Nonequilibrium mode-coupling theory for driven granular systems

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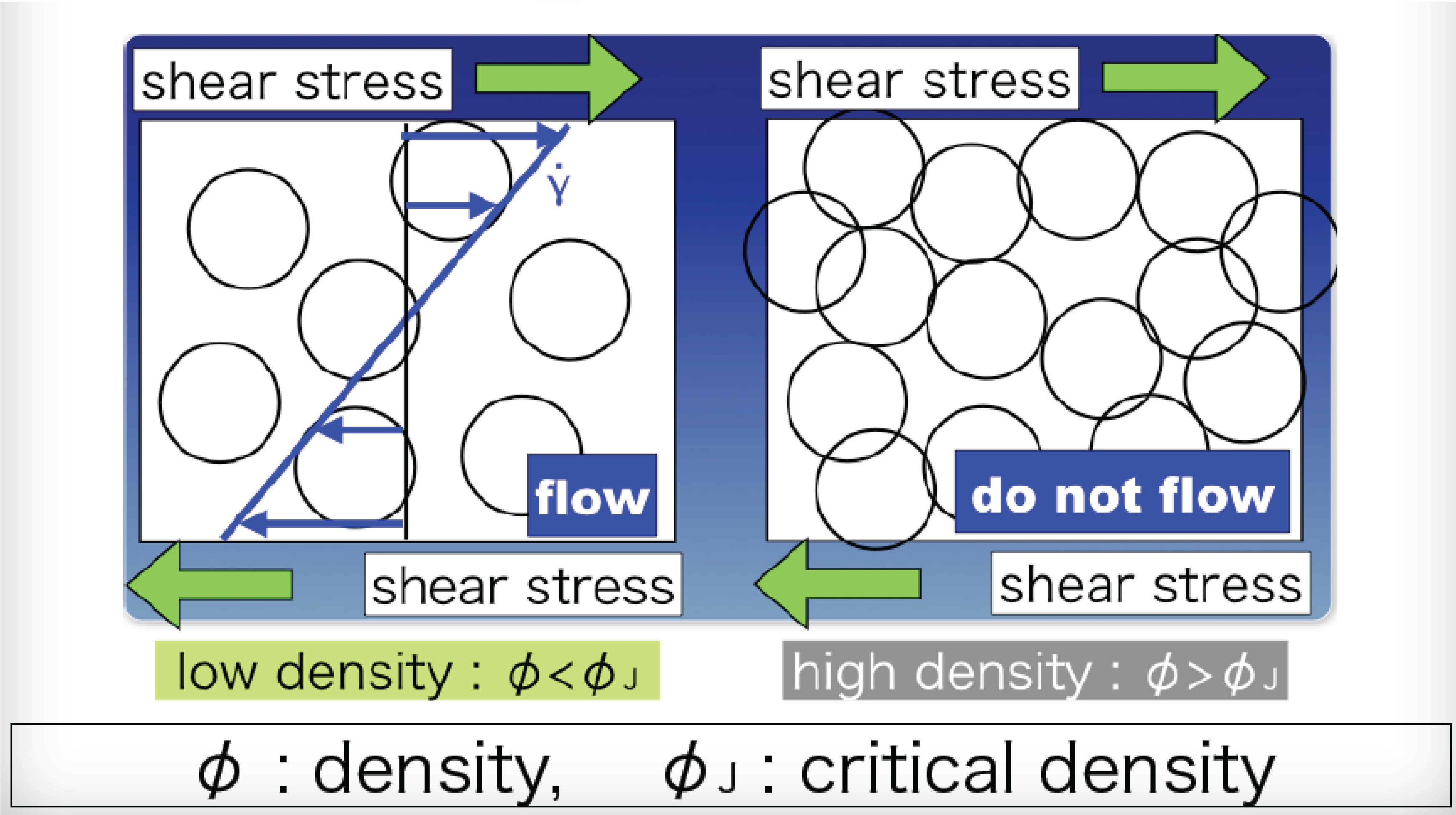
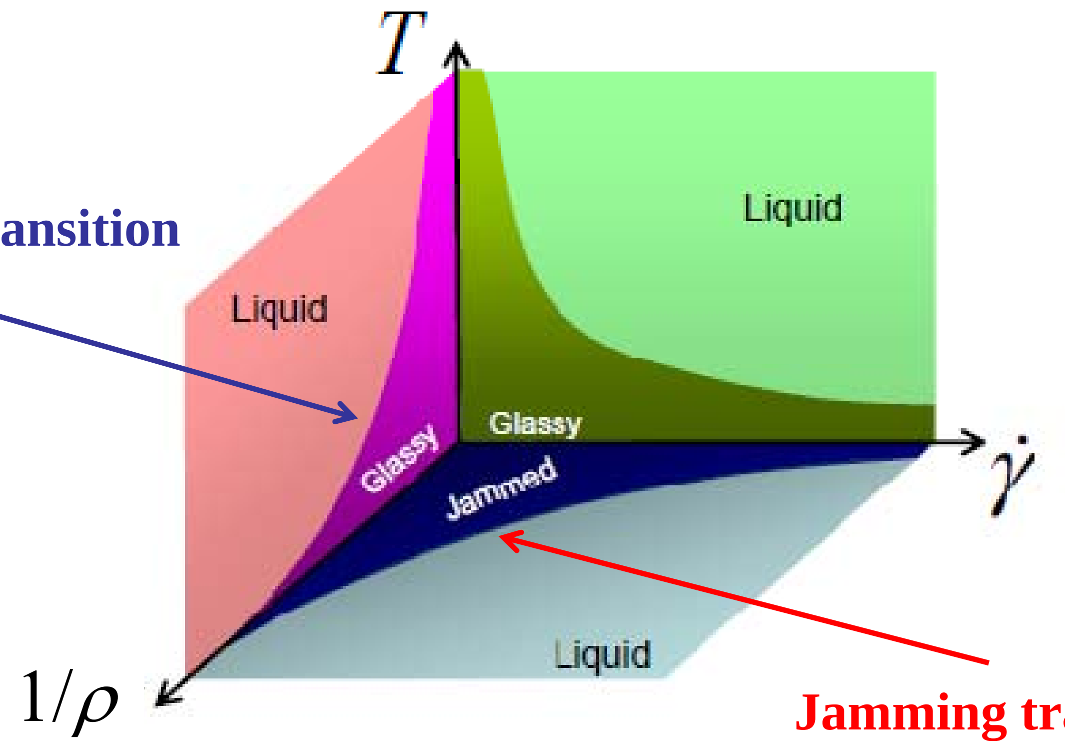
Jamming transition of granular systems



Motivation : unified understanding of jamming phase diagram



Liquid-glass transition

Jamming transition of granular systems

Liu and Nagel, Nature 396, 21 (1998)

Characteristic features of granular systems

- **Dissipative system (inelastic collisions)**
  - **coupled with heat bath of $T = 0$**
- **External load necessary to make it fluidized**
  - **e.g., shearing, shaking**
- **Intrinsic nonequilibrium system**
  - **linear response theory not applicable**
  - **no detailed balance**

    time-reversal symmetry broken

    Langevin equation not applicable

Liquid theory for linear transport coefficients

- Green-Kubo relation

$$D = \int_0^\infty dt \left\langle v_z(t) v_z(0) \right\rangle , \quad \eta = \frac{1}{k_B T V} \int_0^\infty dt \left\langle \sigma_{xy}(t) \sigma_{xy}(0) \right\rangle$$

- Generalized Langevin equation (Mori-Zwanzig equation)

$$\frac{\partial}{\partial t} Z(t) + \int_0^t ds\, M(t-s) Z(s) = 0 \;\text{ for }\; Z(t) = \left\langle v_z(t) v_z(0) \right\rangle$$

- Approximate theory for memory kernel (e.g. mode-coupling theory)

$$M(t) = \frac{\rho k_B T}{6\pi^2 m} \int dk\, k^4 c(k)^2 F_s(k,t) F(k,t)$$

steady-state properties arbitrarily far from equilibrium?

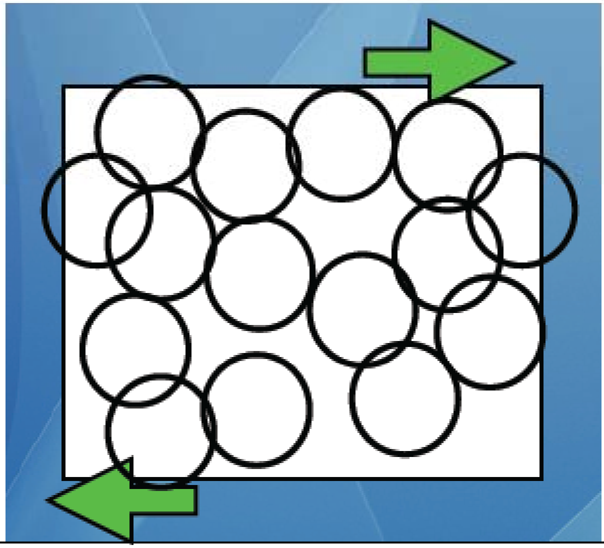
Nonequilibrium mode-coupling theory (MCT) for sheared granular systems

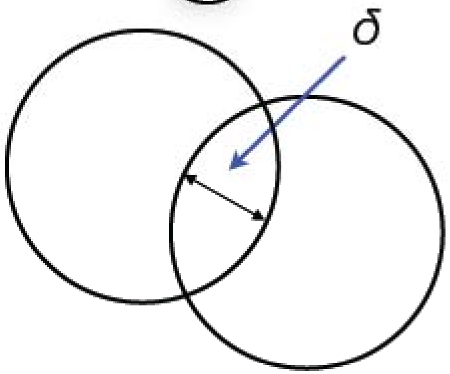
1. **Generalized Green-Kubo relation**
   for nonequilibrium steady-state properties
   in terms of **transient time-correlation function**

2. **Mori-Zwanzig equation of motion**
   for transient time-correlation function

3. **Mode-coupling approximation**

Model (frictionless grains)





$\Delta=1$ (Linear model)

$\Delta=3/2$ (Hertz model)

Interaction Force：$F=k\delta^{\Delta}$

Compressed Length：δ

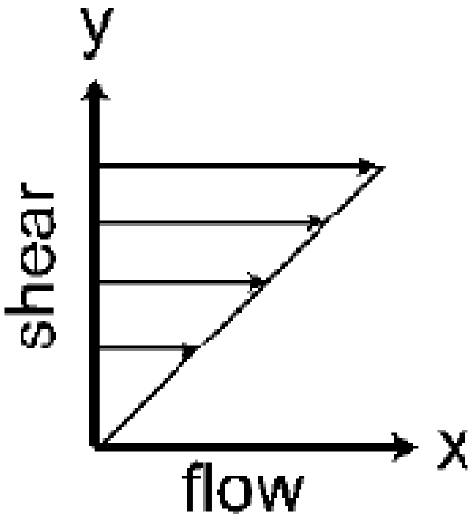
The exponent for the interaction：Δ

Dissipative force between the contacting particles

SLLOD equations of motion

- **SLLOD equations of motion**

$$\dot{\boldsymbol{r}}_i = \boldsymbol{p}_i / m + \boldsymbol{\kappa} \cdot \boldsymbol{r}_i$$
$$\dot{\boldsymbol{p}}_i = \sum_{j \neq i} \left(\boldsymbol{F}_{ij}^{\mathrm{el}} + \boldsymbol{F}_{ij}^{\mathrm{vis}} \right) - \boldsymbol{\kappa} \cdot \boldsymbol{p}_i$$



$\dot{\boldsymbol{r}}_i$: velocity

$\boldsymbol{p}_i$: peculiar momentum with respect to $\boldsymbol{u}(\boldsymbol{r}_i) = \boldsymbol{\kappa} \cdot \boldsymbol{r}_i$

$\boldsymbol{\kappa}$: shear rate tensor

$$\kappa_{\lambda\mu} = \dot{\gamma}\, \delta_{\lambda x}\, \delta_{\mu y}$$

$\boldsymbol{F}_{ij}^{\mathrm{el}} = \hat{\boldsymbol{r}}_{ij}\, \Theta(d - r_{ij}) f(d - r_{ij})$: conservative force $\left(\text{e.g. } f \sim x,\ f \sim x^{3/2}\right)$

$\boldsymbol{F}_{ij}^{\mathrm{vis}} = -\hat{\boldsymbol{r}}_{ij}\, \Theta(d - r_{ij}) \zeta(d - r_{ij}) (\boldsymbol{g}_{ij} \cdot \hat{\boldsymbol{r}}_{ij})$: dissipative force $\left(\text{e.g. } \zeta = \text{const},\ \gamma \sim x^{1/2}\right)$

with $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$ and $\boldsymbol{g}_{ij} = \dot{\boldsymbol{r}}_i - \dot{\boldsymbol{r}}_j$

Liouville equation

- **Liouville equation for the phase-space variable $A(\boldsymbol{\Gamma})$ with $\boldsymbol{\Gamma} = (\boldsymbol{r}^N, \boldsymbol{p}^N)$**

$$\frac{d}{dt}A(\boldsymbol{\Gamma}) = \dot{\boldsymbol{\Gamma}} \cdot \frac{\partial}{\partial \boldsymbol{\Gamma}} A(\boldsymbol{\Gamma}) \equiv iL\,A(\boldsymbol{\Gamma})$$

$$\text{formal solution}\ :\ A(\boldsymbol{\Gamma}(t)) = \exp(iLt)(\boldsymbol{\Gamma}(0))$$

- **Liouville equation for the phase-space distribution function $f(\boldsymbol{\Gamma},t)$**

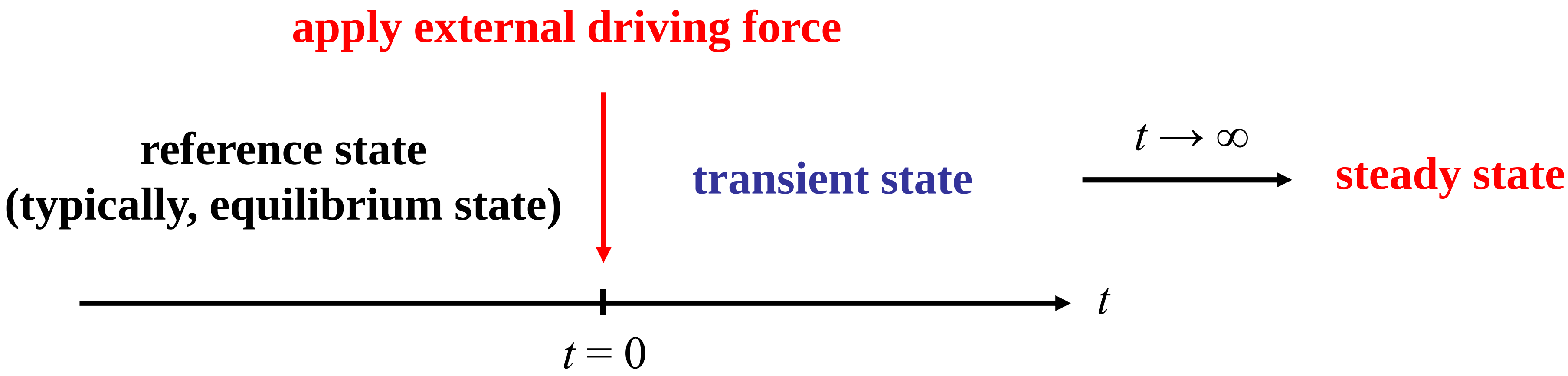
$$\frac{\partial}{\partial t} f(\boldsymbol{\Gamma},t) = -\left[\dot{\boldsymbol{\Gamma}} \cdot \frac{\partial}{\partial \boldsymbol{\Gamma}} + \left(\frac{\partial}{\partial \boldsymbol{\Gamma}} \cdot \dot{\boldsymbol{\Gamma}}\right)\right] f(\boldsymbol{\Gamma},t) \equiv -iL^* f(\boldsymbol{\Gamma},t)$$

$$iL^* = iL + \Lambda \quad \text{with} \quad \Lambda = \frac{\partial}{\partial \boldsymbol{\Gamma}} \cdot \dot{\boldsymbol{\Gamma}} = -\frac{1}{m}\sum_i \sum_{j \neq i} \Theta(d - r_{ij})\zeta(d - r_{ij})$$

$$\text{formal solution}\ :\ f(\boldsymbol{\Gamma},t) = \exp(-iL^* t) f(\boldsymbol{\Gamma},0)$$

Reference state for granular systems?

- Conventional method for handling external driving force

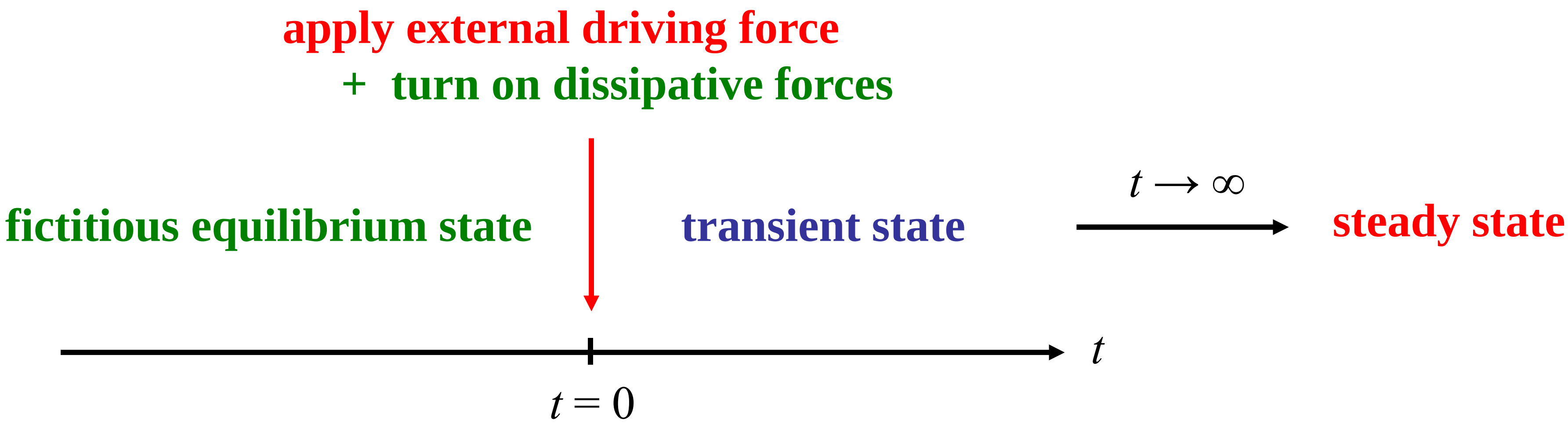


- **Naïve quiescent equilibrium state does not exist for granular systems due to the presence of inelastic collisions !**

Our recipe

reference state : fictitious equilibrium state

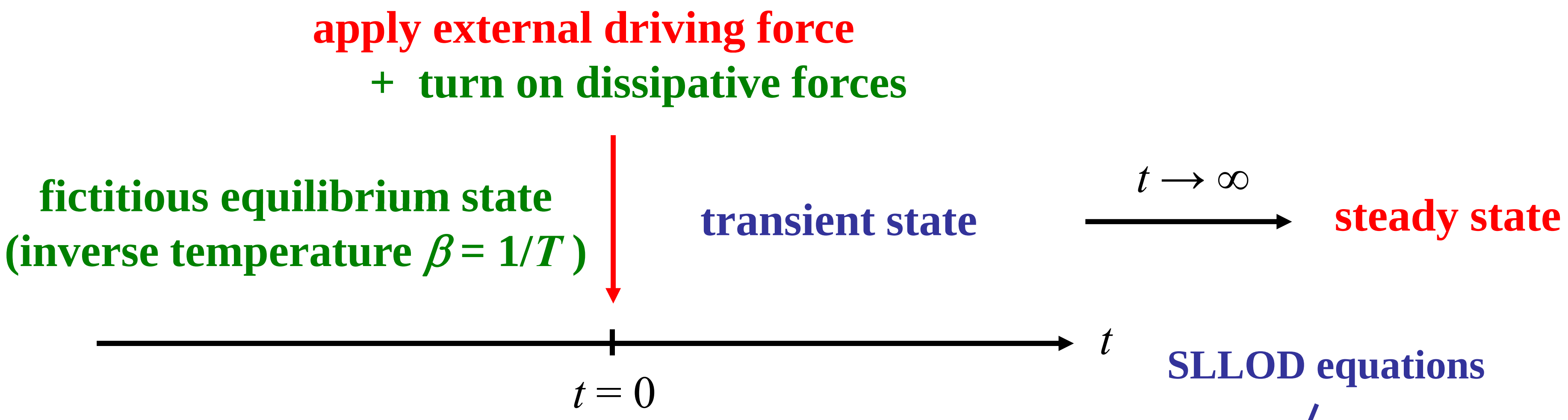
in which dissipative forces are turned off



Does it make sense? **Yes !**

steady-state properties do not depend on the choice of the reference state

Implementation of our recipe



- nonequilibrium phase-space distribution function : $f(\boldsymbol{\Gamma}, t) = \exp(-iL^* t)\, f_{\rm eq}(\boldsymbol{\Gamma}; \beta)$
- nonequilibrium average : $\langle A(t) \rangle_\beta \equiv \int d\boldsymbol{\Gamma}\, A(\boldsymbol{\Gamma})\, f(\boldsymbol{\Gamma}, t)$
- steady-state average : $\langle A \rangle_{\rm ss} \equiv \lim_{t\to\infty} \langle A(t) \rangle_\beta$
- identity : $e^{-iL^* t} = 1 + \int_0^t ds\, e^{-iL^* s} (-iL^*)$

Generalized Green-Kubo relation

(S.-H. Chong, M. Otsuki, and H. Hayakawa, Phys. Rev. E 81, 041130 (2010))

$$\langle A \rangle_{\mathrm{ss}} = \langle A(0) \rangle_\beta + \int_0^\infty ds \, \langle A(s) \Omega(0) \rangle_\beta$$

↑ **transient time-correlation function**

- **Dissipation function**

$$\Omega = -\beta \dot{\gamma} \sigma_{xy} - 2\beta R - \Lambda \quad \text{with} \quad \begin{cases} \sigma_{xy} = \sum_i \left[\dfrac{p_i^x p_i^y}{m} + x_i \sum_{j \neq i} \left(F_{ij}^{\mathrm{el},\, y} + F_{ij}^{\mathrm{vis},\, y} \right) \right] \\ R = \dfrac{1}{4} \sum_i \sum_{j \neq i} \Theta(d - r_{ij}) \zeta(d - r_{ij}) (\boldsymbol{g}_{ij} \cdot \hat{\boldsymbol{r}}_{ij})^2 \\ \Lambda = -\dfrac{1}{m} \sum_i \sum_{j \neq i} \Theta(d - r_{ij}) \gamma(d - r_{ij}) \end{cases}$$

- **e.g. steady-state shear stress :** $\sigma_{xy}^{\mathrm{ss}} \equiv -(1/V) \lim_{t \to \infty} \langle \sigma_{xy}(t) \rangle_\beta$

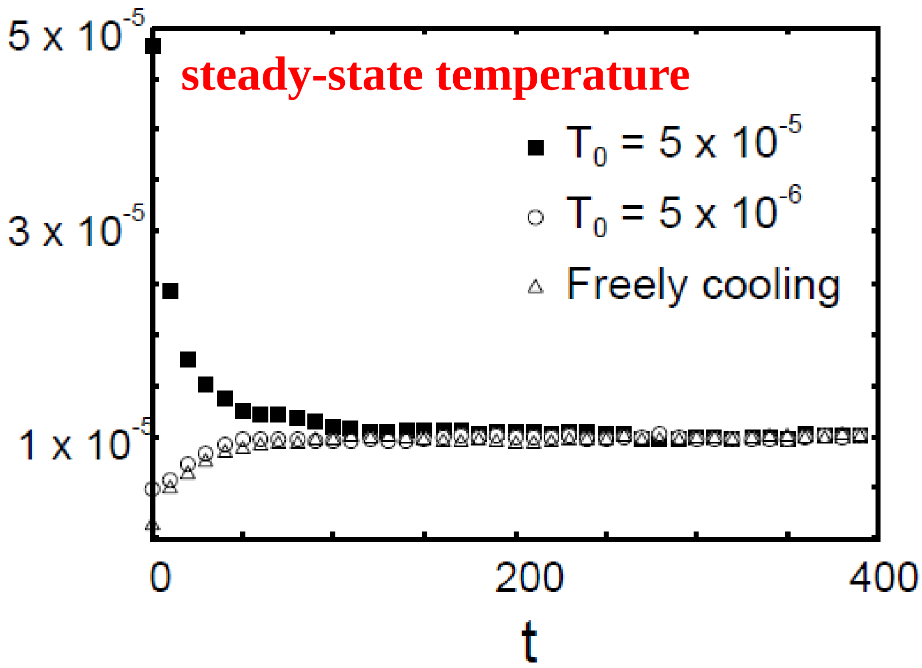
$$\sigma_{xy}^{\mathrm{ss}} = \frac{\beta \dot{\gamma}}{V} \int_0^\infty ds \, \langle \sigma_{xy}(s) \sigma_{xy}(0) \rangle_\beta + \frac{2\beta}{V} \int_0^\infty ds \, \langle \sigma_{xy}(s) R(0) \rangle_\beta + \frac{1}{V} \int_0^\infty ds \, \langle \sigma_{xy}(s) \Lambda(0) \rangle_\beta$$

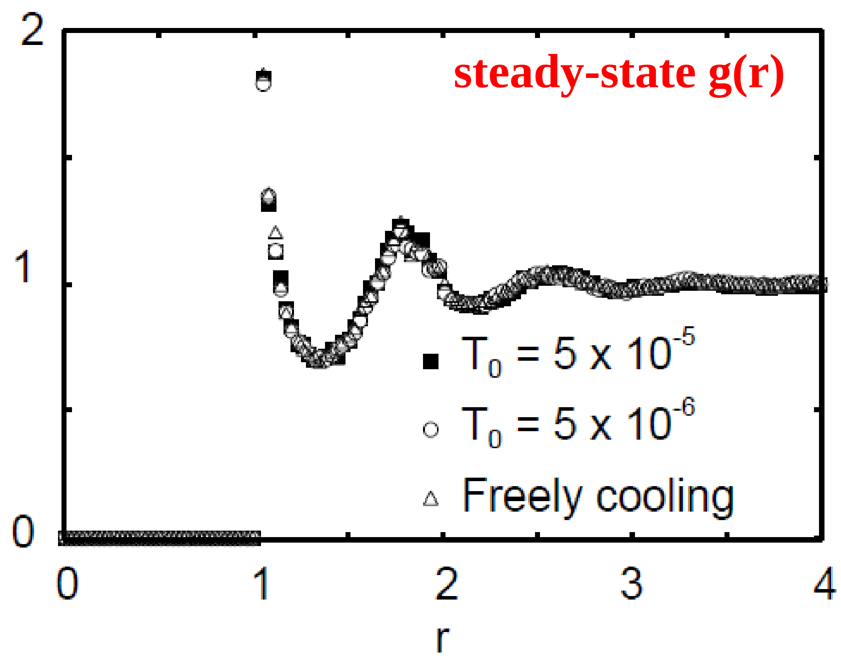
Justification of our recipe

- One can show that $\frac{\partial}{\partial\beta}\langle A(t)\rangle_\beta = \langle A(t)\rangle_\beta \langle H_0(0)\rangle_\beta - \langle A(t) H_0(0)\rangle_\beta$

- For systems that exhibit ***mixing*** $\left(\lim_{t\to\infty}\langle A(t)B(0)\rangle = \langle A(t)\rangle\langle B(0)\rangle\right)$

  there holds $\lim_{t\to\infty}\frac{\partial}{\partial\beta}\langle A(t)\rangle_\beta = 0$, i.e., $\langle A\rangle_{ss} = \lim_{t\to\infty}\langle A(t)\rangle_\beta$ is independent of β.





Remarks for the rest of the steps

- **Anisotropic nature of the sheared system**

$$C_{\lambda\mu}(\mathbf{q},t) \neq \hat{q}_\lambda \hat{q}_\mu C_L(q,t) + (\delta_{\lambda\mu} - \hat{q}_\lambda \hat{q}_\mu) C_T(q,t) \quad (\lambda, \mu = x, y, z)$$

- **Non-Hermitian nature of the Liouville operator**

$$\langle [iLA(t+\tau)] B(t)^* \rangle = -\langle A(t+\tau) [iLB(t)^*] \rangle + \langle A(t+\tau) B(t)^* \Omega(0) \rangle$$

- **Velocity-dependent dissipative force**

couplings to $\rho(k)\, j(p)$ as well as the ones to $\rho(k)\, \rho(p)$

must be taken into account in the mode-coupling approximation

MCT equations for transient density correlator

- **Zwanzig-Mori equation of motion**

$$A_{\boldsymbol{q}}^{\lambda\mu} = \frac{\rho}{m}\int d\boldsymbol{r}\left(1-e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\right)\hat{r}^{\lambda}\hat{r}^{\mu}\,\Theta(d-r)\gamma(d-r)g(r)$$

$$\left[\frac{\partial}{\partial t} - \boldsymbol{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial \boldsymbol{q}}\right]F_{\boldsymbol{q}}(t) = \boldsymbol{q}\cdot\boldsymbol{H}_{\boldsymbol{q}}(t)$$

dissipative force

anisotropy due to shear

$$\left[\frac{\partial}{\partial t} - \boldsymbol{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial \boldsymbol{q}}\right]H_{\boldsymbol{q}}^{\lambda}(t) = -\left(q_{\lambda}\frac{v^2}{S_q} + B_{\boldsymbol{q}}^{\lambda}\right)F_{\boldsymbol{q}}(t) - A_{\boldsymbol{q}}^{\lambda\mu}H_{\boldsymbol{q}}^{\mu}(t) - \left[\boldsymbol{\kappa}\cdot\boldsymbol{H}_{\boldsymbol{q}}(t)\right]_{\lambda}$$

$$-\int_0^t ds\, M_{\boldsymbol{q}}^{\lambda\mu}(s)H_{\boldsymbol{q}(s)}^{\mu}(t-s) - \int_0^t ds\, L_{\boldsymbol{q}}^{\lambda}(s)F_{\boldsymbol{q}(s)}(t-s)$$

non-Hermitian nature of i*L*

- **MCT expression for the memory kernel**

$$M_{\boldsymbol{q}}^{\lambda\mu}(t) = \frac{\rho}{2(2\pi)^3 v_T^2}\int d\boldsymbol{k}\left[V_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{(\mathrm{el})\lambda} - V_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{(\mathrm{vis})\lambda}\right]V_{\boldsymbol{q}(t),\boldsymbol{k}(t),\boldsymbol{p}(t)}^{(\mathrm{el})\mu}F_{\boldsymbol{k}}(t)F_{\boldsymbol{p}}(t)$$

$$+\frac{1}{(2\pi)^3 v_T^2}\int d\boldsymbol{k}\, D_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{\lambda\nu}V_{\boldsymbol{q}(t),\boldsymbol{k}(t),\boldsymbol{p}(t)}^{(\mathrm{el})\mu}F_{\boldsymbol{k}}(t)H_{\boldsymbol{p}}^{\nu}(t) + \cdots$$

$$V_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{(\mathrm{el})\lambda} = v_T^2\left(k_{\lambda}c_k + p_{\lambda}c_p\right),\quad V_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{(\mathrm{vis})\lambda} = \left(C_{\boldsymbol{k}}^{\lambda} + C_{\boldsymbol{p}}^{\lambda}\right)/\rho,\quad D_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{\lambda\mu} = A_{\boldsymbol{p}}^{\lambda} - A_{\boldsymbol{k}}^{\lambda}$$

Implications of the theory

$$M_{\boldsymbol{q}}^{\lambda\mu}(t)=\frac{\rho}{2(2\pi)^3 v_T^2}\int d\boldsymbol{k}\left[\underline{V_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{(\mathrm{el})\lambda}}-\underline{V_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{(\mathrm{vis})\lambda}}\right]\underline{V_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{(\mathrm{el})\mu}}\,F_{\boldsymbol{k}}(t)F_{\boldsymbol{p}}(t)+\cdots$$

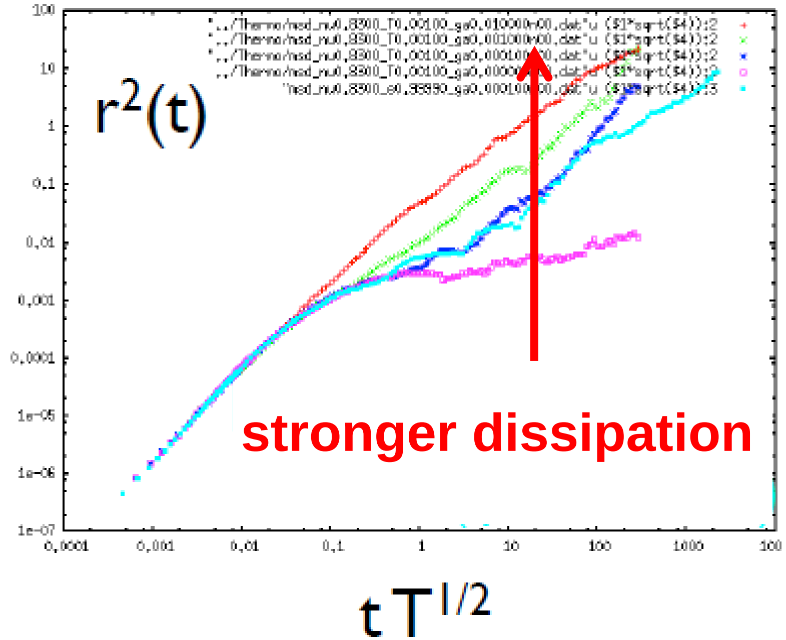
elastic force (cage effect) — dissipative force

- Vanishing of the plateau

  due to the dissipative force

- Singular behavior near

  the jamming transition point



$$g(r)=A\delta(r-d)+\cdots \;\rightarrow\; V_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{p}}^{(\mathrm{el})\lambda}=O(1/k)\;\rightarrow\;\lim_{t\to\infty}F_{\boldsymbol{q}}(t)/S_q=1\quad\text{for all } q$$

Summary

- **Nonequilibrium mode-coupling theory is developed for driven, dense granular systems.**
- **The theory is of the same quality as that for the glass transition.**
- **It is hoped that the theory is useful for a unified understanding of the glass transition and the jamming transition.**