Kinetic theory for dilute cohesive granular gases with a square well potential

Satoshi Takada
Yukawa Institute for Theoretical Physics, Kyoto University

Shear thickening

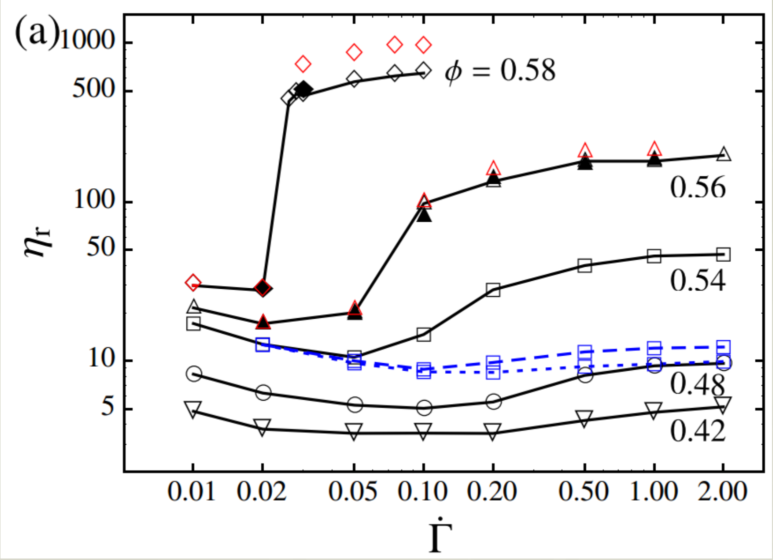
Why can we run on fluid?
⇒ Shear viscosity increases as the shear rate increases.

There are many papers studying shear thickening.

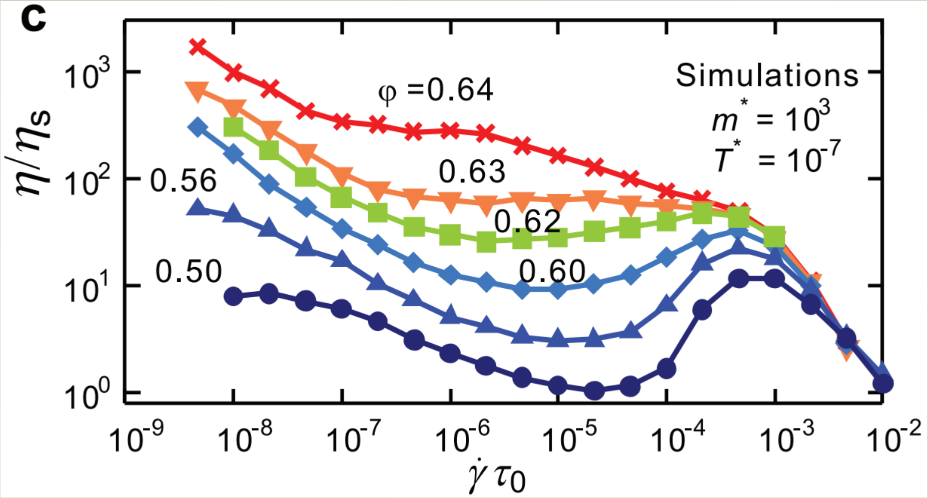
Shear thickening

- Dense suspension
  Discontinuous shear thickening
- For $0.3 < \phi < 0.4$,
  Continuous shear thickening

Seto et al. PRL, **111**, 218301 (2013)



Kawasaki et al. EPL **107**, 28009 (2014)

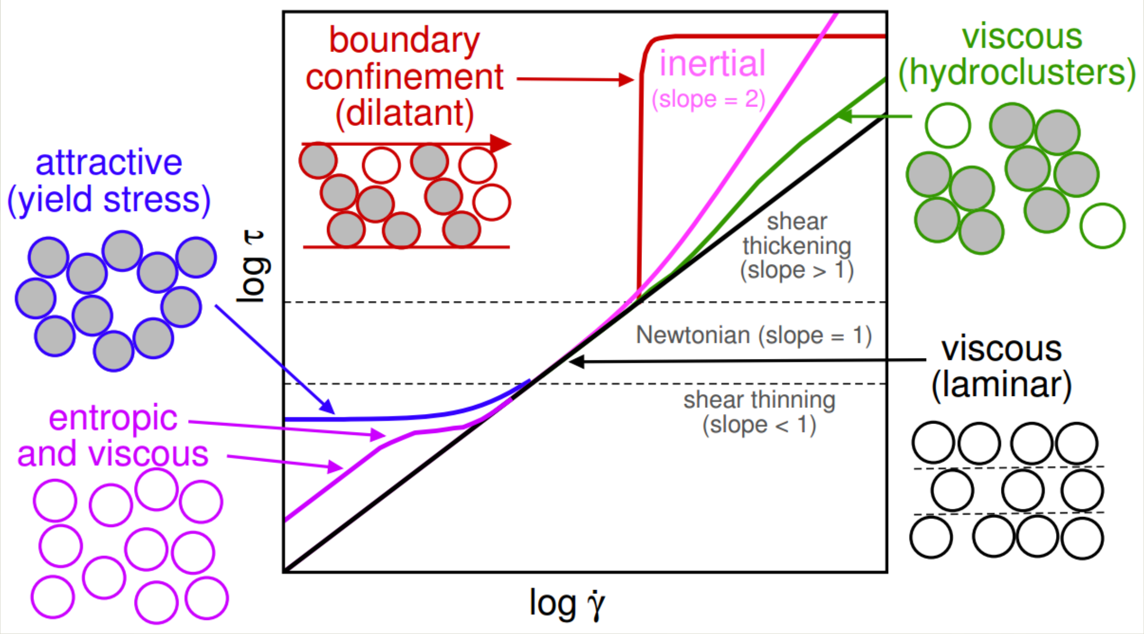


Mechanism

Many mechanisms have been proposed to explain shear thickening.

- hydroclusters
- dilatant
- …

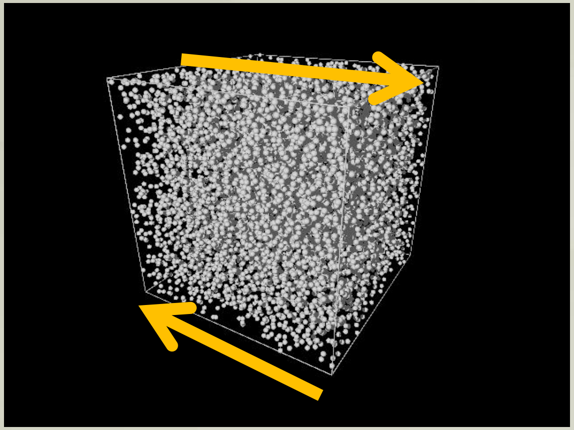
Brown & Jaeger, Rep. Prog. Phys. **77**, 046602 (2014)



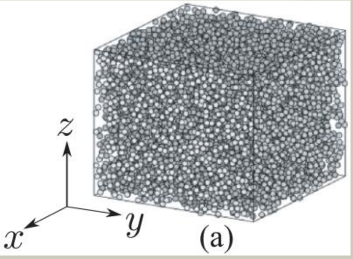
Molecular dynamics simulation under a plane shear

S. Takada, K. Saitoh, & H. Hayakawa, Phys. Rev. E, **90**, 062207 (2014)

Lennard-Jones potential
+ dissipation

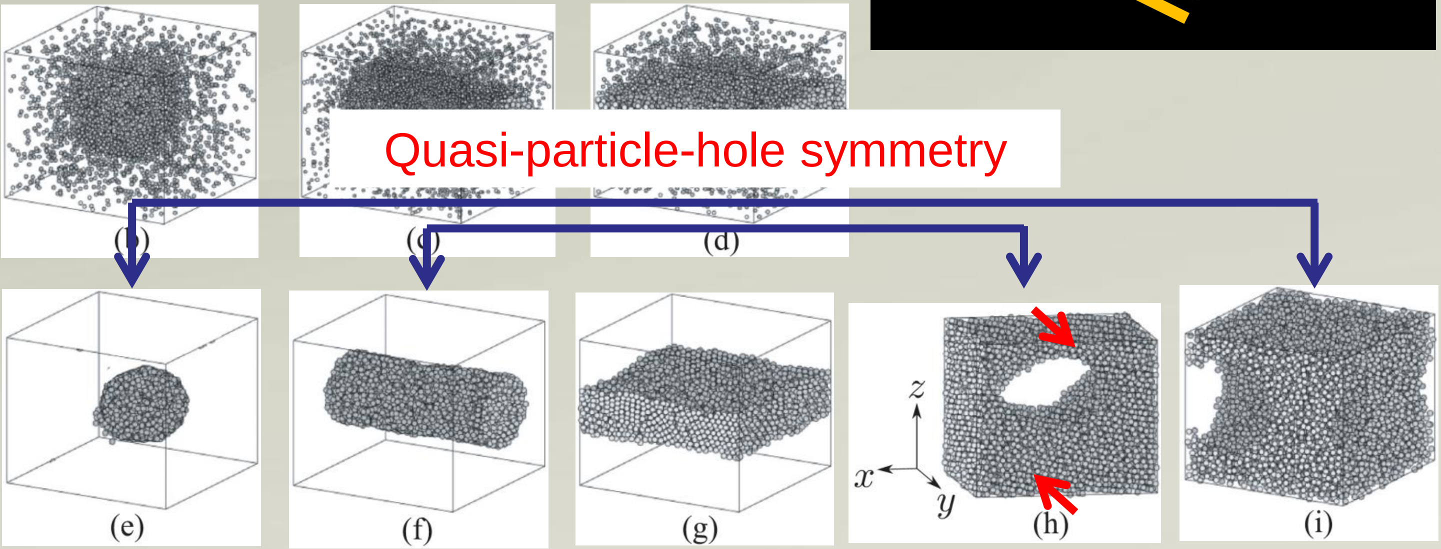


uniform



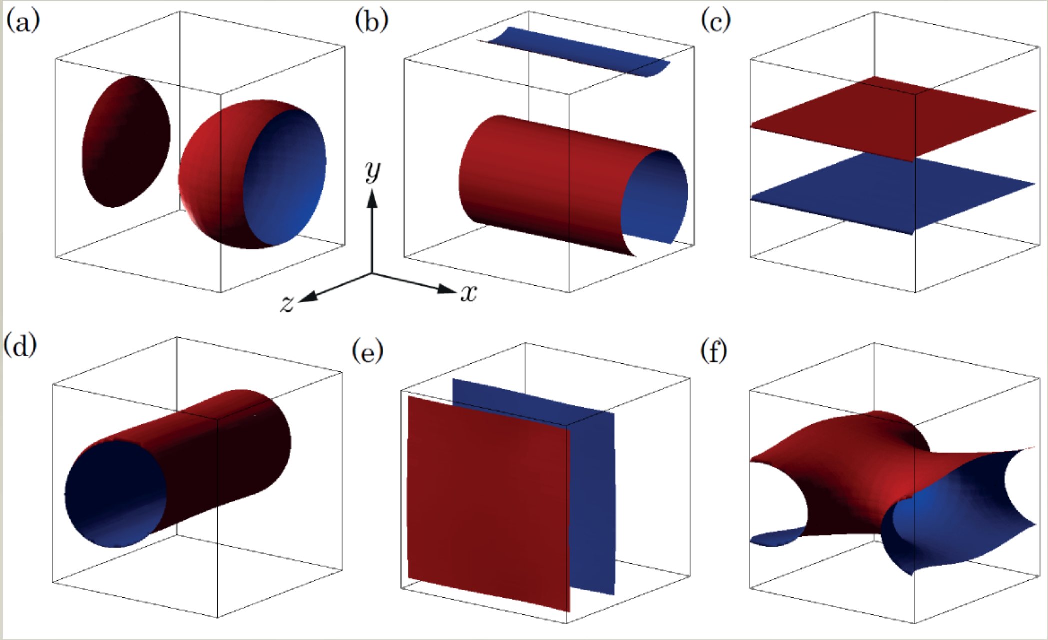
coexistence

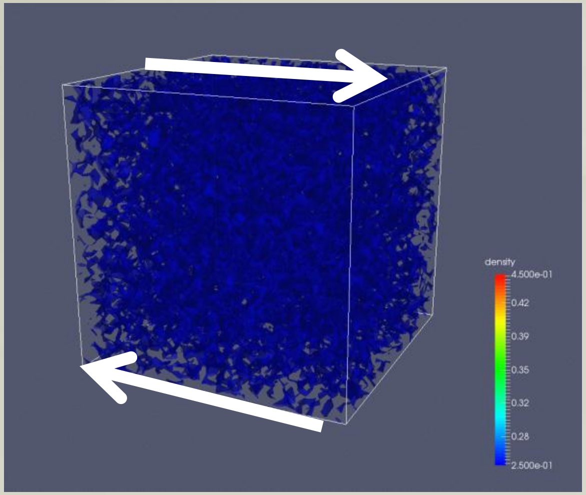
cluster



Hydrodynamics for cohesive system
based on dynamic van der Waals model

$$p = \frac{nT}{1 - v_0 n} - \varepsilon v_0 n^2$$





Qualitatively similar patterns as MD simulation.

Motivation of this work

Theoretical explanation of shear thickening is poor.
Can we derive shear thickening theoretically?

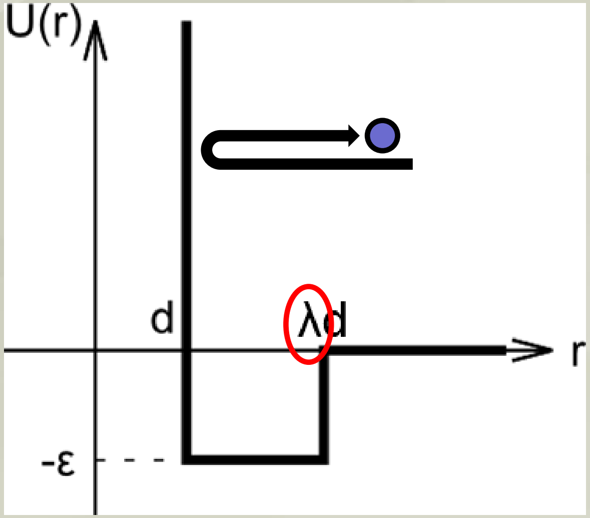
Nonequilibrium statistical mechanics approach to explain shear thickening

- Especially for dilute cohesive system
- Development of kinetic theory based on Boltzmann equation for cohesive granular gases
- Derivation of shear viscosity

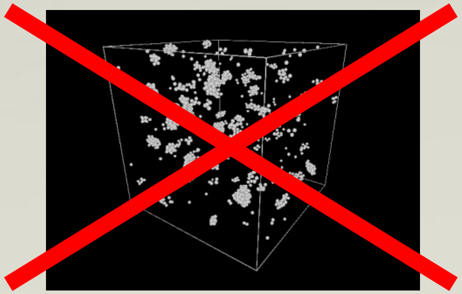
Setup

- Monodisperse particles (mass: m, diameter d)
- Square-well potential

$$U(r) = \begin{cases} \infty & (r < d) \\ -\varepsilon & (d < r < \lambda d) \\ 0 & (r > \lambda d) \end{cases}$$



- Collision
  - inelastic (restitution coeff. e) at $r = d$
  - elastic (otherwise)
- Dilute limit： $nd^3 \ll 1$ (n: density)
- Weakly inelastic limit： $e \lesssim 1$



Assumption：We ignore the trapping process.

Boltzmann equation

Santos et al. PRE (2004)

Starting point:
Boltzmann equation under a plane shear

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

Velocity distribution function = (lowest order of Grad expansion)

$$f(\boldsymbol{V}) = f_{\mathrm{M}}(\boldsymbol{V}) \left[1 + \frac{m}{2T}\left(\frac{P_{ij}}{nT} - \delta_{ij}\right) V_i V_j\right]$$

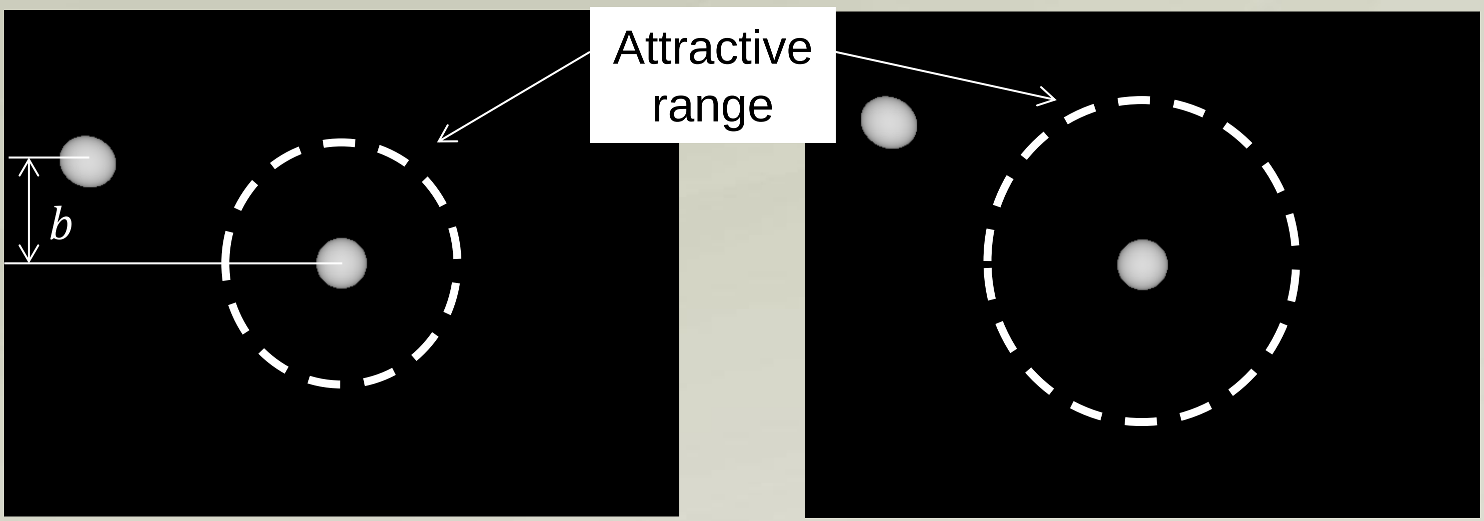
$f_{\mathrm{M}}(V)$: Maxwell distribution

$I(f, f)$: collision integral

Scattering process

> ☛ Landau Lifshitz "Mechanics"
> refractive index $\nu = \sqrt{1 + \dfrac{4\varepsilon}{mv^2}}$

- Hard core system…inelastic
- Cohesive system…depending on b and v,
  (a) inelastic collision
  (b) grazing collision (no dissipation)
  Acceleration in the well (energy conservation)



(a) Inelastic collision $(b < \nu d)$

(b) Grazing collision $(\nu d < b < \lambda d)$

Boltzmann equation

YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

Boltzmann equation considering two types of collisions

$$\left(\frac{\partial}{\partial t} - \dot{\gamma} V_y \frac{\partial}{\partial V_x}\right) f(\boldsymbol{V}, t) = I_{\text{hard core}}(f, f)(f, f) + I_{\text{grazing}}(f, f)$$

Inelastic collisions Grazing collisions

Time evolution of stress tensor

$$\partial_t P_{ij} + \dot{\gamma}(\delta_{ix} P_{yj} + \delta_{jx} P_{iy}) = -\Lambda_{ij}$$

$$\Lambda_{ij} \equiv -m \int d\boldsymbol{v} V_i V_j I(f, f)$$

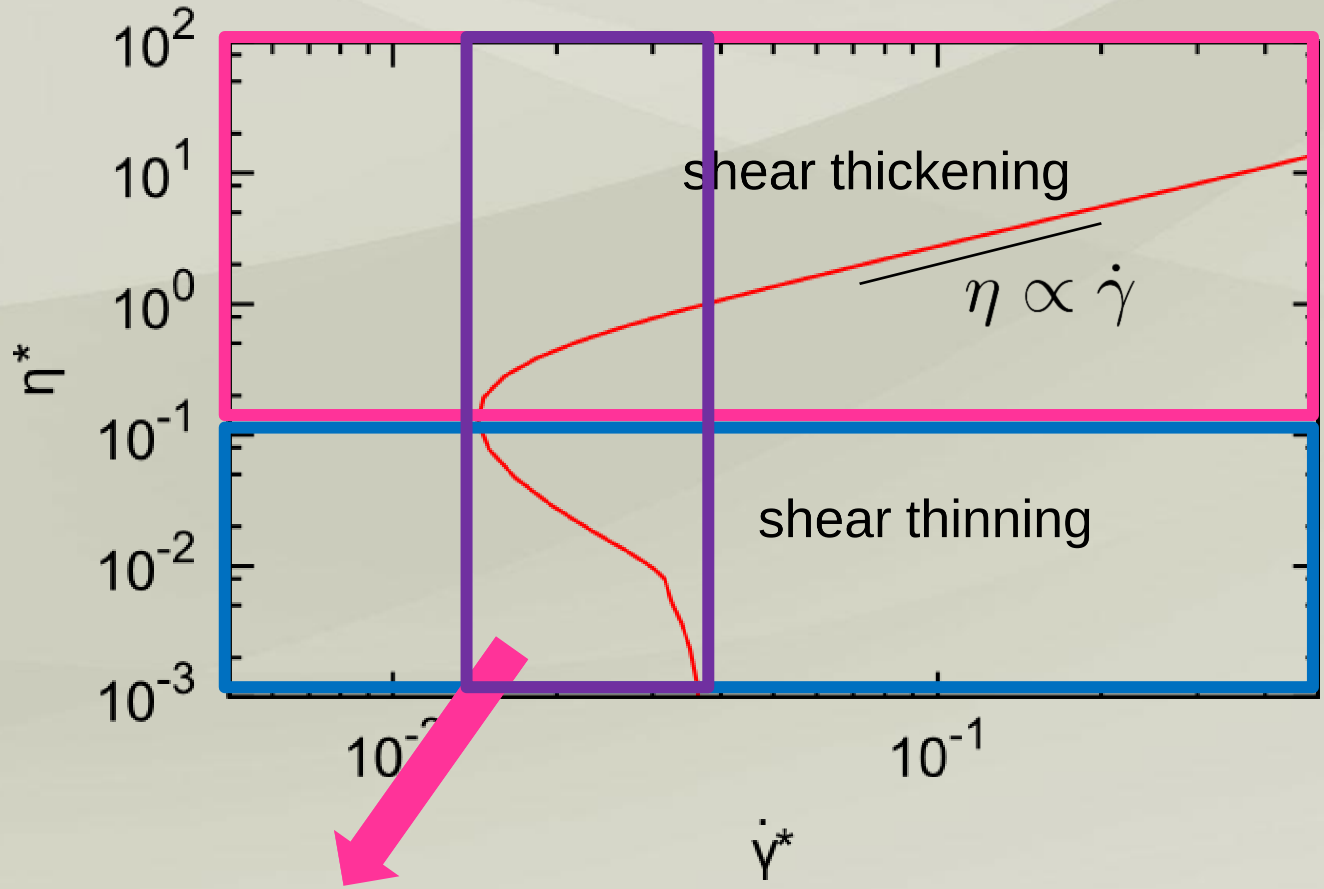
$$= \nu_1 (P_{ij} - p\delta_{ij}) + \nu_2 p \delta_{ij}$$

We focus only on the steady state.

$$\dot{\gamma}_{\rm s} = \sqrt{\frac{3}{2} \frac{\nu_1^2 \nu_2}{\nu_1 - \nu_2}}, \quad P_{xy,\rm s} = -\frac{p}{\nu_1} \sqrt{\frac{3}{2} \nu_2 (\nu_1 - \nu_2)}$$

$$\eta_{\rm s} = -\frac{P_{xy,\rm s}}{\dot{\gamma}_{\rm s}} = \frac{(\nu_1 - \nu_2) p}{\nu_1^2}$$

Shear viscosity vs. shear rate



parameter

$nd^3 = 0.01$

$\lambda = 2.5$

$e = 0.99$

shear thickening & shear thinning?

Question:
Which branch is stable in this region?

Linear stability analysis

To check the stability,
we perform a linear stability analysis around the steady state.

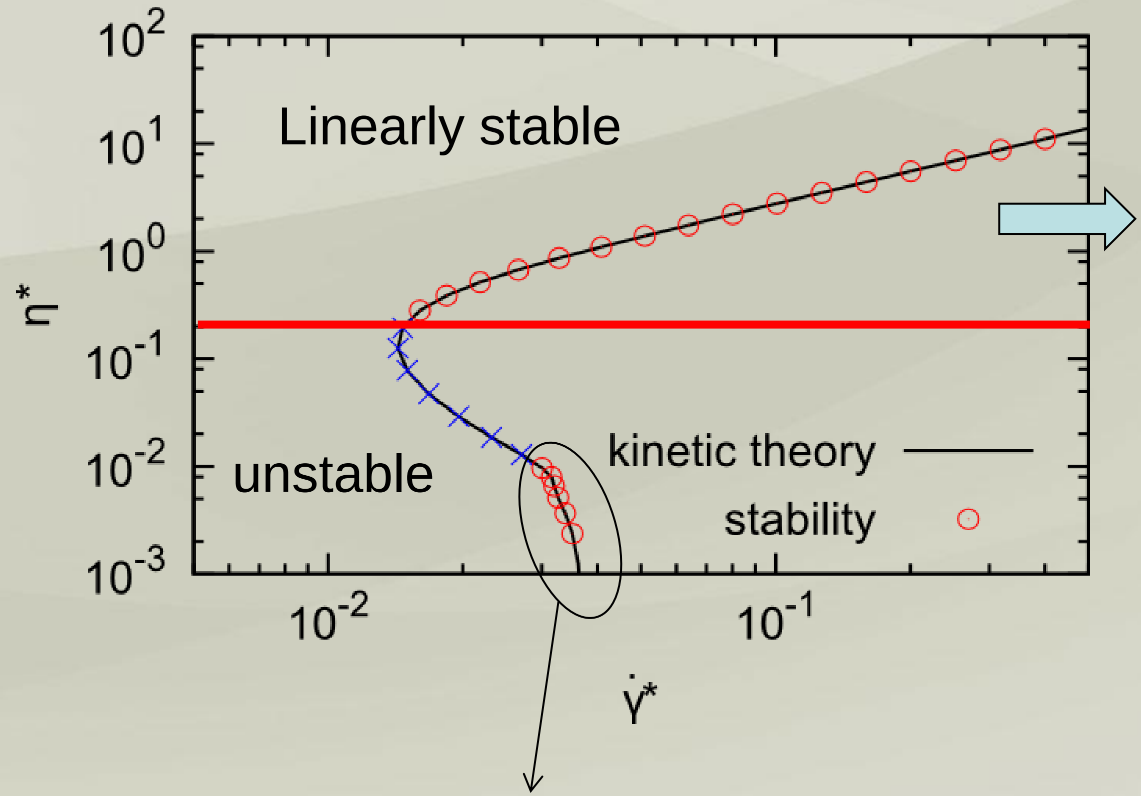
$$\partial_t P_{ij} + \dot{\gamma}(\delta_{ix} P_{yj} + \delta_{jx} P_{iy}) = -\Lambda_{ij}$$

We add a small perturbation

$$P_{ij} = P_{ij,\mathrm{s}} + \hat{P}_{ij}, \quad T = T_\mathrm{s} + \hat{T}$$

If $\hat{P}_{ij}, \hat{T} \to 0 \quad (t \to \infty)$, this state is stable.
Otherwise, unstable.

Linear stability analysis



The upper branch is stable.
⇒ shear thickening !

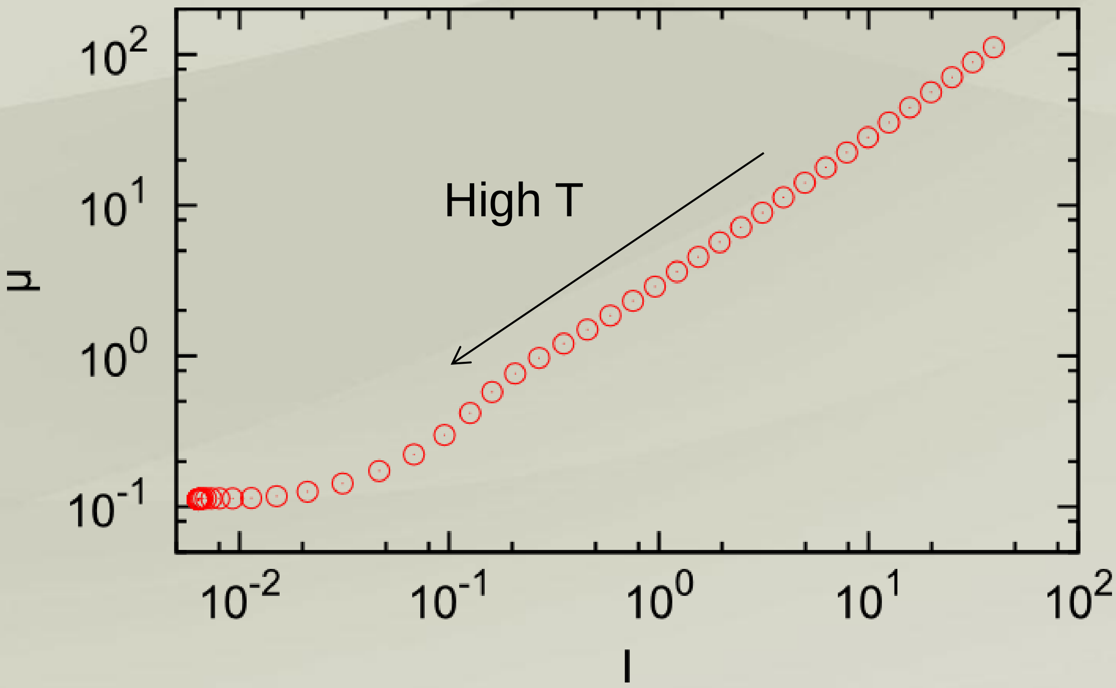
Do we need further analysis to check the stability of this region?
⇒ Future work

μ-I rheology

We also check μ-I rheology.

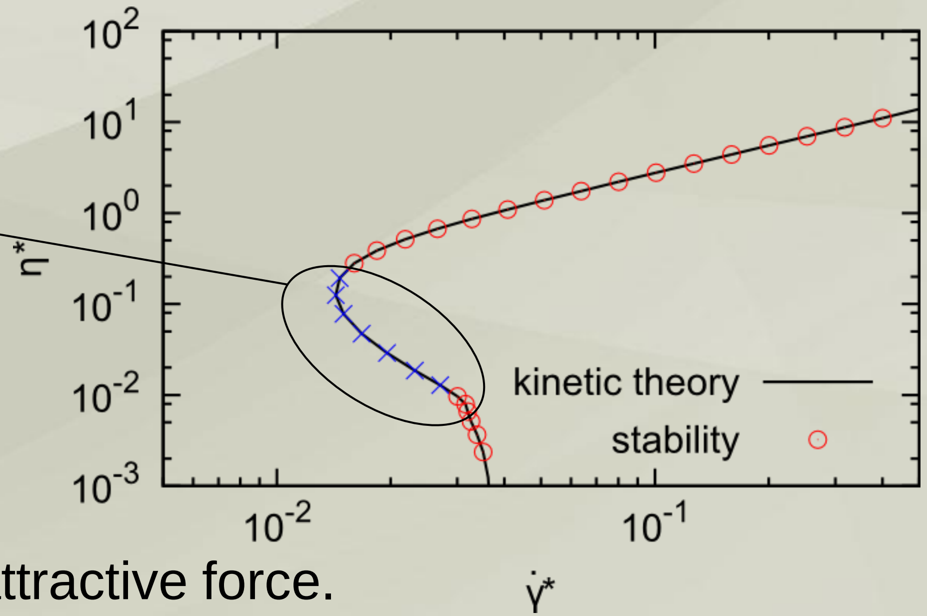
$$I = \frac{d\dot{\gamma}}{\sqrt{p/mn}}$$

$$\mu \equiv \frac{|P_{xy}|}{p}$$



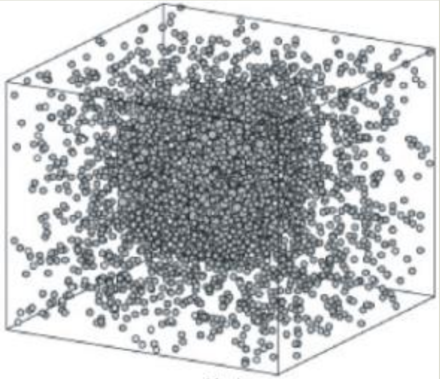
Discussion

What happens in
the shear thinning region?



Shear is weak.

Particles might form clusters due to attractive force.
= The system cannot be keep uniform.



(b)

Event-driven simulation is needed.
We have not implemented a code…

Summary

We have

- obtained the shear viscosity for the system under a plane shear.
- found that the shear viscosity becomes two-values function near the intermediate temperature.
- found that shear thickening region is stable from the linear stability analysis.

Future perspective

- Can we check the validity of our theory by performing an event-driven simulation?