Jacobian analysis for frictional amorphous solids under quasi-static shear

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Introduction Amorphous solids

Amorphous materials

Forms

Sands

Bubbles

Solid-like ←

Frictionless amorphous solids

Frictional amorphous solids

[2]

Previous researches for frictionless solids

Definition of Hessian $H_{ij}^{\alpha\beta}$

$$H_{ij}^{\alpha\beta} = \frac{\partial^2 U}{\partial r_i^\alpha \partial r_j^\beta} = -\frac{\partial F_i^\alpha}{\partial r_j^\beta},$$

U : Potential energy,

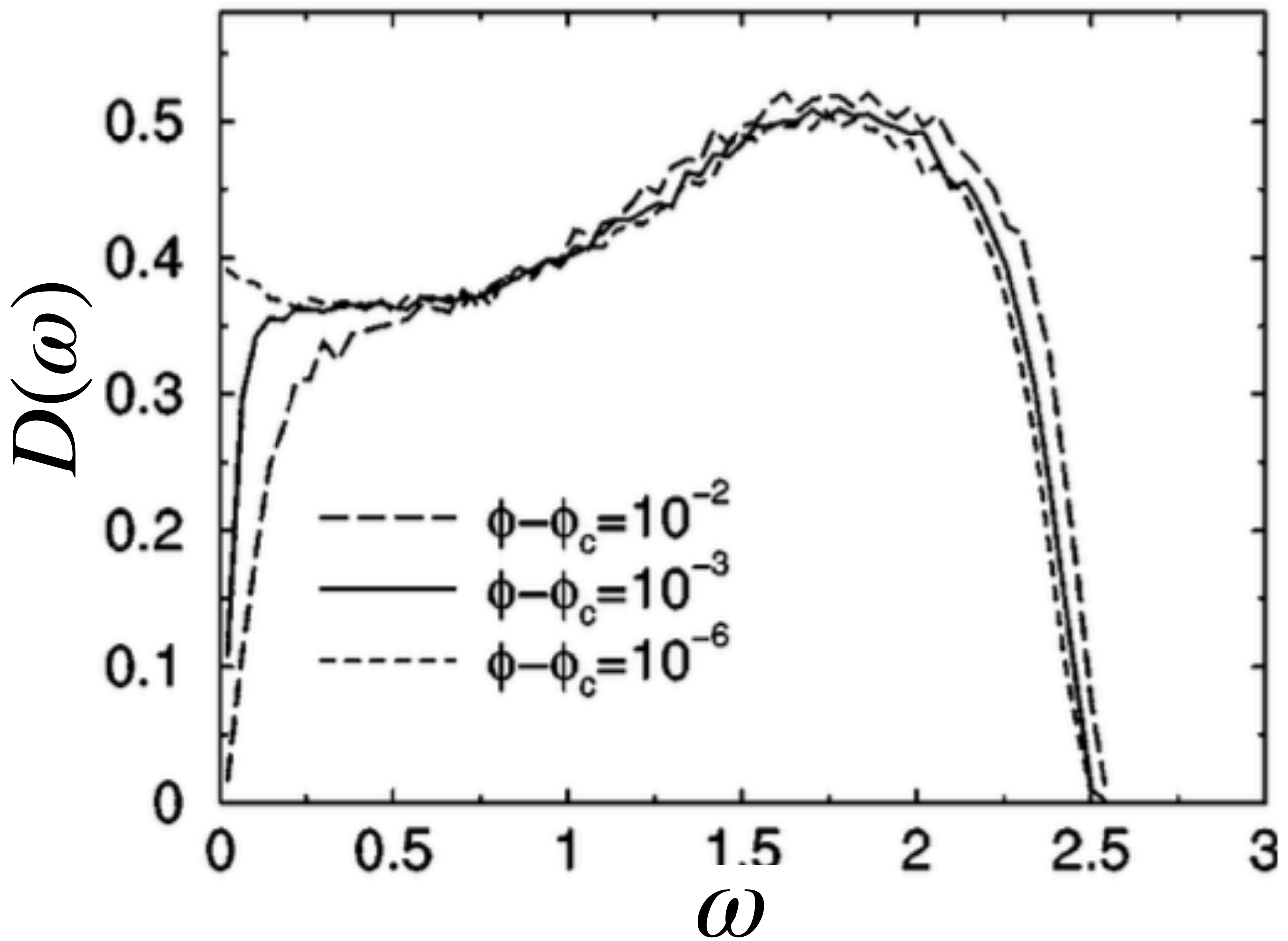
F_i^α : α component of force acting on i-th particle,

r_i^α : α component of i-th particle coordinate.

We obtain DOS from eigenvalues of H.

*Note that zero eigenmodes are related floppy mode or transnational mode.

$D(\omega)$: Density of state (DOS)



C. S. O'Hern et al., Phys. Rev. E **68**, *011306 (2003).*

Previous researches for frictional solids

Definition of Jacobian $J_{ij}^{\alpha\beta}$

$$J_{ij}^{\alpha\beta} = -\frac{\partial \tilde{F}_i^\alpha}{\partial q_j^\beta},$$

$\tilde{F}_i^\alpha$: α component of generalized force acting on i-th particle $\vec{F}_i = (F_i^x, F_i^y, T_i)^T$,

q_i^α : α component of generalized i-th particle coordinate $q_i := (r_i^x, r_i^y, \theta_i)$,

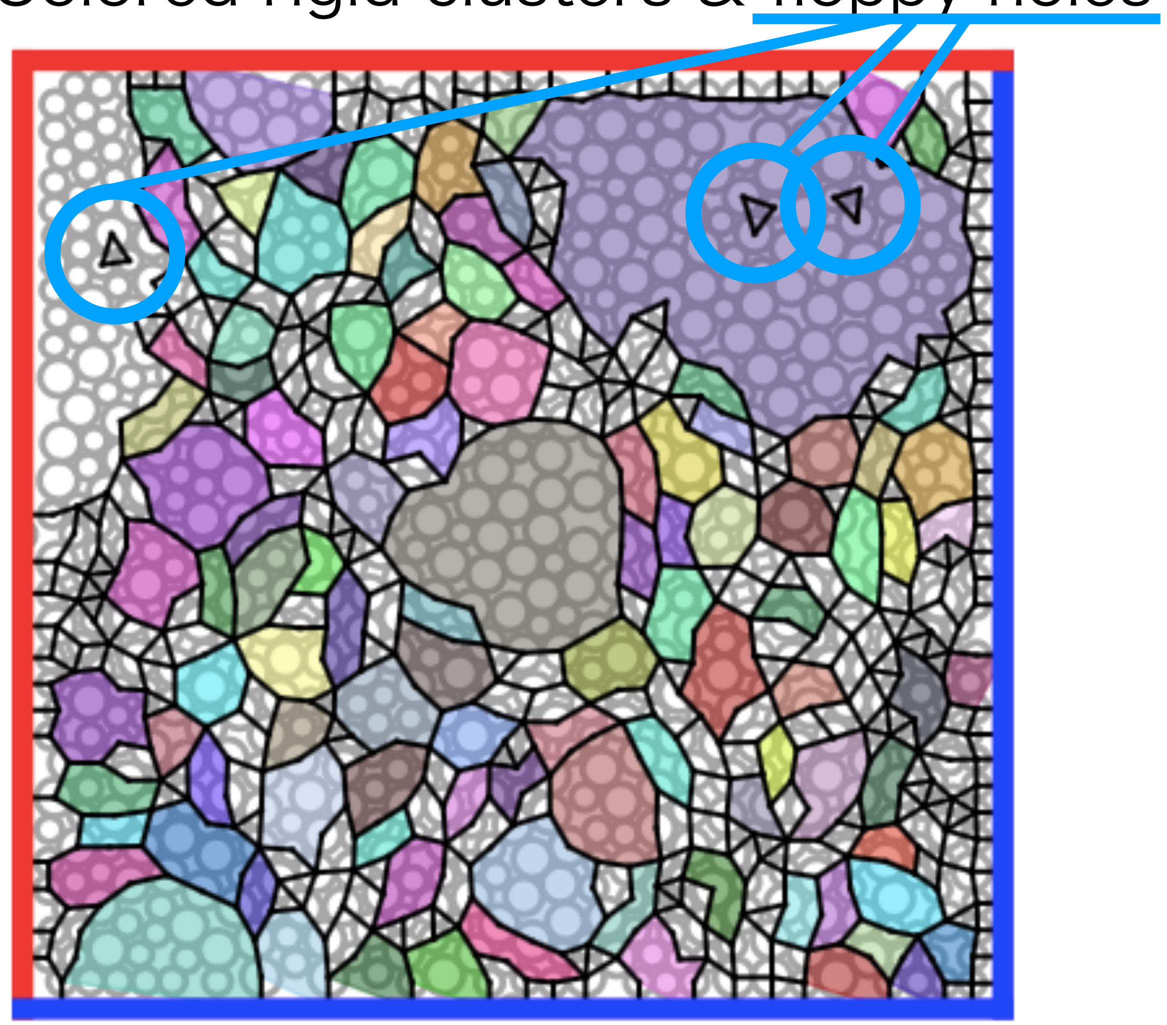
T_i : Torque of i th particle,

θ_i : Rotational degree of i th particle.

They identify the floppy hole* from Jacobian's zero eigenvalue

*Floppy hole: NOT contribute rigidity

Colored rigid clusters & floppy holes



K. Liu et al., Phys. Rev. Lett. ***126***, *088002 (2021).*

Previous researches for frictional solids

Definition of Jacobian $J_{ij}^{\alpha\beta}$

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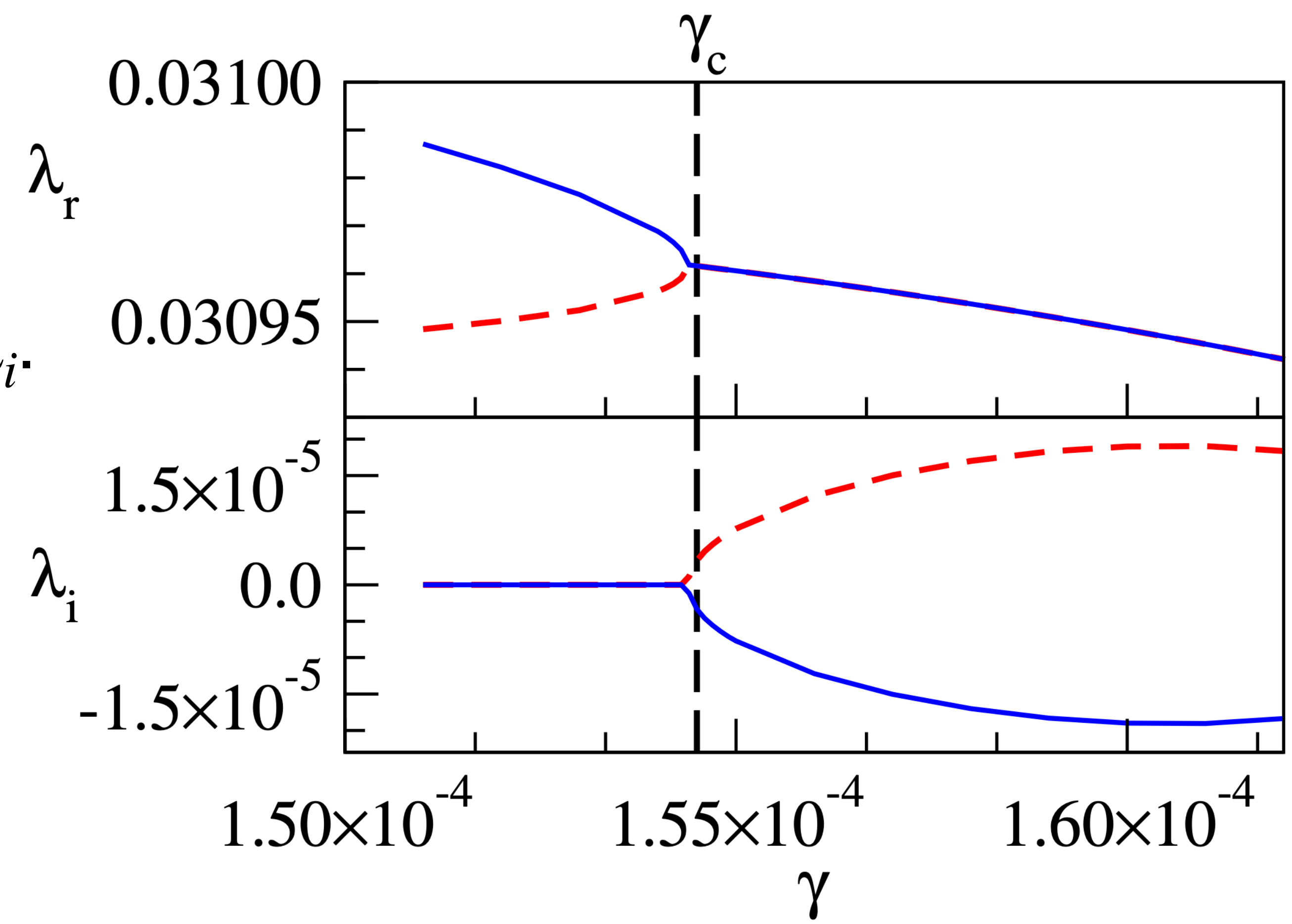
AQS, Frictional particles



Jacobian is an asymmetric matrix.

->It has complex eigenvalue $\lambda = \lambda_r + i\lambda_i$.

->Imaginary parts contribute to oscillatory instability*.

*J. Chattoraj et al., Phys. Rev. Lett. **123**, 098003 (2019).

Introduction

	Frictionless materials	Frictional materials
Tool for stability analysis (dynamical matrix)	Hessian: $H_{ij}^{\alpha\beta} = \dfrac{\partial^2 U}{\partial r_i^\alpha \partial r_j^\beta}$	Jacobian: $J_{ij}^{\alpha\beta} = -\dfrac{\partial \tilde{F}_i^\alpha}{\partial q_j^\beta}$
To determine floppy mode	○	○
Oscillatory instability	×	○
Shear rigidity G formula with dynamical matrix	○	?

G can be obtained from $H_{ij}^{\alpha\beta}$, Hessian's eigenvalues & Hessian's eigenvectors*.

*A. Lemaître & C. Maloney, J. Stat. Phys. **123**, 2 (2006).

Question?

Can we predict G by Jacobian?

Purpose

To obtain the prediction of G in the limit $\gamma \to 0$

Our numerical protocol

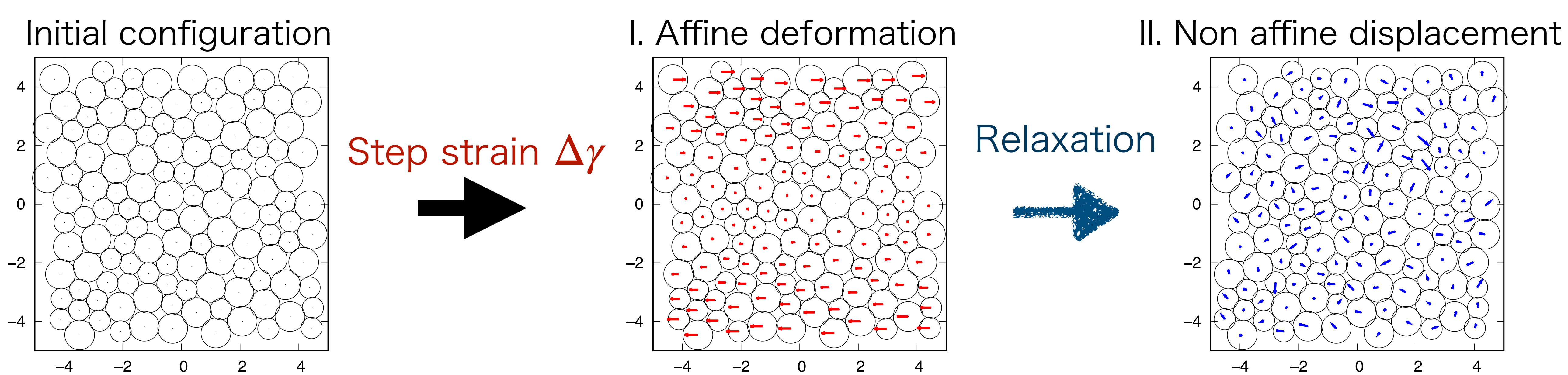
Preparation of initial configuration

1. Preparing the frictionless configuration at density ϕ with energy minimization by FIRE*
2. Incorporating the tangential forces
3. Relaxation by dissipation until $|F_i^\alpha| < F_{\rm Th}$

*E. Bitzek et al., Phys. Rev. Lett., 97, 170201 (2006).

Athermal quasistatic shear protocol

I. Applying affine shear deformation $\Delta\gamma$ to the system with Lees-Edwards periodic boundary condition
II. Relaxation by dissipation until $|F_i^\alpha| < F_{\rm Th}$



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Numerical methods

Equation of motion

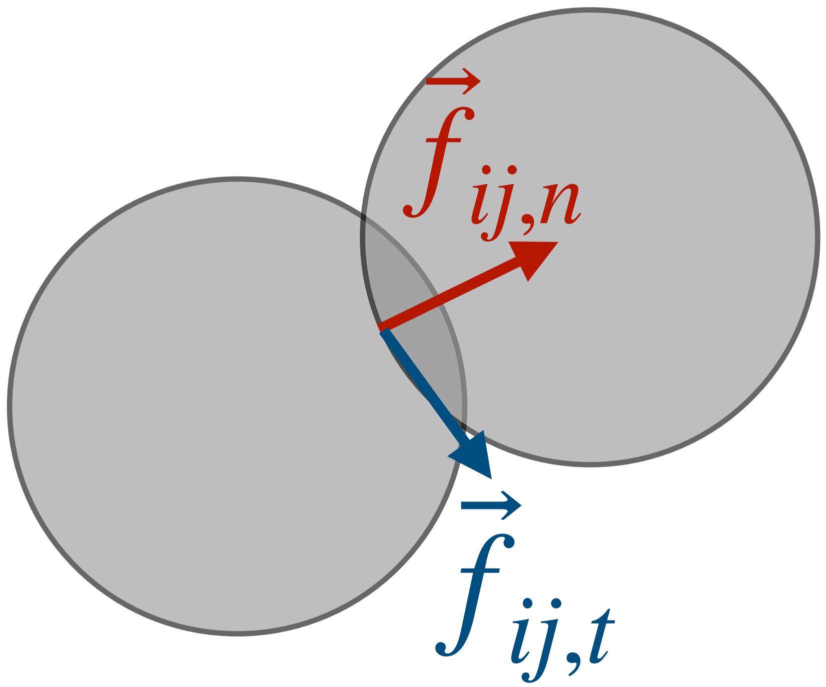
$$m_i \frac{d^2 \vec{x}_i}{dt^2} = \vec{F}_i$$

$$I_i \frac{d^2 \theta_i}{dt^2} = T_i$$

$\vec{F}_i$: Force of i particle

T_i : Torque of i particle

θ_i : rotational degree of i particle



$$\vec{F}_i = \sum_j \left(\vec{f}_{N,ij} + \vec{f}_{T,ij} \right) \Theta(a_i + a_j - r_{ij}),$$

$$\vec{f}_{N,ij} = k_N \xi_{N,ij}^{3/2} \vec{n}_{ij} - \eta_N \vec{v}_{N,ij},$$

$$\vec{f}_{T,ij} = -k_T \xi_{N,ij}^{1/2} \vec{\xi}_{T,ij} - \eta_T \vec{v}_{T,ij}$$

*nonslip model

Our simulated system

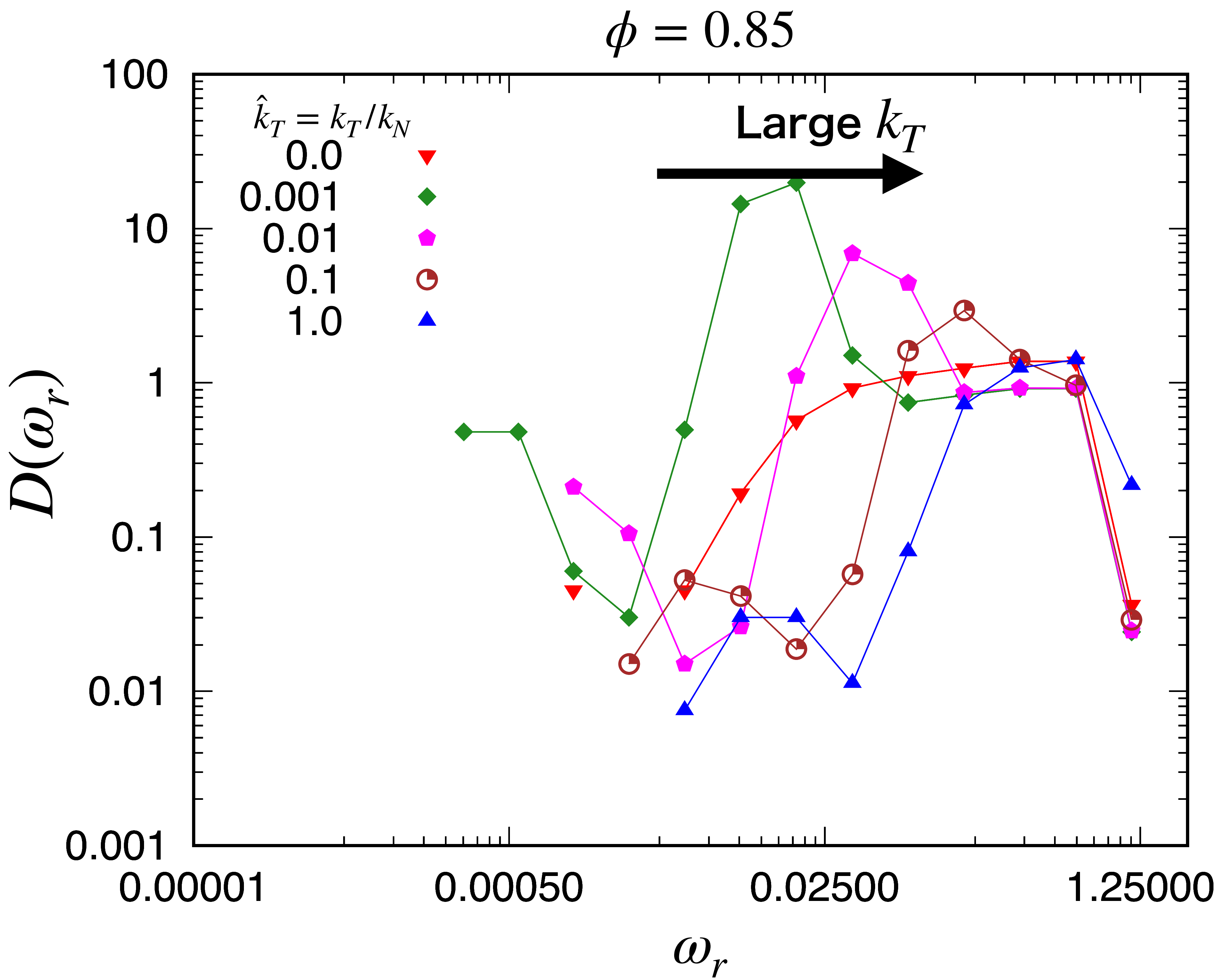
2 dimensional binary disks ($N = 128$),

Step strain: $\Delta\gamma = 10^{-10}$,

Threshold value of mechanical equilibrium condition: $F_{\mathrm{Th}}/(k_N d_0) = 10^{-14}$,

Density $0.80 \leq \phi \leq 0.90$, Tangential ratio $0.0 \leq k_T/k_N \leq 10.0$.

Density of State



As k_T increases, low frequency part moves high frequency region*

*C. F. Schreck et al., Phys. Rev. E, **85**, 061305 (2012).

Expression of G by J

We obtain shear modulus G by J:

$$G(0) = \frac{1}{2L^2}\sum_{i,j(i\neq j)}\left[\underbrace{y_{ij}^2(0)J_{N,ij}^{xx}(0)}_{\text{Affine shear modulus}} + \underbrace{\sum_{\kappa=x,y} y_{ij}(0)J_{ij}^{\kappa x}(0)\frac{du_{ij}^{\kappa}(0)}{d\gamma} + y_{ij}(0)J_{ij}^{\ell x}(0)\left(\frac{du_i^{\ell}(0)}{d\gamma}+\frac{du_j^{\ell}(0)}{d\gamma}\right)}_{\text{Non affine shear modulus}}\right] \cdots \quad (1)$$

Affine shear modulus Non affine shear modulus

with $J_{ij}^{\alpha\beta} = -\frac{\partial f_{ij}^{\beta}}{\partial q_i^{\alpha}}$, $J_{N,ij}^{\alpha\beta} = -\frac{\partial f_{N,ij}^{\beta}}{\partial q_i^{\alpha}}$, $u_{ij}^{\alpha} := u_i^{\alpha} - u_j^{\alpha}$, $u_i^{\alpha}(0) = q_i^{\alpha}(\Delta\gamma) - q_i^{\alpha}(0) - \Delta\gamma\delta_{\alpha x}$: non affine displacement.

Calculation methods of G

Cauchy's expression

$$G = \frac{d\sigma_{xy}}{d\gamma}, \quad \sigma_{xy} = -\frac{1}{L^2}\sum_i\sum_{j>i} f_{ij}^x y_{ij},$$

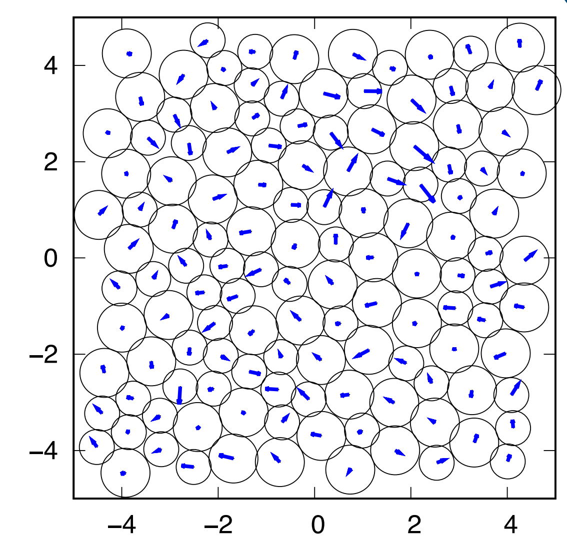
f_{ij}^x : x component of forces from j to i particle,

y_{ij} : y component of displacements from j to i particle.

It needs $f_{ij}^x(0)$, $y_{ij}(0)$, $f_{ij}^x(\Delta\gamma)$, $y_{ij}(\Delta\gamma)$.

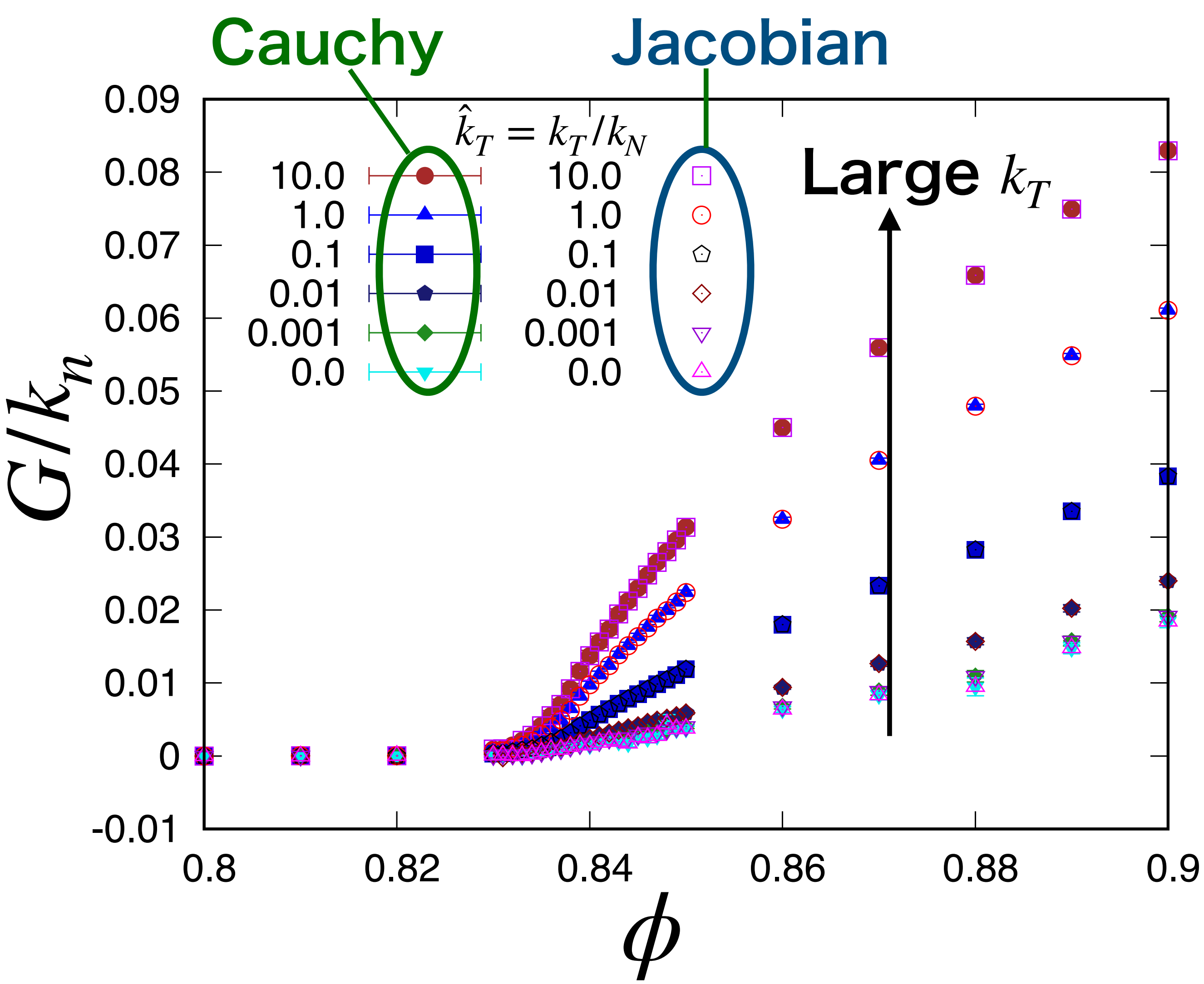
Jacobian's expression

Eq. (1) needs $J_{ij}^{\alpha\beta}(0)$, $y_{ij}(0)$, $u_i^{\alpha}(0)$

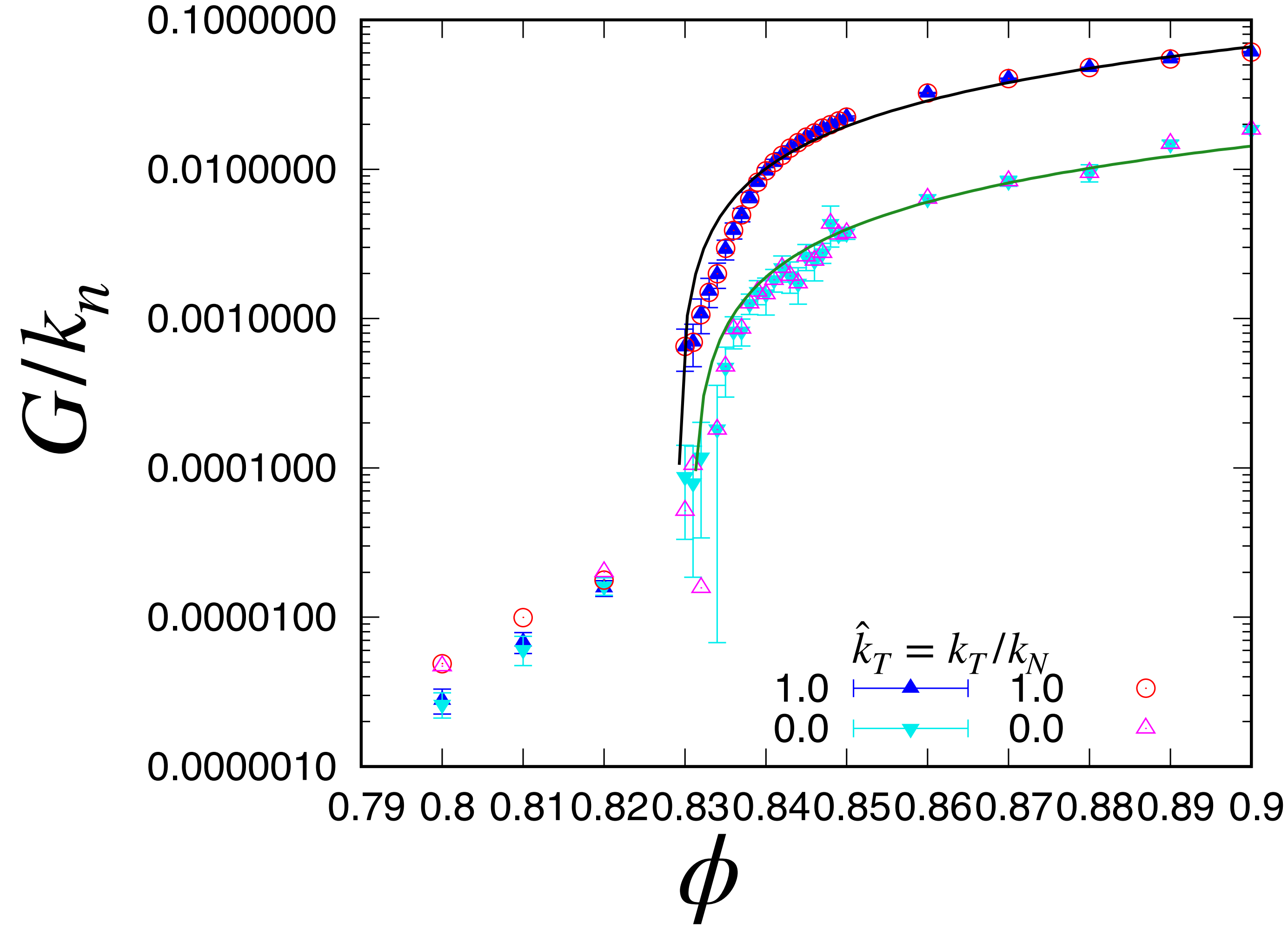


Non affine displacement: $u_i^{\alpha}(0)$

ϕ-dependence



Fitted by $G(\phi) = G_0 + c(\phi - \phi_J)^\alpha$ with $\alpha = 1$



Jacobian's expression reproduces ϕ dependence.

$G(\phi)$ has a linear dependence of $\phi - \phi_J$*.

*C. S. O'Hern et al., Phys. Rev. Lett., **88**, 7 (2002), E. Somfai et al., Phys. Rev. E, **75**, 020301(R) (2007).

Eigenfunction expansion for $k_T = 0$

We obtain shear modulus G by H:

$$G(0) = \frac{1}{2L^2} \sum_{i,j(i\neq j)} \left[y_{ij}^2(0) H_{ij}^{xx}(0) + \sum_{\kappa=x,y} y_{ij}(0) H_{ij}^{\kappa x}(0) \frac{du_{ij}^{\kappa}(0)}{d\gamma} \right] \quad \cdots \quad (2)$$

with Hessian: $H_{ij}^{\alpha\beta} = -\frac{\partial f_{N,ij}^{\beta}}{\partial q_i^{\alpha}} = \frac{\partial^2 U_N}{\partial q_i^{\alpha} \partial q_j^{\beta}} \quad (\alpha, \beta = x, y).$

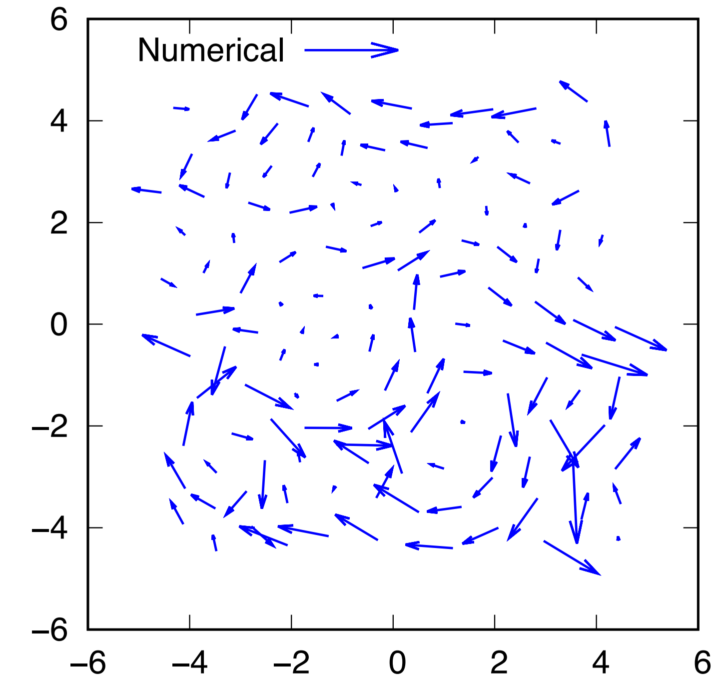
Eigenfunction expansion of $|du/d\gamma\rangle$ by H*:

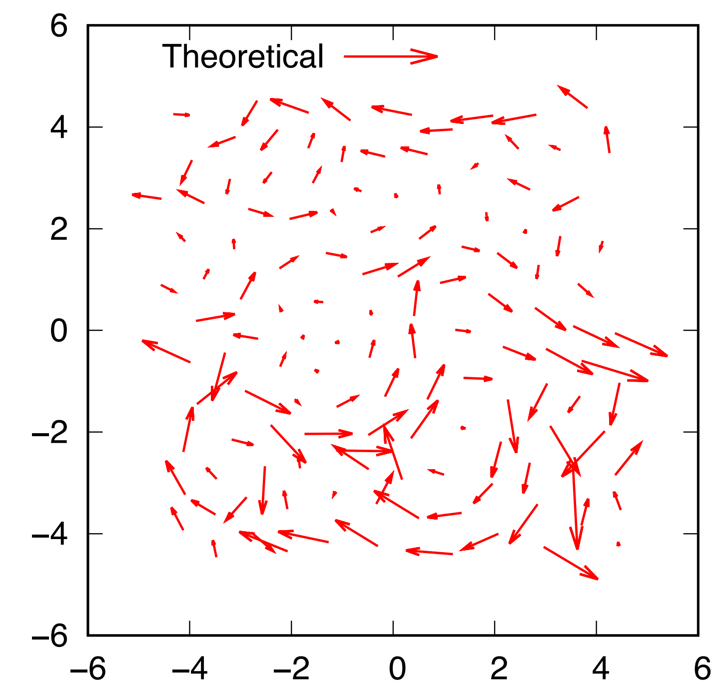
$$\left| \frac{du}{d\gamma} \right\rangle = \sum_n \frac{\langle n | \Xi \rangle}{\lambda_n} | n \rangle \quad \cdots \quad (3)$$

*A. Lemaître & C. Maloney, J. Stat. Phys. **123**, 2 (2006).

where $\lambda_n, |n\rangle$: n-th eigenvalue & vector, $|\Xi\rangle = \begin{bmatrix} \sum_{j\neq 1} H_{1j}^{xx} \\ \sum_{j\neq 1} H_{1j}^{xy} \\ \vdots \\ \sum_{j\neq N} H_{Nj}^{xx} \\ \sum_{j\neq N} H_{Nj}^{xy} \end{bmatrix}$

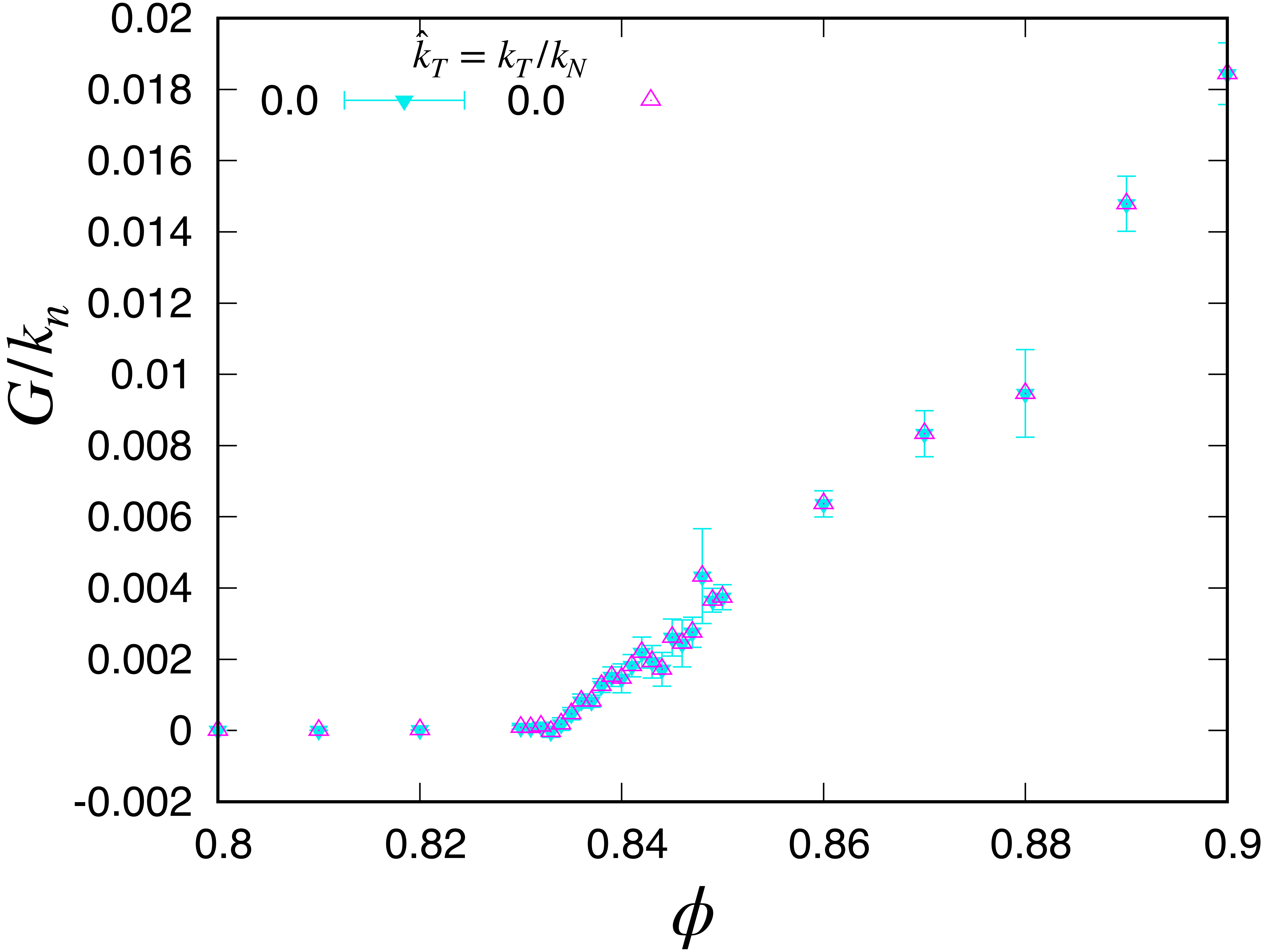
Non affine displacement $k_t = 0$





We can predict G from initial information by using Eqs. (2) & (3).

ϕ-dependence for $k_T = 0$ (frictionless)



We can predicts $G(\phi)$ from initial information.

Eigenfunction expansion for small k_T

We ignore the tangential part of J for small k_T :

$$J = J_N + J_T \simeq J_N \quad (k_T \ll k_N) = H,$$

where $J_N := -\dfrac{\partial f_N}{\partial q}, J_T := -\dfrac{\partial f_T}{\partial q}$.

We use Hessian's formula

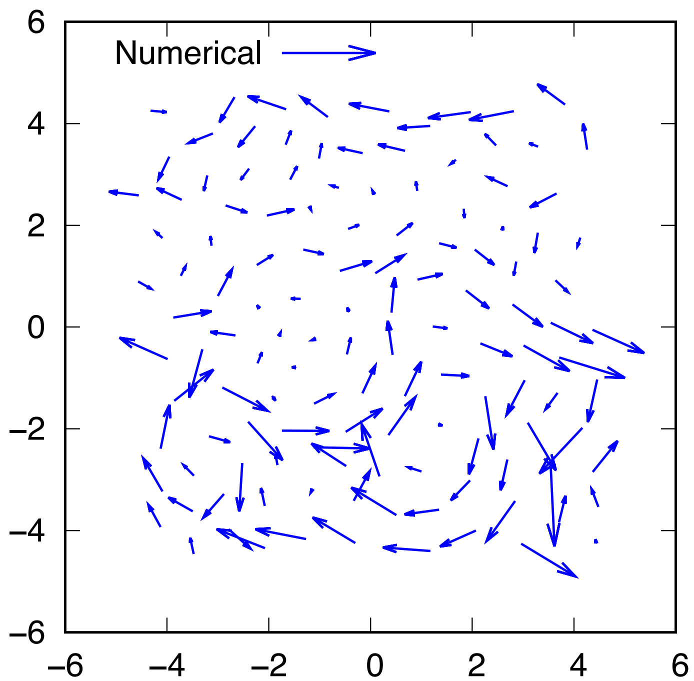
$$G(0) = \frac{1}{2L^2}\sum_{i,j(i\neq j)}\left[y_{ij}^2(0)H_{ij}^{xx}(0) + \sum_{\kappa=x,y} y_{ij}(0)H_{ij}^{\kappa x}(0)\frac{du_{ij}^{\kappa}(0)}{d\gamma}\right] \quad \cdots \quad (2)$$

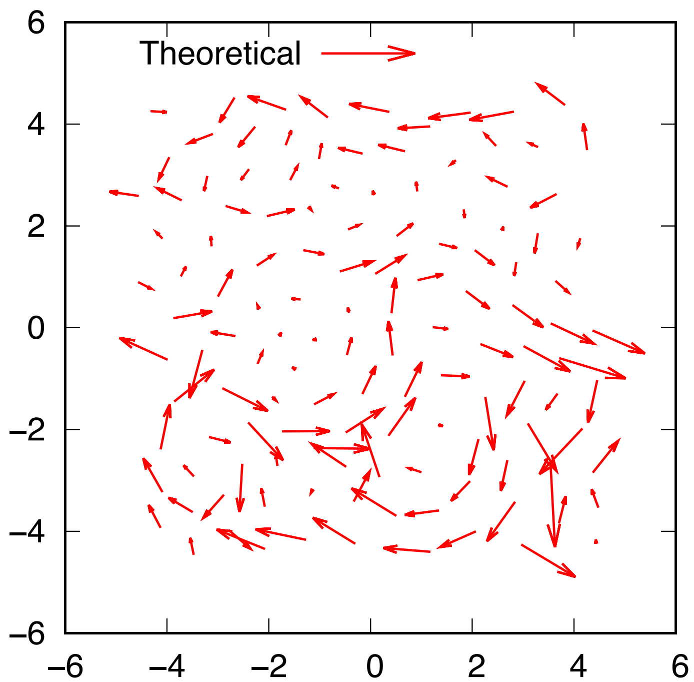
$$\left|\frac{du}{d\gamma}\right\rangle = \sum_n \frac{\langle n|\Xi\rangle}{\lambda_n}|n\rangle \quad \cdots \quad (3)$$

Can we predict G from initial information

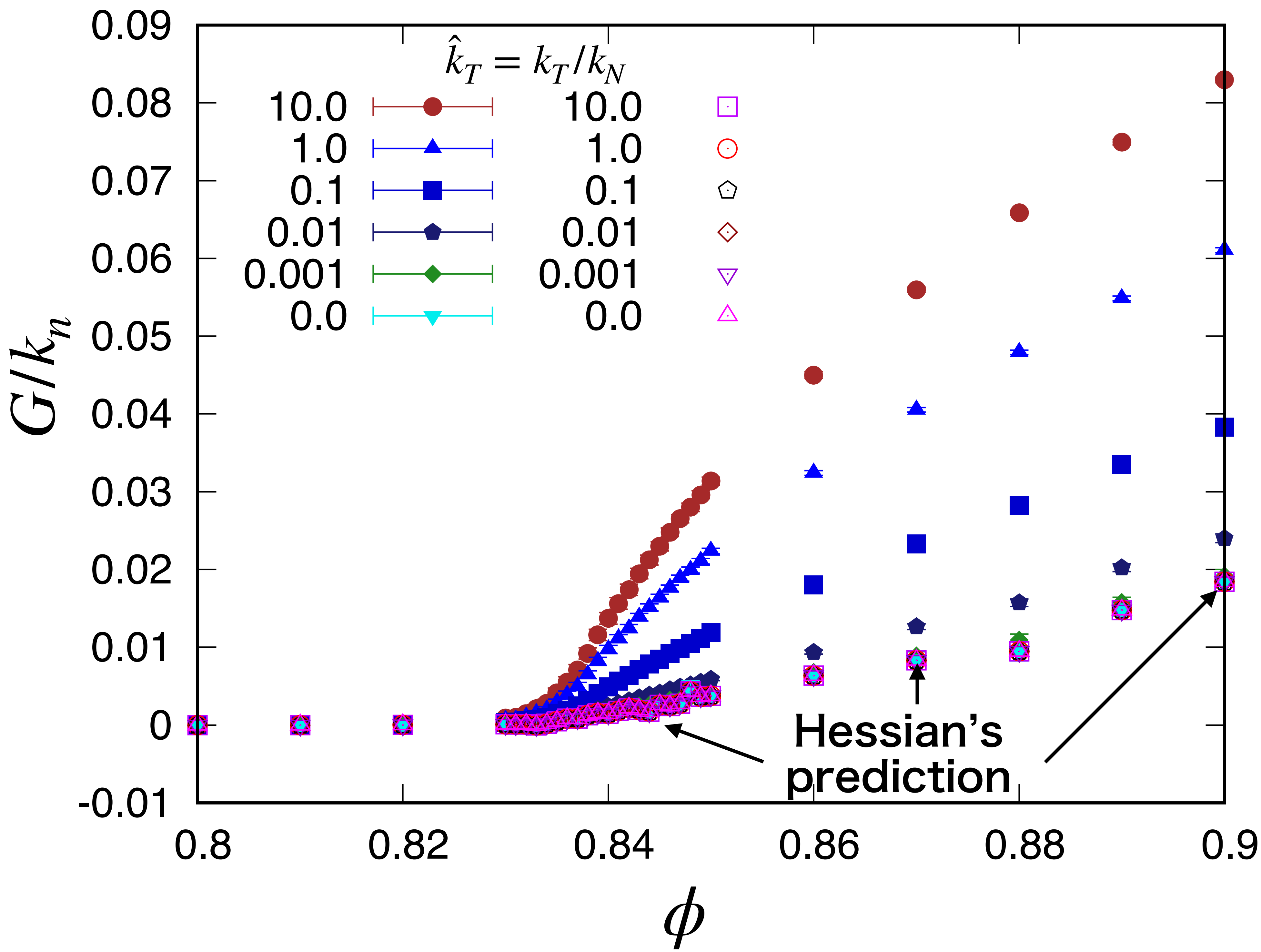
by using Eqs. (2) & (3)?

Non affine displacement $k_t = 0.001$





ϕ-dependence for $0 \leq k_t/k_n \leq 1.0$



Hessian's approach predicts G at $\hat{k}_T = 0.001$.

<u>We have to consider the tangential part for $k_T \geq 0.01$.</u>

Summary

Frictional amorphous solids under quasi-static shear are analyzed using the Jacobian.

Density of state $D(\omega_r)$ in the limit $\gamma \to 0$

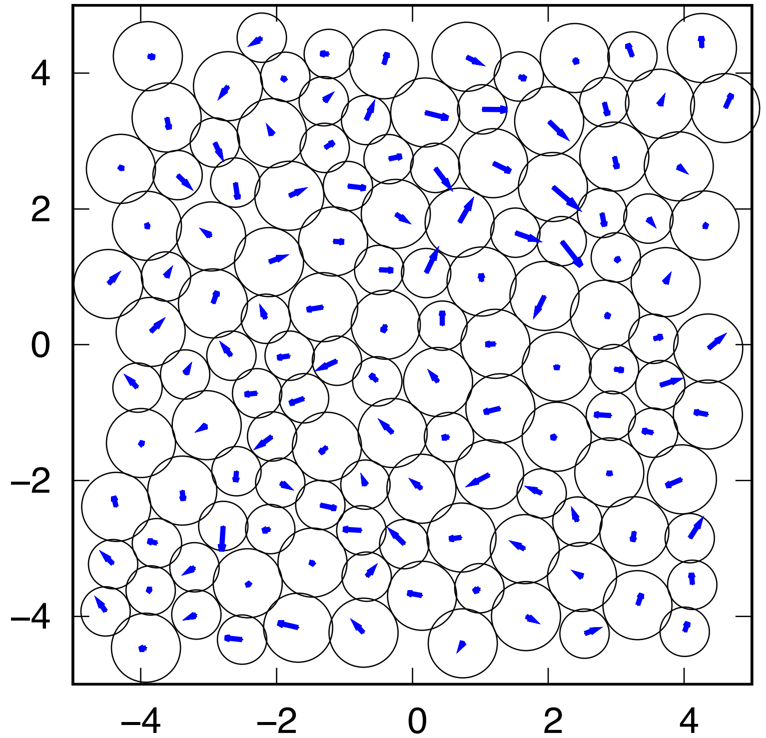
- **As k_T increases, low frequency part moves high frequency region**

Shear modulus G in the limit $\gamma \to 0$

- **Jacobain's representation can reproduce G.**
- **Hessian'a approach predict G for $k_T \leq 0.001$.**

Future work

- Expanding non affine displacements $u_i^\alpha(0)$ by eigenfunctions of Jacobian



Non affine displacement: $u_i^\alpha(0)$