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Different singularities in the functions of extended kinetic theory at the origin of the yield stress in granular flows

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We use previous results from discrete element simulations of simple shear flows of rigid, identical spheres in the collisional regime to show that the volume fraction-dependence of the stresses is singular at the shear rigidity. Here, we identify the shear rigidity, which is a decreasing function of the interparticle friction, as the maximum volume fraction beyond which a random collisional assembly of grains cannot be sheared without developing force chains that span the entire domain. In the framework of extended kinetic theory, i.e., kinetic theory that accounts for the decreasing in the collisional dissipation due to the breaking of molecular chaos at volume fractions larger than 0.49, we also show that the volume fraction-dependence of the correlation length (measure of the velocity correlation) is singular at random close packing, independent of the interparticle friction. The difference in the singularities ensures that the ratio of the shear stress to the pressure at shear rigidity is different from zero even in the case of frictionless spheres: we identify that with the yield stress ratio of granular materials, and we show that the theoretical predictions, once the different singularities are inserted into the functions of extended kinetic theory, are in excellent agreement with the results of numerical simulations. © *2015 AIP Publishing LLC.* [http://dx.doi.org/10.1063/1.4905461]

I. INTRODUCTION

One of the most striking macroscopic features of granular materials is the existence of an asymptotic value of the ratio of the shear stress to the pressure at vanishing motion (and large volume fraction), often identified as the yield stress ratio, μ_s, which discriminates between fluid-like and solid-like behaviour. In many models of dense granular flows,[1–3] the value of μ_s is treated as a parameter and obtained on the basis of fitting with experiments and/or simulations. Using molecular dynamics simulations on simple shear flows of identical spheres, it has been shown[4] that μ_s depends on the interparticle friction coefficient μ, and that, due to geometric effects, it is different from zero even in the case of frictionless particles.[5]

Here, we use extended kinetic theory,[3,6–10] i.e., kinetic theory of granular gases that takes into account the breaking of molecular chaos at volume fractions ν larger than the freezing point 0.49,[11] to describe the simple shear flow (Fig. 1) of identical, rigid spheres at volume fractions less than the shear rigidity value ν_s, i.e., the largest volume fraction at which a randomly collisional granular material can be sheared without force chains spanning the entire domain: when this happens, the stresses become rate-independent (quasi-static regime). Hence, our ν_s coincides with the critical volume fraction measured by Chialvo, Sun, and Sundaresan[4] in their simulations, which is only a function of μ (Fig. 2). For frictionless spheres, ν_s is equal to 0.636.

If, as we believe, extended kinetic theory is all we need to quantitatively predict granular shear flows at volume fractions less than ν_s (in the collisional regime, where collisions can be in general either sticking or sliding[12]), and if there is a continuous transition from the rate-dependent (collisional) to the rate-independent (quasi-static) regime for increasing volume fraction, we should be able to theoretically predict μ_s, as the value of the stress ratio at $\nu = \nu_s$.

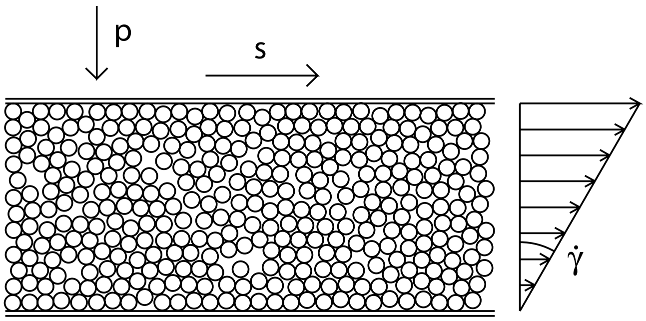

FIG. 1. Simple shear flow configuration.

II. THEORY

Without loss of generality, we take the particle density and diameter to be one. We employ the constitutive relations proposed by Garzó and Dufty,[13] as modified by Jenkins and Berzi,[8] to express the pressure

$$p = f_1 T, \tag{1}$$

the shear stress

$$s = f_2 T^{1/2}\dot{\gamma}, \tag{2}$$

and the rate of energy dissipation in collisions,

$$\Gamma = \frac{f_3}{L} T^{3/2}. \tag{3}$$

Here, T is the granular temperature (one third of the mean square of the particle velocity fluctuations) and $\dot{\gamma}$ is the shear rate. The dissipation rate is present in the fluctuation energy balance which, for simple shearing, reduces to

$$s\dot{\gamma} = \Gamma, \tag{4}$$

i.e., the fluctuation energy produced by the shear stress is entirely dissipated in collisions.

The functions f_1, f_2, and f_3, in the dense limit, i.e., for volume fractions larger than say 0.4, when the streaming component of the stresses is negligible, are derived from those reported in Jenkins and Berzi[8] and summarized in Table I. All of them are proportional to G, the product of ν

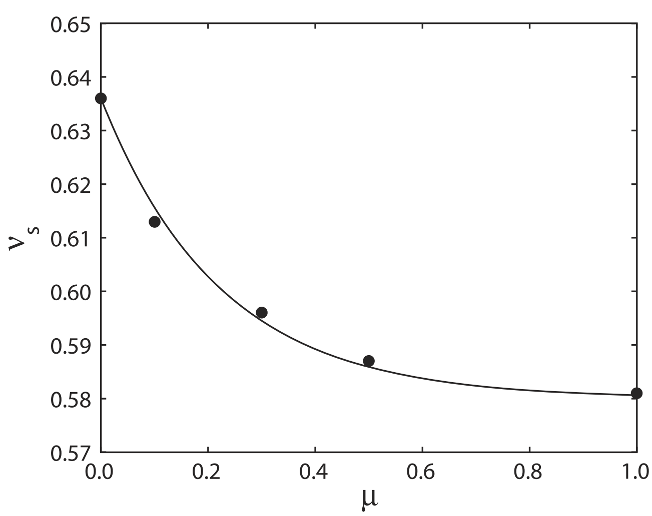

FIG. 2. Numerical (symbols) values of ν_s against μ obtained from Chialvo, Sun, and Sundaresan.[4] The data can be fitted with the expression $\nu_s = 0.58 + (0.636 - 0.58)\exp(-4.5\mu)$ (solid line).

TABLE I. Functions of extended kinetic theory in the dense limit.

$$f_1 = 2(1+e_n)\nu G$$
$$f_2 = \frac{8J}{5\pi^{1/2}}\nu G$$
$$f_3 = \frac{12}{\pi^{1/2}}\nu G(1-e^2)$$
$$G = \nu g_0$$
$$J = \frac{1+e_n}{2} + \frac{\pi}{4}\frac{(3e_n-1)(1+e_n)^2}{[24-(1-e_n)(11-e_n)]}$$
$$e = e_n - \frac{3}{2}\mu \exp(-3\mu)$$
$$g_0 = \mathrm{f}\frac{2-\nu}{2(1-\nu)^3} + (1-\mathrm{f})\frac{2}{\nu_s-\nu}$$
$$\mathrm{f} = \begin{cases} 1 & \text{if } \nu < 0.4, \\ \dfrac{\nu^2 - 0.8\nu + \nu_s(0.8-\nu_s)}{0.8\nu_s - 0.16 - \nu_s^2} & \text{otherwise,} \end{cases}$$
$$L^* = \left(\frac{f_2}{f_3}\right)^{1/2}\left[\frac{26(1-e)}{15}\left(\frac{\nu-0.49}{\nu_{rcp}-\nu}\right)+1\right]^{3/2}$$

and the radial distribution function at contact g_0. For the latter, we adopt the expression suggested by Vescovi *et al.*,[14] which has been tested against numerical simulations of frictionless spheres. The functions f_1 and f_2 depend also on the normal coefficient of restitution e_n, i.e., the negative of the ratio of post- to pre-collisional normal relative velocity between two impending spheres. As in Ref. 12, we treat the possibility of linear momentum being transferred to angular momentum for frictional particles as an additional dissipation of fluctuation energy, using an effective coefficient of restitution e, which depends on the coefficient of normal restitution, the coefficient of tangential restitution in a sticking collision e_t, and the interparticle friction μ in the function f_3 of the dissipation rate.[15] When $e_t = 1$, Chialvo and Sundaresan[15] suggest the expression of Table I.

Figs. 3 and 4 depict the functions $f_1 = p/T$ and $f_2 = s/\left(T^{1/2}\dot{\gamma}\right)$ calculated from the numerical values of stresses, granular temperature, and shear rate reported in Refs. 15 and 16 for $e_n = 0.7$ and $e_t = 1$ at different values of the interparticle friction. The latter has a strong influence on the value of volume fraction at which the functions f_1 and f_2 diverge. Interestingly, the singularity is the same for both functions and coincides with the values of ν_s reported in Fig. 2. Indeed, the lines in Figs. 3 and 4, which notably reproduce the data, represent the expressions of Table I when the radial distribution function at contact has the form proposed by Vescovi *et al.*[14] for frictionless spheres,

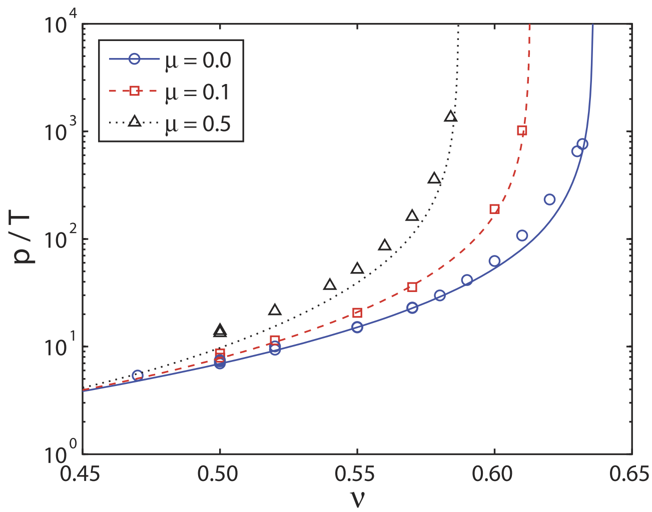

FIG. 3. Numerical (symbols, after Mitarai and Nakanishi[16] and Chialvo and Sundaresan[15]) and theoretical (lines) ratio of pressure to granular temperature (function f_1) as a function of the volume fraction for $e_n = 0.7$, $e_t = 1$, and different values of the interparticle friction.

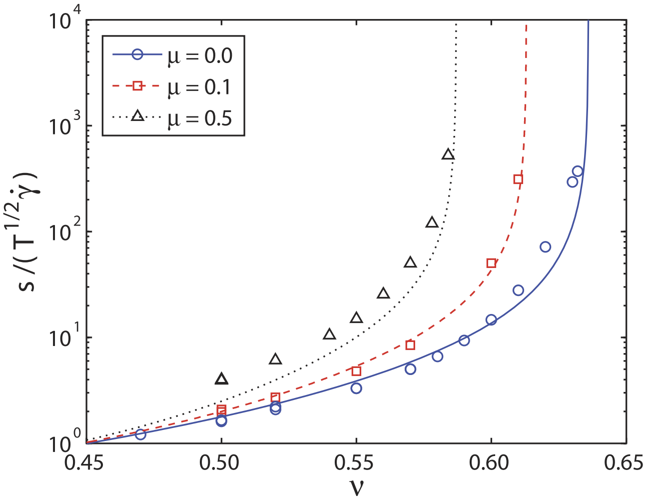

FIG. 4. Same as in Fig. 2, but for the ratio of shear stress to the product of shear rate and square root of granular temperature (function f_2).

where ν_s is used instead of 0.636 (Table I). The volume fraction at shear rigidity is therefore the volume fraction at which the radial distribution function at contact diverges in shearing flows, and the functions f_1, f_2, and f_3 of kinetic theory are singular. More refined interpretations of this singularity must take into account the anisotropy in the pair distribution of contacting spheres induced by the shearing.

The quantity L in Eq. (3) is the correlation length of extended kinetic theory, accounting for the decrease in the collisional energy dissipation due to the presence of correlated motion among the particles (breaking of molecular chaos), which occurs when $\nu > 0.49$.[6,7,10,16,17] Its expression comes from an heuristic balance[6] between the shearing that tends to build correlation and the agitation of the particles that tends to destroy the correlation, and, for plane shear flows, reads

$$L = \max\left(1, L^* \frac{\dot{\gamma}}{T^{1/2}}\right), \tag{5}$$

where L^* is a function of the volume fraction and the effective coefficient of restitution (for consistency, given that the correlation length appears in the constitutive expression of the dissipation rate). Berzi[10] has suggested an expression for L^* on the basis of previous results of event-driven simulations of simple shear flows of frictionless spheres;[16] a simplified version of it is reported in Table I, with $\nu_{rcp} = 0.64$ the volume fraction at random close packing.[11] When L is equal to one diameter (for $\nu \leq 0.49$), the molecular chaos assumption is valid and extended kinetic theory reduces to classic kinetic theory. From Eqs. (2)–(5) and Table I, when $\nu > 0.49$,

$$\frac{\dot{\gamma}}{T^{1/2}} = \left[\frac{15\left(1 - e^2\right)}{2J} \frac{1}{L^*}\right]^{1/3}. \tag{6}$$

Equation (6) and the expressions of Table I can then be employed to determine the ratio of the shear stress to the pressure

$$\frac{s}{p} = \frac{4J}{5\pi^{1/2}(1 + e_n)} \left[\frac{15\left(1 - e^2\right)}{2J}\right]^{1/3} \frac{1}{L^{*1/3}}. \tag{7}$$

Equation (7) shows that the stress ratio can be different from zero at $\nu = \nu_s$ only if the function L^* is not singular there. From Eqs. (5) and (6), we also obtain that, in simple shear flows,

$$L = \left[\frac{15\left(1 - e^2\right)}{2J}\right]^{1/3} L^{*2/3}, \tag{8}$$

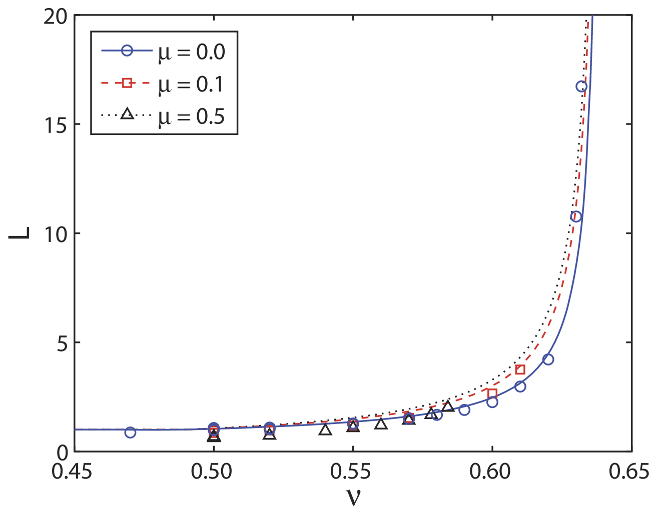

FIG. 5. Numerical (symbols, after Mitarai and Nakanishi[16] and Chialvo and Sundaresan[15]) and theoretical (lines) correlation length as a function of the volume fraction for $e_n = 0.7$, $e_t = 1$, and different values of the interparticle friction.

i.e., that the correlation length has the same singularity of L^*. The correlation length can be calculated indirectly as $L = f_3 T^{3/2}/(s\dot{\gamma})$, using Eqs. (3) and (4), from measurements of shear stress, granular temperature, shear rate, and volume fraction in numerical simulations, assuming that the functions f_3 and g_0 are those of Table I. The comparison between the values of L obtained from the numerical simulations of Refs. 15 and 16, and Eq. (8) shows a good agreement (Fig. 5). It also confirms that the singularity in L, and consequently in L^*, does not depend on the interparticle friction, suggesting that the anisotropy induced by the shearing does not play a significant role in the velocity correlation.

Being ν_{rcp} (the singularity of L^*) always greater than ν_s (the singularity in the radial distribution function at contact) for every μ, the stress ratio at $\nu = \nu_s$ is always different from zero. We can obtain μ_s from Eq. (7), with L^* calculated from the expression of Table I at $\nu = \nu_s$. We compare the theoretical values of the yield stress ratio μ_s against the data measured in numerical simulations[4] in Fig. 6. Once again, the agreement is remarkable. It is worthwhile to emphasize that the tiny difference between ν_{rcp} and 0.636, ignored in Ref. 14, is enough to correctly predict the non-zero value of μ_s even in the case of frictionless spheres.[5]

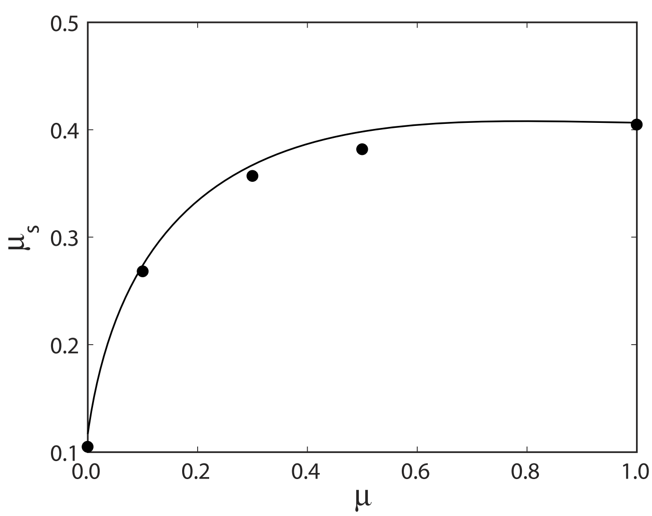

FIG. 6. Numerical (symbols, after Chialvo, Sun, and Sundaresan[4]) and theoretical (lines) yield stress ratio as a function of the interparticle friction.

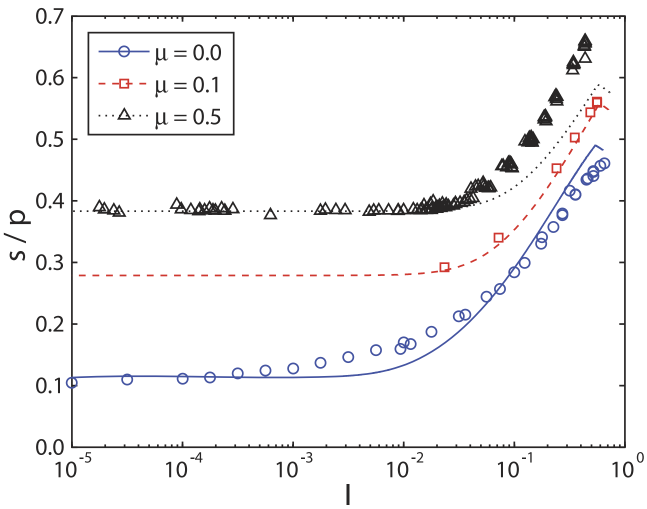

FIG. 7. Numerical (symbols, after Refs. 4, 5, 15, and 16) and theoretical (lines) stress ratio as a function of the inertial parameter for different values of the interparticle friction.

Equation (7) indicates that, in simple shear flows, the stress ratio is a unique function of the volume fraction. If we divide both sides of Eq. (6) by $f_1^{1/2}$, we obtain

$$\frac{\dot{\gamma}}{p^{1/2}} = \frac{1}{f_1^{1/2}}\left[\frac{15\left(1-e^2\right)}{2J}\frac{1}{L^*}\right]^{1/3}, \tag{9}$$

where the term on the left hand side is the inertial parameter I.[1] Equation (9) indicates that, in simple shear flows, also the inertial parameter is a unique function of the volume fraction. Obviously, Eqs. (7) and (9) can be formally rewritten to obtain the stress ratio and the volume fraction as unique functions of the inertial parameter. This is often referred to as the GDR MiDi rheology, that here has been obtained as a special case of the more general extended kinetic theory. Such a description is not valid if the fluctuation energy balance does not reduce to production equal to dissipation (Eq. (4)): for instance, when energy diffusion is important (close to solid boundaries[18]). A modification of the GDR MiDi approach, with the inclusion of a diffusive-like term, to take care of non-locality has been recently proposed.[19] Energy diffusion is naturally included in the context

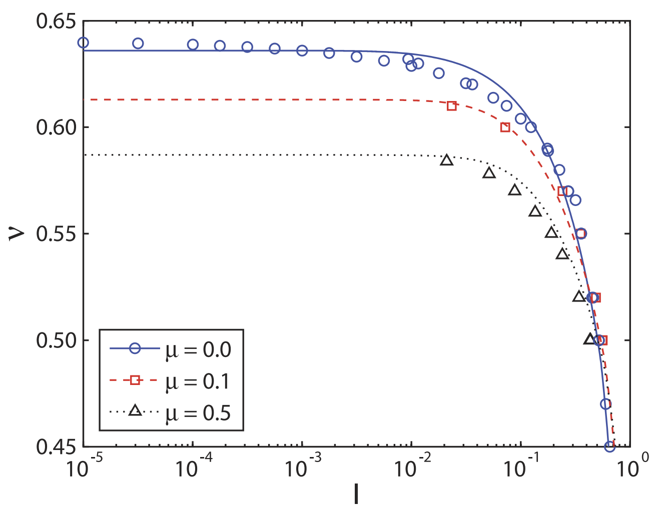

FIG. 8. Same as in Fig. 7, but for the volume fraction as a function of the inertial parameter.

of kinetic theory, so that there is no need for such *ad hoc* modifications. Figs. 7 and 8 show that extended kinetic theory notably reproduces the results of numerical simulations on simple shear flows,[4,5,15,16] even in the case of frictional spheres for $\nu \leq \nu_s$, if the different singularities in the radial distribution function at contact and L^* are taken into account.

In the more general situation in which the fluctuation energy production is not equal to the energy dissipation, the stress ratio results, when $\nu > 0.49$,

$$\frac{s}{p} = \frac{4J}{5\pi^{1/2}(1+e_n)} \frac{L}{L^*}. \tag{10}$$

Equation (10) shows that even at $\nu = \nu_s$, the stress ratio can be less than μ_s if the correlation length decreases. The fact that the correlation length decreases with increasing granular temperature (that destroys the correlation) gives a hint on how agitation can induce the vanishing of the yield stress, as observed in recent experiments.[20,21] Of course, extended kinetic theory must be completed by including the role of force chains[22] to deal also with the quasi-static regime ($\nu > \nu_s$), before claiming to have a comprehensive model for granular flows.

III. CONCLUSIONS

We have shown that the yield stress ratio in granular materials can be theoretically predicted in the context of extended kinetic theory once the different singularities of the radial distribution function at contact in shearing flows and the volume fraction-dependence of the correlation length are accounted for. This allows extend kinetic theory to be in excellent agreement with the results of numerical simulations on simple shearing of inelastic, frictional, and frictionless particles for volume fractions less than the value at shear rigidity. Although it is intriguing to have a consistent theoretical framework to predict the macroscopic yield stress of granular materials, the microscopic origin of the different singularities, and of the relation between the shear rigidity and the interparticle friction, is still lacking and deserves future work.

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