2\beta^2(p + \beta)}},
\]

(B3d)

\[
A_2 \equiv \frac{\beta^2 D_2}{\sqrt{q^2 + 2\beta^2(p + \beta) - q + \beta^3/2}}}, \quad \frac{\beta^2 D_2}{\sqrt{q^2 + 2\beta^2(p + \beta) - q + \beta^3/2}} = \sqrt{-q + \beta^3/2 + \sqrt{q^2 + 2\beta^2(p + \beta)}}.
\]

(B3e)

Here, \( F(\phi, m) \equiv \int_0^\phi d\phi'/(1 - m \sin^2 \phi')^{1/2} \) and \( \Pi(a, \phi|m) \equiv \int_0^\phi d\phi'/(1 - a \sin^2 \phi')^{1/2} \) are the elliptic integrals of the first and third kind, respectively [75]. We note that the sign of the inside of the square root for \( A_2 \) in Ref. [38] should be minus. Figure 16 shows the velocity dependence of the scattering angle \( \chi \) and the closest distance \( r_{\min} \). We note that these results are obtained without considering three-body collisions and the effect of the drag from the background fluid.

**Appendix C: Convergence of \( \Lambda_{a,\beta}^* \) and \( \Pi_{xy}^* \) in the expansions of \( \tilde{\gamma} \) and the linear theory**

In this appendix, we show how the calculated stress depends on the number of truncation terms \( N_c \) in the set of equations (34). We also present some analytical results of the linear theory with \( N_c = 1 \).

1. Convergence of expansions

In this subsection, we present how the expansions of \( \Lambda_{a,\beta}^* \) and \( \Pi_{xy}^* \) in the set of equations (34) converge as the number of \( N_c \) increases.

We plot the theoretical viscosity \( \eta^* \) against \( \tilde{\gamma}^* \) for various \( N_c \) in Fig. 17 with \( \varphi = 0.30, \xi_{env} = 1.0, \) and \( \varepsilon^* = 10^4 \). Viscosity is almost converged for \( N_c \geq 2 \), whereas the results of the linear theory with \( N_c = 1 \) are more comparable to the simulation results than those with \( N_c \geq 2 \). We note that it is possible to obtain analytic expressions of \( \eta^* \) and \( \theta \) in the case of \( N_c = 1 \) as shown in the next subsection, whereas it is impossible to obtain the analytic expressions if we adopt \( N_c \geq 2 \).

2. Linear theory

In this subsection, we show the explicit forms when we consider only the terms up to the linear order with respect to the expansion parameter \( \tilde{\gamma} \) (i.e., \( N_c = 1 \)) in the set of equations (34). A set of dynamical equations (21) in the
FIG. 16. Velocity dependence of (a) the scattering angle \( \chi \) and (b) the closest distance \( r_{\text{min}} \) against the dimensionless relative speed \( v^* \) for \( b^* \equiv b/d = 0.4, 0.6, \) and 0.8. Here, we have introduced \( r_{\text{min}}^* \equiv r_{\text{min}}/d \).

FIG. 17. Plots of \( \eta^* \) against \( \dot{\gamma}^* \) for \( \varphi = 0.30, \xi_{\text{env}} = 1.0, \) and \( \varepsilon^* = 10^4 \) when we control the truncation \( N_c = 1 \) (solid line), 2 (dashed line), and 6 (crosses).
steady state with \( N_c = 1 \) is reduced to (see also Ref. [36]):

\[
\frac{2}{3} \dot{\gamma}^* C \Pi_{xy} = 2(\theta - 1),
\]

\[
2 \dot{\gamma}^* \Pi_{xy} = (2 + \nu^*_\text{soft}) \Delta \theta,
\]

\[
2 \dot{\gamma}^* \varepsilon \Pi_{xy} = (2 + \nu^*_\text{soft}) \delta \theta,
\]

\[-(2 + \nu^*_\text{soft}) \Pi_{xy} = \dot{\gamma}^* \left( \frac{2}{3} \Delta \theta - \frac{1}{3} \varepsilon \delta \theta - C \theta \right),
\]

where we have introduced \( \nu^*_\text{soft} \equiv \nu_{\text{soft}} / \zeta \) and

\[
C \equiv 1 + \frac{8}{5} \varphi g_0 \Omega^*_{2,2},
\]

\[
D \equiv 1 - \frac{4}{35} \varphi g_0 \Omega^*_{2,2},
\]

\[
E \equiv 1 - \frac{16}{35} \varphi g_0 \Omega^*_{2,2}
\]

The set of solutions of Eqs. (C1) is given by

\[
\Pi_{xy} = \frac{3}{\dot{\gamma}^* C} (\theta - 1),
\]

\[
\Delta \theta = \frac{3}{C} 2(\theta - 1),
\]

\[
\delta \theta = \frac{3 \varepsilon}{C} 2(\theta - 1).
\]

Substituting Eqs. (C3) into Eq. (C1d), we obtain the expression of \( \dot{\gamma}^* \) as

\[
\dot{\gamma}^* = \sqrt{-\frac{3(1 - \theta^{-1})(2 + \nu^*_\text{soft})}{C F}},
\]

where

\[
F = \frac{2}{3} \frac{\Delta \theta}{\theta} - \frac{1}{3} \varepsilon \frac{\delta \theta}{\theta} - C = \frac{2 D - E^2}{C} 2(1 - \theta^{-1}) + \nu^*_\text{soft} - C.
\]

Equation (C4) is used to determine \( \dot{\gamma}^* \) under a given set of \( \varphi \) and \( \theta \). Once we fix \( \theta \), we can derive the other rheological quantities \( \Pi_{xy} \), \( \Delta \theta \), and \( \delta \theta \) from Eqs. (C3a)–(C3c), respectively. Correspondingly, the dimensionless contact shear stress is given by

\[
\Pi^c_{xy} = \frac{8}{5} \varphi g_0 \Omega^*_{2,2} \left( \Pi_{xy} + \frac{1}{\sqrt{\pi}} \frac{\dot{\gamma}^*}{\xi_{\text{env}} \sqrt{\theta}} \right).
\]

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