

お体ガスおよびサスペンション系の レオロジーに及ぼす影響についての理論的研究



http://web.tuat.ac.jp/~takada/

16pB19-4

(農工大工)

日本物理学会第77回年次大会(2022年)

Granular Materials

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Macroscopic matters (µm~km) (Quantum effects are negligible.)





Examples:

sand, toner particles, coffee, volcanic PM2.5, Saturn's ring...

Behavior is different from usual gas, liquid, or solid Example: Brazil nut effect Larger particles move up.





Flow of granular materials

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Surface flow of sand mountains

Only particles near the surface can flow (liquid-like).



• Other particles do not move (solid-like). Coexistence of both states in one system. Existence of the jamming density φ_{I}

- $\varphi < \varphi_{\rm I}$: liquid-like response
- $\varphi > \varphi_{\rm I}$: solid-like response



Viscosity

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• Viscosity $\eta(\varphi) \equiv \frac{\sigma(\varphi)}{\dot{\gamma}}$: characterizes noneq. transport

Example: Suspension Dilute case (Einstein, 1906): $\frac{\eta_s(\varphi)}{n_0} = 1 + \frac{5}{2}\varphi$ ($\varphi \le 0.03$)

Solvent viscosity: η_0 Shear rate: $\dot{\gamma}$





Dense case (near jamming): $\frac{\eta_s(\varphi)}{\eta_0} = \left(1 - \frac{\varphi}{\varphi_m}\right)^{-2}$ (empirical) Shear rate dependent viscosity

Shear thickening (thinning): Viscosity becomes large (small) as y increases.

Example: granular gas $\eta \propto \dot{\gamma}$ (Bagnold scaling)

Shear thickening

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• Discontinuous shear thickening (DST): viscosity discontinuously increases.



⇒ DST is studied in many contexts and setups.

DST for dense systems (simulations)

• Mutual friction is important. M. Otsuki & H. Hayakawa, Phys. Rev. E **83**, 051301 (2011) R. Seto, et al., Phys. Rev. Lett. **111**, 218301 (2013)

DST for colloidal systems (experiments)

Normal stress difference

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is also important. C. D. Cwalina & N.J. Wagner, J. Rheol. **58**, 949 (2014)

"Inertial effect" is often ignored for suspension. (overdamped) If this is not ignored, system is called as "inertial suspensions" (a model of aerosols or colloid)

 $\begin{pmatrix} 10^{-2} \\ 10^{-3} \\ 10^{-4} \\ * \\ 10^{-5} \\ 10^{-6} \\ 10^{-7} \\ 10^{-8} \\ 10^{-6} \\ 10^{-5} \\ \cdot \\ \gamma \\ \end{pmatrix}$



Previous studies of inertial suspension

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System: frictionless, Stokes' drag

- - Find the two theorem is the term of t
 - > No thickening for $\varphi \gtrsim 0.63$
 - **※ Only contact** contribution

Rheology of dilute gas-solid suspensions without thermal noise Tsao and Koch, JFM 296, 211 (1995) Quenched-Ingnited transition DST-like transition for temperature but not for viscosity





Our previous works

Kinetic theoretical approach considering the thermal noise (Hard-core system)

- Boltzmann-Enskog theory well describes monodisperse systems up to $\varphi \leq 0.50$.
- DST-like transition in the dilute system
 H. Hayakawa and S. Takada, PTEP 2019, 083301 (2019)
- DST-like to CST-like as the density B. Hayakawa, S. Takada, and V. Garzó, PRE 96, 042903 (2017)
- Mpemba effect in the relaxation process
 S. Takada, H. Hayakawa, and A. Santos, Phys. Rev. E 103, 032901 (2021)



Motivation

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We would like to know

Impact of softness of particles on the rheology

		Suspension		Granular system
		Hard-core	Soft-core	Soft-core
Theory & Sim.	Dilute	Hayakawa & Takada PTEP (2019)		Our study
	Moderately dense	Hayakawa, Takada, & Garzó PRE (2017), Takada, Hayakawa, Santos, & Garzó PRE (2020)	Our study	
Sim.	Dense		Kawasaki, Ikeda, & Berthier EPL (2014)	

Our theoretical tool: Kinetic theory

Why kinetic theory?

Kinetic theory of granular gases

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Ogawa; Savage and Jeffrey, 1978~1981 Beginning of application of inelastic Boltzmann equation to granular system

Brey et al., 1998

Application of Chapman-Enskog method to inelastic Boltzmann equation

Transport coefficients for dilute system

Garzó & Dufty, 1999

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Extension to finite density (Enskog equation)



S. Chialvo and S. Sundaresan, Phys. Fluid. **25**, 0706503 (2013)

Kinetic theory is a powerful tool to treat the system for $\phi < 0.5$

Model and setup (Suspension)



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Langevin model for suspensions

Langevin equation:
$$\frac{dp_i}{dt} = \sum_j F_{ij} - \zeta p_i + m\xi_i$$

Boltzmann equation for the inertial suspension



shear

drag from the solvent particle interaction

Collision integral: $J[V|f, f] = \int dV_2 \int d\hat{k}\sigma_s(\chi, V_{12})V_{12}$



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× $[f(\mathbf{r}_1, \mathbf{V}_1', t)f(\mathbf{r}_2, \mathbf{V}_2', t) - f(\mathbf{r}_1, \mathbf{V}_1, t)f(\mathbf{r}_2, \mathbf{V}_2, t)]$ $\sigma_{\rm s}(\chi, V_{12})$: collision cross section

determined from the scattering problem Softness appears here.

(Dimensionless) control parameters: 1 Packing fraction: φ 2 Shear rate: $\dot{\gamma}^* \equiv \dot{\gamma}/\zeta$

(3) Particle softness: $\varepsilon^* \equiv \frac{\varepsilon}{m\sigma^2/2}$ (4) Env. temp.: $\xi_{env} \equiv$

$$\sqrt{\frac{T_{\rm env}}{m}}\frac{1}{\zeta\sigma}$$

Softness of particles

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Scattering analysis

$$\theta = \int_0^{u_0} \frac{b du}{\sqrt{1 - b^2 u^2 - \frac{4}{mv^2} U\left(\frac{1}{u}\right)}}$$

= $\sin^{-1} \frac{b}{\sigma} + C_1 F(\phi, v) + C_2 \Pi(a; \phi | v) + C_3 \tan^{-1} \gamma + C_2 \Pi(a; \phi | v)$



Introduction of Omega integral:

$$\Omega_{2,2}^{*}(T^{*}) \equiv \int_{0}^{\infty} dy \, y^{7} e^{-y^{2}} \int_{0}^{1} db^{*} b^{*} \sin^{2} \chi \left(b^{*}, 2y \sqrt{T^{*}} \right)$$

The ratio of the coll. freq. of soft particles
 to that of hard-core particles

 $\Omega_{2,2}^* = \nu_{\rm soft} / \nu_{\rm HC}$

• Low T: hard-core like $(\Omega_{2,2}^* \simeq 1)$

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• High T: softer and softer $(\Omega_{2,2}^* \to 0)$



Enskog kinetic equation for the inertial suspension

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

Evolution equation for the kinetic stress:

 $\frac{\partial}{\partial t}P_{\alpha\beta}^{k} + \dot{\gamma}\left(\delta_{\alpha x}P_{y\beta}^{k} + \delta_{\beta x}P_{y\alpha}^{k}\right) = -2\zeta\left(P_{\alpha\beta}^{k} - nT_{\rm env}\delta_{\alpha\beta}\right) - \Lambda_{\alpha\beta}$

Kinetic stress: $P_{\alpha\beta}^{k} = m \int d\mathbf{V} V_{\alpha} V_{\beta} f(\mathbf{V}, t)$ Moment of the collision integral: $\Lambda_{\alpha\beta} = -m \int d\mathbf{V} V_{\alpha} V_{\beta} J(\mathbf{V}|f, f)$ This equation is NOT closed!

<u>Closure</u>: Grad's moment method $f(\mathbf{V}) = f_{\rm M}(\mathbf{V}) \left(1 + \frac{m}{2T} \left(\frac{P_{\alpha\beta}^k}{nT} - \delta_{\alpha\beta} \right) V_{\alpha} V_{\beta} \right)$

Maxwellian distribution $f_{\rm M}(V) = n \left(\frac{m}{2\pi T}\right)^{\frac{3}{2}} \exp\left(-\frac{mV^2}{2T}\right)$

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A set of dynamic equations:

$$\frac{d\theta}{d\tau} = -\frac{2}{3}\dot{\gamma}^*\Pi_{xy}^* + 2(1-\theta)$$

$$\frac{d\Delta\theta}{d\tau} = -2\dot{\gamma}^*\Pi_{xy}^* - (\nu^* + 2)\Delta\theta$$

$$\frac{d\Pi_{xy}^*}{d\tau} = \dot{\gamma}^* \left(\frac{1}{3}\Delta\theta - \theta\right) - (\nu^* + 2)\Pi_{xy}^*$$
Dimensionless quantities

$$\theta = \frac{T}{T_{env}}$$
: temperature

$$\Delta\theta = \frac{\Delta T}{T_{env}}$$
: anisotropic temperature

$$\Pi_{xy}^* = \frac{P_{xy}^k}{nT_{env}}$$
: kinetic shear stress

$$\nu^* = \frac{95}{5\sqrt{\pi}}\Omega_{2,2}^*\varphi\xi_{env}\sqrt{\theta}$$

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$$\dot{\gamma}^{*} = (\nu^{*} + 2) \sqrt{\frac{3(\theta - 1)}{\nu^{*}\theta + 2}}$$
$$\eta^{*} = -\frac{\Pi_{xy}^{*}}{\dot{\gamma}} = \frac{\nu^{*}\theta + 2}{(\nu^{*} + 2)^{2}}$$

All quantities are written as a function of the temperature.

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Steady rheology

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- DST-like behavior even for soft system
- 2 step DST-like behaviors for harder system
- Shear thinning in high shear regime
- Kinetic theory reproduces the sim. results.





"Does this behavior survive even in denser situations?"

Extension to denser system

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Enskog kinetic equation for the inertial suspension

$$\left(\frac{\partial}{\partial t} \left(\dot{\gamma} V_{y} \frac{\partial}{\partial V_{x}} \right) f(V,t) = \zeta \frac{\partial}{\partial V} \cdot \left(\left[V + \frac{T_{\text{env}}}{m} \frac{\partial}{\partial V} \right] f(V,t) + J_{\text{E}}(V|f,f) \right)$$

Shear drag from the solvent particle interaction Collision integral: $J_{\rm E}[V|f,f] = \int dV_2 \int d\hat{k} \sigma_{\rm s}(\chi,V_{12})V_{12}[f^{(2)}(\boldsymbol{r},\boldsymbol{r}+r_{\rm min}\hat{k},V_1'',V_2'',t) - f^{(2)}(\boldsymbol{r},\boldsymbol{r}-r_{\rm min}\hat{k},V_1,V_2,t)]$ $\sigma_{\rm s}(\chi,V_{12})$: collision cross section, $f^{(2)}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{V}_1,\boldsymbol{V}_2,t) \simeq g_0 f(r_1,V_1,t) f(r_2,V_2,t)$: decoupling approx.

Closure: Grad's moment method
$$f(\mathbf{V}) = f_{\mathrm{M}}(\mathbf{V}) \left(1 + \frac{m}{2T} \left(\frac{P_{\alpha\beta}^{k}}{nT} - \delta_{\alpha\beta} \right) V_{\alpha} V_{\beta} \right)$$

Maxwellian distribution $f_{\rm M}(\mathbf{V}) = n \left(\frac{m}{2\pi T}\right)^{\frac{3}{2}} \exp\left(-\frac{mV^2}{2T}\right)$

$$\begin{aligned} \frac{\partial \theta}{\partial \tau} &= -\frac{2}{3} \dot{\gamma}^* \Pi_{xy}^* + 2(1-\theta) - \frac{1}{3} \Lambda_{\alpha\alpha}^*, \\ \frac{\partial \Delta \theta}{\partial \tau} &= -2 \dot{\gamma}^* \Pi_{xy}^* - 2 \Delta \theta - \delta \Lambda_{xx}^* + \delta \Lambda_{yy}^*, \\ \frac{\partial \delta \theta}{\partial \tau} &= -2 \dot{\gamma}^* \Pi_{xy}^* - 2 \delta \theta - 2 \delta \Lambda_{xx}^* - \delta \Lambda_{yy}^*, \\ \frac{\partial \Pi_{xy}^*}{\partial \tau} &= -\dot{\gamma}^* (\theta + \Pi_{yy}^*) - 2 \Pi_{xy}^* - \Lambda_{xy}^*, \end{aligned}$$

Denser system

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DST-like behavior survives

- even for finite density. (⇔ CST-like for hard-core system)
- Shear thinning in high shear regime_n*
- Kinetic theory reproduces the sim. results.



Parameters: $\varphi = 0.10, 0.20, 0.30$ $\varepsilon^* = 10^4, \xi_{env} = 1.0$



(= cannot be ignored)

Stokes' + lubrication model

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• More realistic hydrodynamic interaction **Stokes' + lubrication model**: $F_i^{\rm H} = -\sum_j \overleftarrow{\zeta_{ij}} p_j$ $\overrightarrow{\zeta_{ij}}$ has nondiagonal components

$$\zeta_{ij,\alpha\beta} = \begin{cases} \frac{3\pi a\eta_0}{m} \delta_{\alpha\beta} + \sum_{k\neq i} \frac{1}{m} A_{ik,\alpha\beta}^{(1,1)} \Theta(r_c - r_{ik}) & (i = j) \\ -\frac{1}{m} A_{ij,\alpha\beta}^{(1,1)} \Theta(r_c - r_{ij}) & (i \neq j) \end{cases}$$

$$A_{ij,\alpha\beta}^{(1,1)}: \text{ function of } \hat{\mathbf{k}} \equiv \mathbf{r}_{ij} / |\mathbf{r}_{ij}| & (\mathbf{r}_{ij} \equiv \mathbf{r}_j - \mathbf{r}_i) \\ (\not\subseteq \forall \text{ Kim \& Karrila, "Microhydrodynamics"}) \\ r_c \equiv d_{\mathrm{H}} + \lambda: \text{ cutoff length } (\lambda = 0.25d) \end{cases}$$

()-d.

- Scaled viscosity $\tilde{\eta} \equiv \eta/\eta_1$ against the Peclet number $Pe \equiv \frac{3\pi\eta_0 d^3}{4T_{env}}\dot{\gamma}$
 - $\eta \equiv P_{xy}/\dot{\gamma}, \eta_1 = \eta_0 \left(1 + \frac{5}{2}\varphi + 4\varphi^2 + 42\varphi^3\right):$ $\eta_1: \text{Empirical expression of}$

the apparent viscosity in the low shear limit

DST occurs at $Pe \simeq 10$.

Parameters:

$$\varphi = 0.30$$

 $\varepsilon^* = 10^4$, $\xi_{env} = 1.0$



Discussion: Estimation

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Aerosol

 $d \sim 10^{-5} \text{ m}, \rho \sim 1 \text{ g/cm}^3, E \sim 10 \text{ GPa} \Rightarrow m \sim 10^{-12} \text{ kg}$ Viscosity of air: $\eta_0 \sim 10^{-5} \text{ Pa} \cdot \text{s}$ DST takes place at $\dot{\gamma}_c \sim 10^3 \text{ 1/s} \Rightarrow$ shear speed 10 m/s if L = 1 cm

Colloid

- $d \sim 10^{-6} \text{ m}, \rho \sim 1 \text{ g/cm}^3, E \sim 1 \text{ GPa} \Rightarrow m \sim 10^{-14} \text{ kg}$ Viscosity of water: $\eta_0 \sim 10^{-3} \text{ Pa} \cdot \text{s}$ DST takes place at $\dot{\gamma}_c \sim 10^4 \text{ 1/s} \Rightarrow$ shear speed 10^4 m/s if L = 1 cm
- ► Kinetic temperature becomes 10² times larger. Is it possible to achieve this?
 ⇒ This will open for all researchers.



Case for nonlinear drag

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- Question:

What happens if the drag coefficient has velocity dependence?

- By solving scattering problem, the drag coeff. becomes $\zeta(v) = \zeta_0(1 + \gamma v^2)$.
- Change the env. Temperature at t = 0.
- No external force





Velocity distribution func. deviates from the Maxwellian in the relaxation process.

Detect this deviation in terms of a_2

$$\tilde{f}(\boldsymbol{c}) = \tilde{f}_{M}(\boldsymbol{c}) \left(1 + a_{2} \left(\frac{1}{2} c^{4} - \frac{5}{2} c^{2} + \frac{15}{8} \right) \right), \tilde{f}(\boldsymbol{c}) = \frac{v_{T}^{3}}{n} f(\boldsymbol{v}), \boldsymbol{c} \equiv \frac{v}{v_{T}}, v_{T} \equiv \sqrt{\frac{2T}{m}}$$

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$$\frac{\partial}{\partial t}f(\boldsymbol{v}) - \frac{\partial}{\partial \boldsymbol{v}} \cdot \left[\zeta(\boldsymbol{v})\left(\boldsymbol{v} + \frac{k_{\mathrm{B}}T_{\mathrm{env}}}{m}\right)f(\boldsymbol{v})\right] = J[\boldsymbol{v}|f, f],$$

$$\int \frac{d\theta}{d\tau} = -2(\theta - 1)(1 + 5\gamma\theta) - 10\theta^{2}a_{2},$$

$$\frac{da_{2}}{d\tau} = -8\gamma(\theta - 1) - \left[\frac{4}{\theta} - 8\gamma + 44\gamma\theta + \frac{64}{5\sqrt{\pi}}\varphi\xi_{\mathrm{env}}\sqrt{\theta}\Omega_{2,2}^{*}\left(\frac{\theta}{k^{*}}\right)\right]a_{2}.$$

$$\theta = \frac{T}{T_{\mathrm{env}}^{(\mathrm{tat})}}, \quad \theta_{0} = \frac{T_{\mathrm{env}}^{(\mathrm{ini})}}{T_{\mathrm{env}}^{(\mathrm{tat})}}, \quad \tau = \zeta_{0}t.$$

$$\int \frac{\theta(\tau)_{1,0}}{\theta(\tau)_{1,0}} \int \frac{10^{4}}{10^{2}} \int \frac{\theta}{10^{4}} \int \frac{\theta}{10^{$$

Deviation has a peak at a certain time. Softness is not important in the relaxation process. Good agreement with the simulation. 2022/3/16

Extension to granular system

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- Our theory itself can treat only elastic collision.
- Assumption: collisions occur instantaneously. (Hard-core like)

$$\boldsymbol{v}_1' = \boldsymbol{v}_1 - \frac{1+e}{2} (\boldsymbol{v}_{12} \cdot \hat{\boldsymbol{k}}) \hat{\boldsymbol{k}}$$
$$\boldsymbol{v}_2' = \boldsymbol{v}_2 + \frac{1+e}{2} (\boldsymbol{v}_{12} \cdot \hat{\boldsymbol{k}}) \hat{\boldsymbol{k}}$$

Boltzmann equation

$$\left(\frac{\partial}{\partial t} - \dot{\gamma} V_y \frac{\partial}{\partial V_x}\right) f(V, t) = J(V|f, f)$$

Softness

Collision integral: $J[V|f, f] = \int dV_2 \int d\hat{k} \sigma_s(\chi, V_{12}) V_{12}$ $\times \left[\frac{1}{e^2} f(r_1, V'_1, t) f(r_2, V'_2, t) - f(r_1, V_1, t) f(r_2, V_2, t) \right]$

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Hard-core like treatment



Results:

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Deviations from the Bagnold scaling

$$T_{\rm B} = \frac{5\pi(2+e)}{432(1-e)(1+e)^2(3-e)^2} \frac{1}{\varphi} m\sigma^2 \dot{\gamma}^2,$$

$$\Delta T_{\rm B} = \frac{25\pi(2+e)}{432(1+e)^2(3-e)^3} \frac{1}{\varphi^2} m\sigma^2 \dot{\gamma}^2,$$

$$\eta_{\rm B} = \frac{5(2+e)}{72(1+e)^2(3-e)^3} \sqrt{\frac{5(2+e)}{3(1-e)}} \frac{1}{\varphi} \frac{m}{\sigma} \dot{\gamma}.$$





Summary

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- We have developed the kinetic theory of soft-core suspension and granular gases.
- Suspension:
 - Softness induced DST-like behaviors for frictionless system
 - DST-like behaviors can occur twice.
 - Second DST-like behavior survives even for finite density.
 - Deviation from the Maxwellian if the drag coeff. has vel. dependence.
- Granular gas:
 - Deviation from the Bagnold scaling
 - No solution for larger shear rate