JPS autumn meeting, 15pB19-10
ZOOM, 2022/03/15

準静的剪断下における摩擦のあるアモルファス固体の固有関数解析

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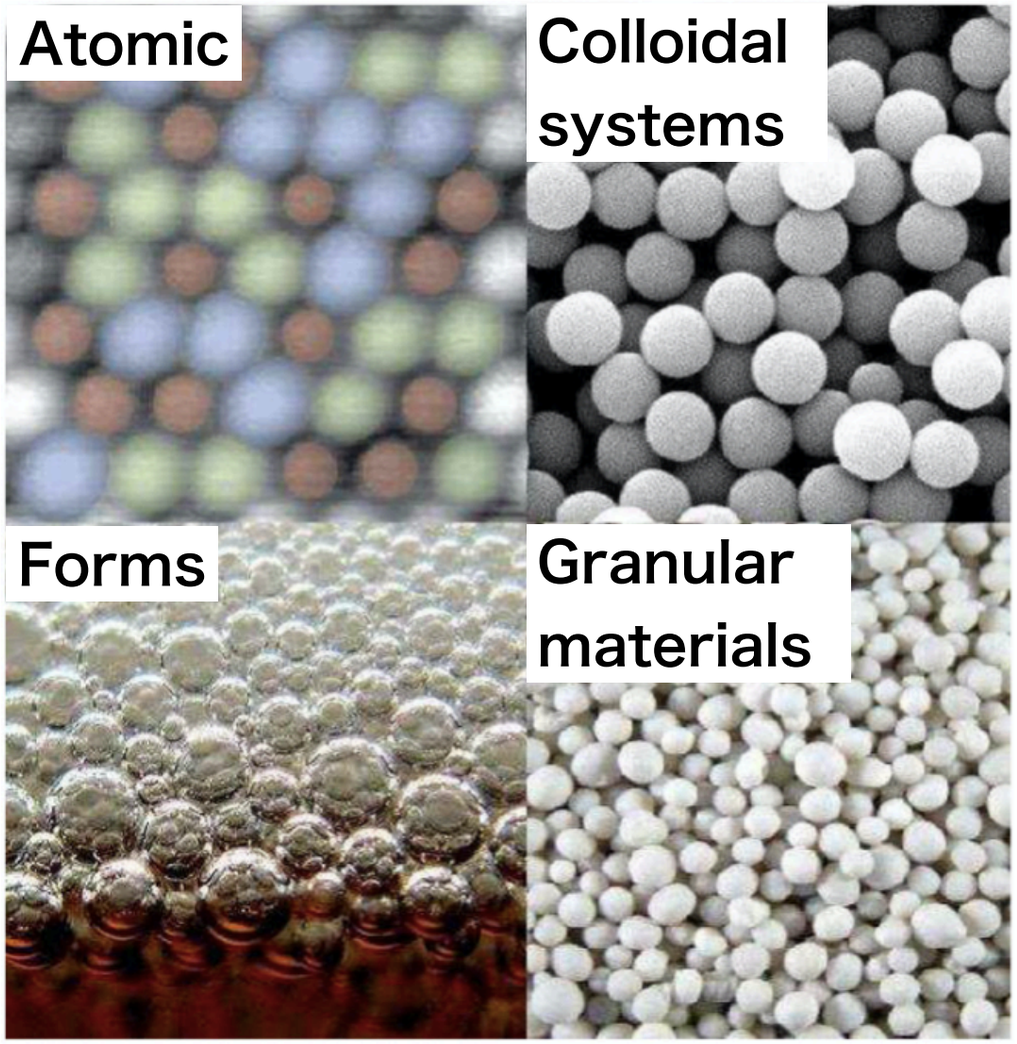
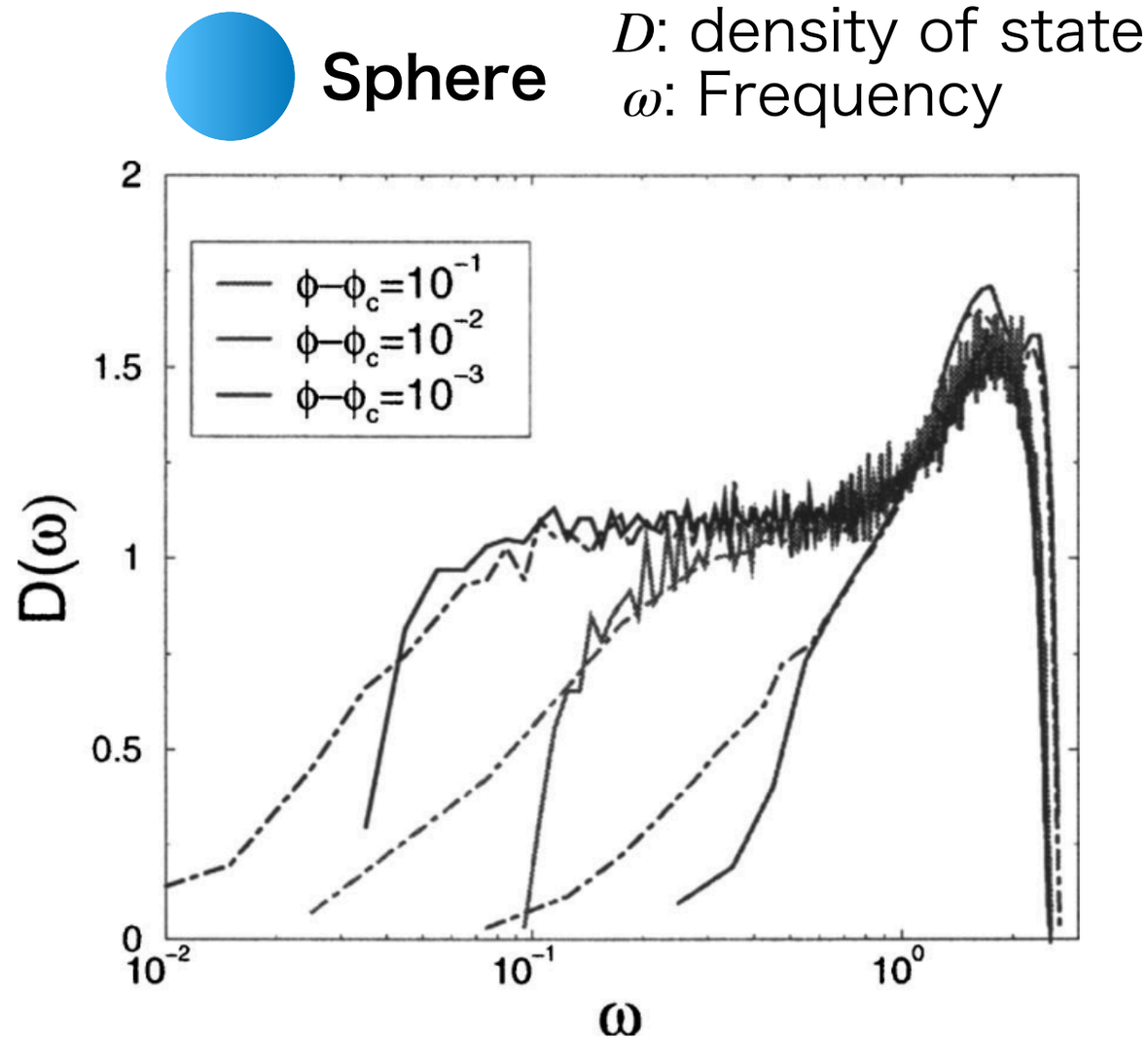
Introduction

Amorphous solids



L. Berthier and G. Biroli, Rev. Mod. Phys., ***83***, *587 (2011).*



M. Wyart, L. E. Silbert, S. R. Nagel, and T. A. Witten, Phys. Rev. E, ***72****, 051306 (2005).*

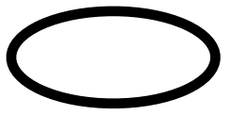
They have rigidity above jamming density.

Many researchers have investigated the density of state (DOS) for frictionless amorphous solids

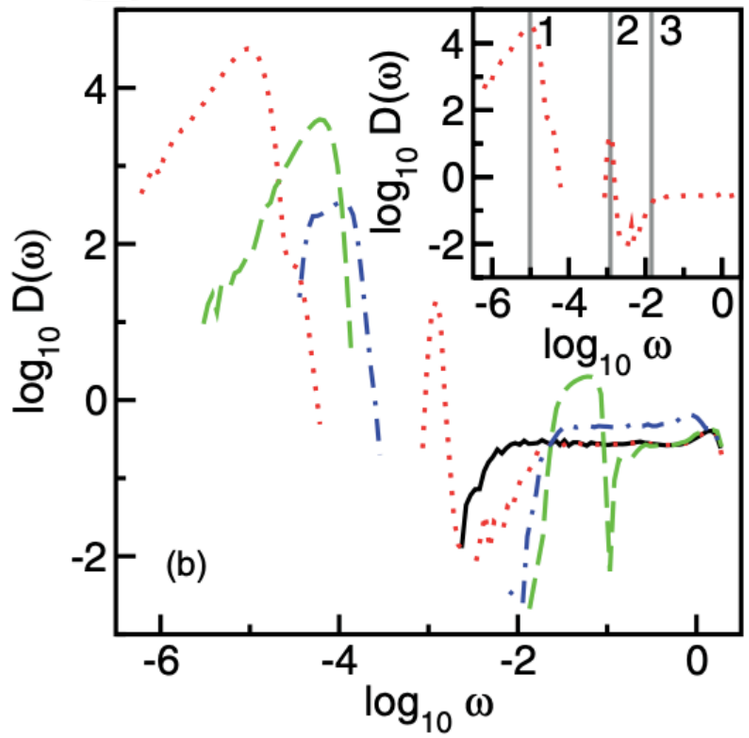
[2]

Introduction

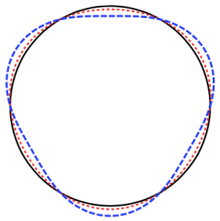
Effects of rotation?



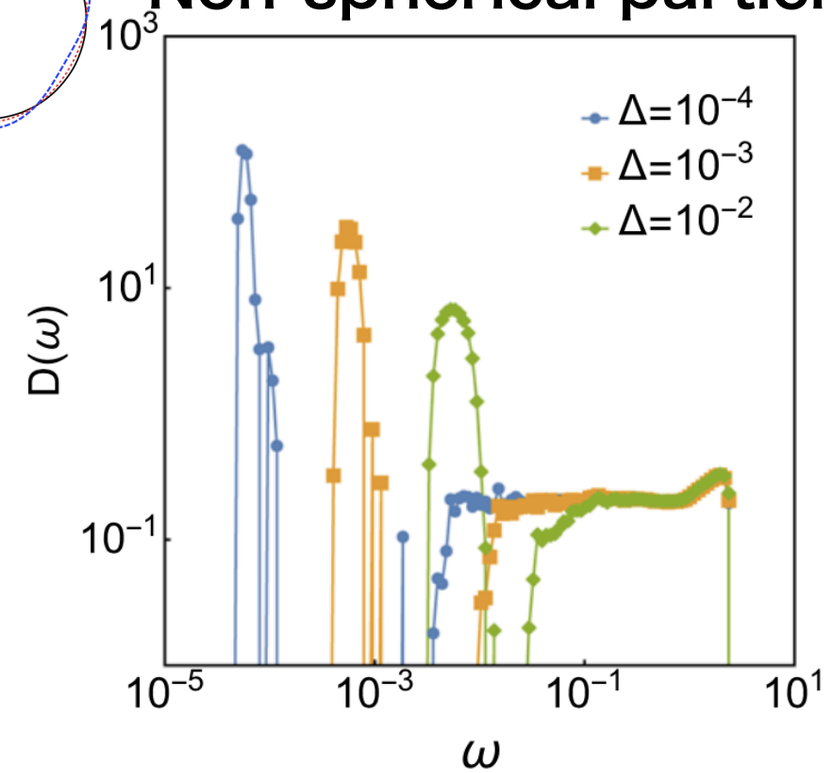
Ellipses



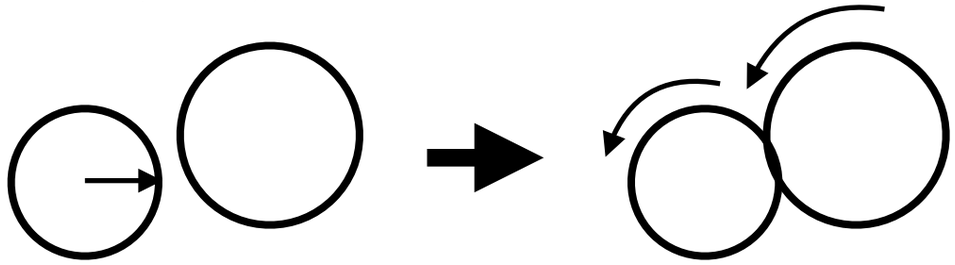
*C. F. Schreck et al., Phys. Rev. E, **85**, 061305 (2012).*



Non-spherical particles



*H. Ikeda, Eur. Phys. J. E **44**, 120 (2021).*



Question?

What about DOS for frictional amorphous materials?

Rigidity formula* exists? **C. E. Maloney & A. Lemaître, Phys. Rev. E, **74**, 016118 (2006).*

Purpose

To investigate DOS and rigidity of frictional amorphous materials

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 $-\eta \vec{v}_{ij}$ until $|F_i^\alpha| < F_{\mathrm{Th}}$

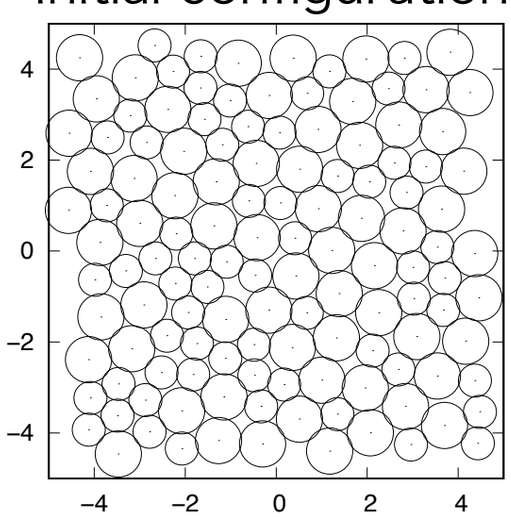
*E. Bitzek et al., Phys. Rev. Lett., 97, 170201 (2006).

Athermal quasistatic shear protocol

I. Applying affine shear deformation $\Delta\gamma$ to the system with Lees-Edwards periodic boundary condition

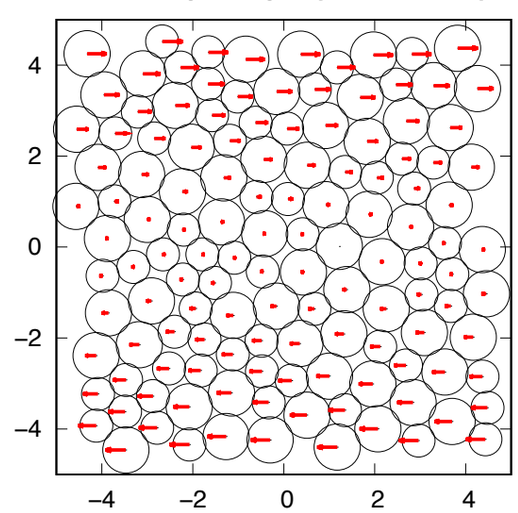
II. Relaxation by dissipation $-\eta \vec{v}_{ij}$ until $|F_i^\alpha| < F_{\mathrm{Th}}$

Initial configuration



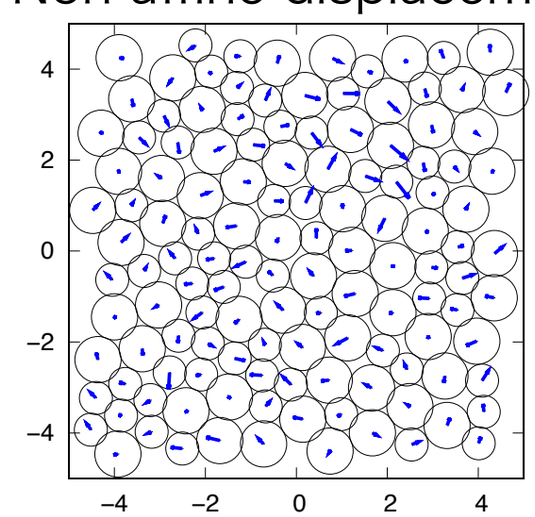
Step strain $\Delta\gamma$

I. Affine deformation



Relaxation by $-\eta \vec{v}_{ij}$

II. Non affine displacement



[4]

Numerical methods

Equation of motion

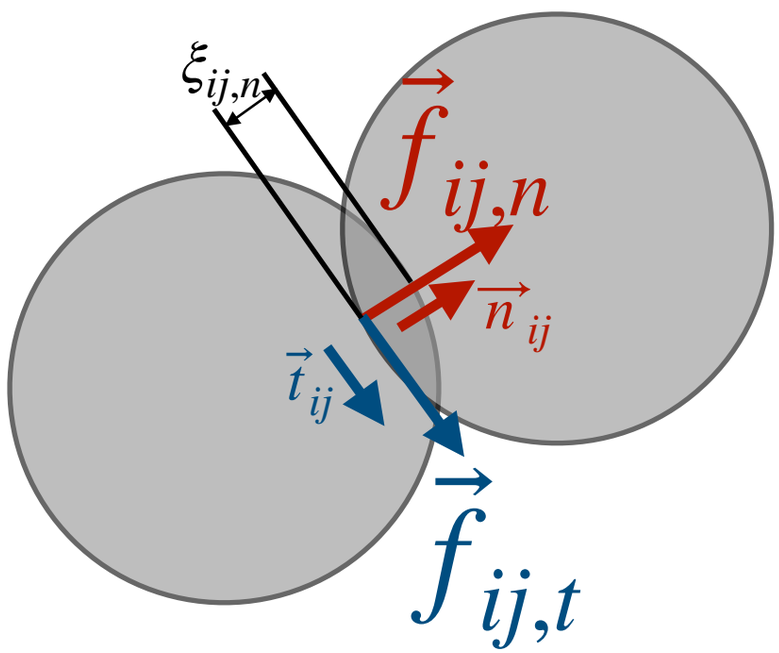
$$m_i \frac{d^2 \vec{x}_i}{dt^2} = \vec{F}_i,$$

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

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

T_i : Torque of i particle

θ_i : rotational degree of i particle



$$\vec{F}_i = \sum_j \left(\vec{f}_{ij,n} + \vec{f}_{ij,t} \right) \Theta(\xi_{ij,n}),$$

$$\vec{f}_{ij,n} = k_n \xi_{ij,n}^{3/2} \vec{n}_{ij} - \eta \vec{v}_{ij,n},$$

$$\vec{f}_{ij,t} = -k_t \xi_{ij,n}^{1/2} \xi_{ij,t} \vec{t}_{ij} - \eta \vec{v}_{ij,t}$$

*nonslip model

Our simulated system

2 dimensional binary disks ($N = 1024$),

Step strain: $\Delta\gamma = 10^{-6}$,

Threshold value of mechanical equilibrium condition: $F_{\mathrm{Th}}/(k_n d_0^{3/2}) = 10^{-14}$,

Density $0.80 \leq \phi \leq 0.90$, Tangential ratio $0.0 \leq k_t/k_n \leq 10.0$.

Density of state

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

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

$$J_{ij}^{\alpha\beta} := -\frac{\partial \tilde{F}_i^\alpha}{\partial q_j^\beta}, \xrightarrow{\text{If } \tilde{F}_i^\alpha = -\frac{\partial U}{\partial q_i^\alpha}} J_{ij}^{\alpha\beta} := -\frac{\partial \tilde{F}_i^\alpha}{\partial q_j^\beta} = \frac{\partial^2 \tilde{U}}{\partial q_i^\alpha \partial q_j^\beta} =: H_{ij}^{\alpha\beta},$$

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

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

T_i : Torque of i particle,

θ_i : Rotational degree of i particle.

Eigenvalue equation:

$$J|R_n\rangle = \lambda_n |R_n\rangle$$

$$\downarrow$$

$$\omega_n = \sqrt{\lambda_n}$$

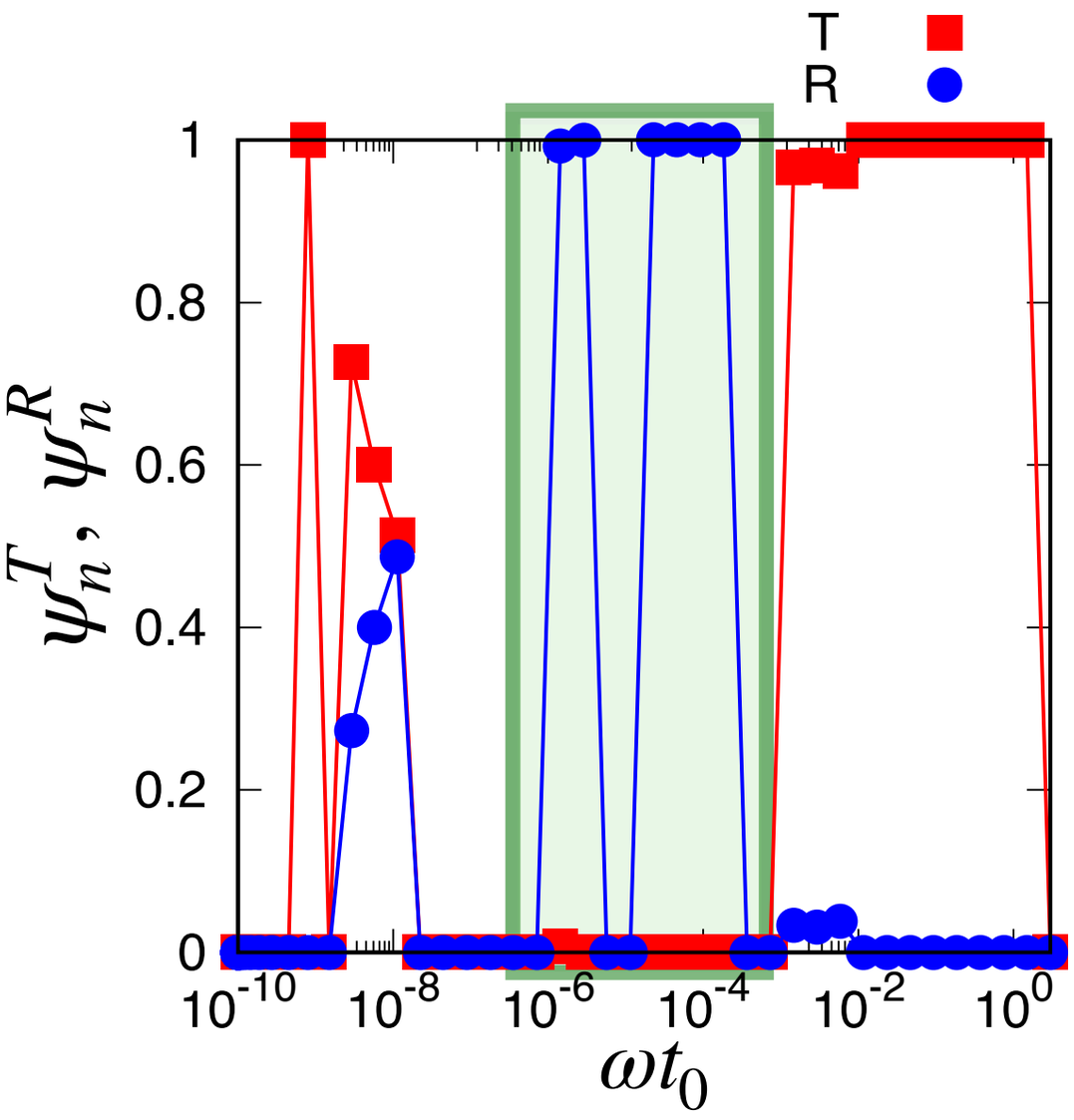
ω_n: eigen frequency

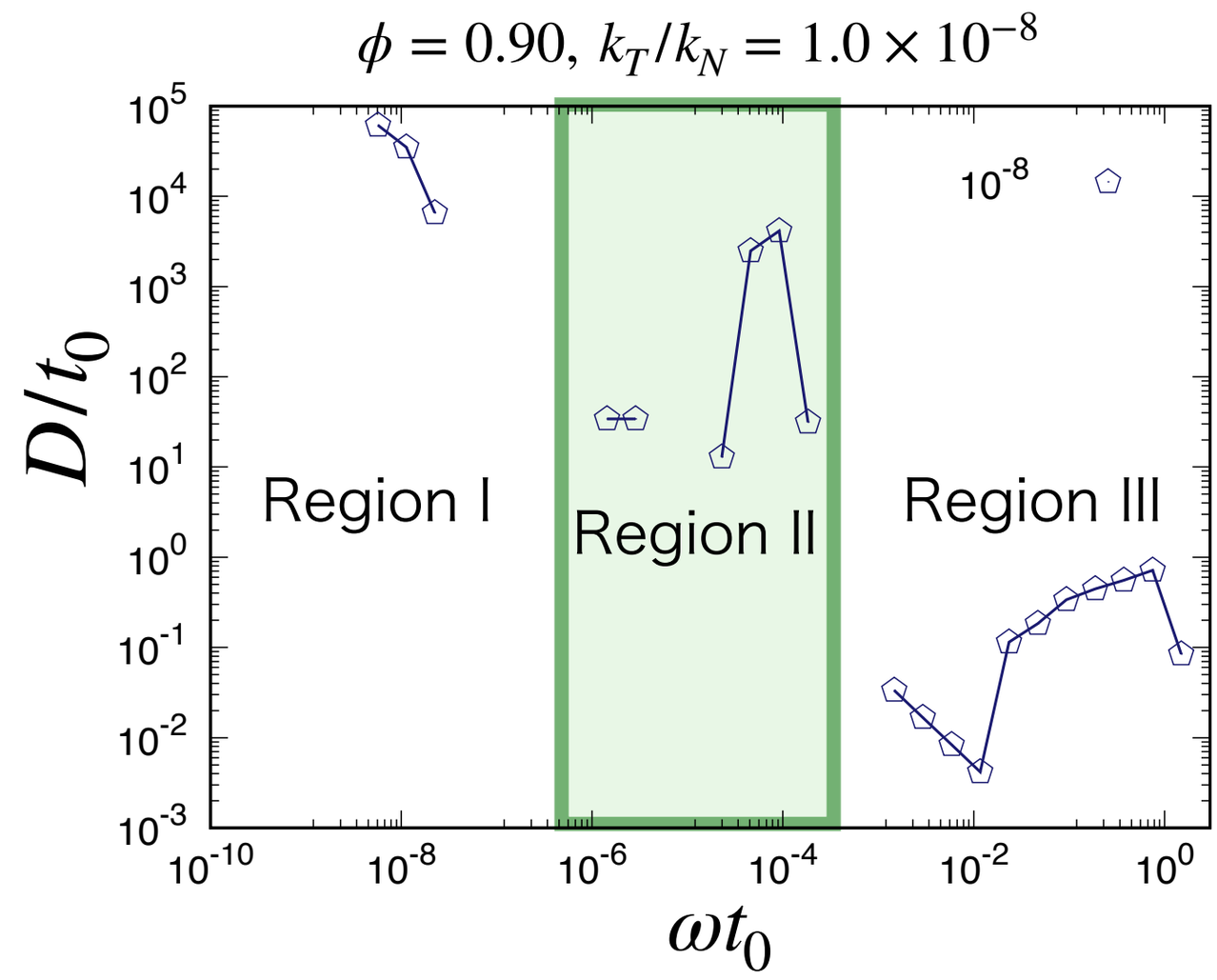
$\Rightarrow$ We obtain $D(\omega)$ from distribution of ω_n.

Density of State: Region II

$$\psi_n^T := \sum_{i=1}^{N} \left[(R_{n,i}^x)^2 + (R_{n,i}^y)^2 \right], \quad \psi_n^R := \sum_{i=1}^{N} (R_{n,i}^\ell)^2 = 1 - \psi_n^T$$

$R_{n,i}^\alpha$: $(i,\ \alpha)$ component of n-th eigenvector $(i = 1,2,\cdots,N,\ \alpha = x, y, \ell)$





Region II consists of rotational modes*.

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

[7]

Density of State: Region II

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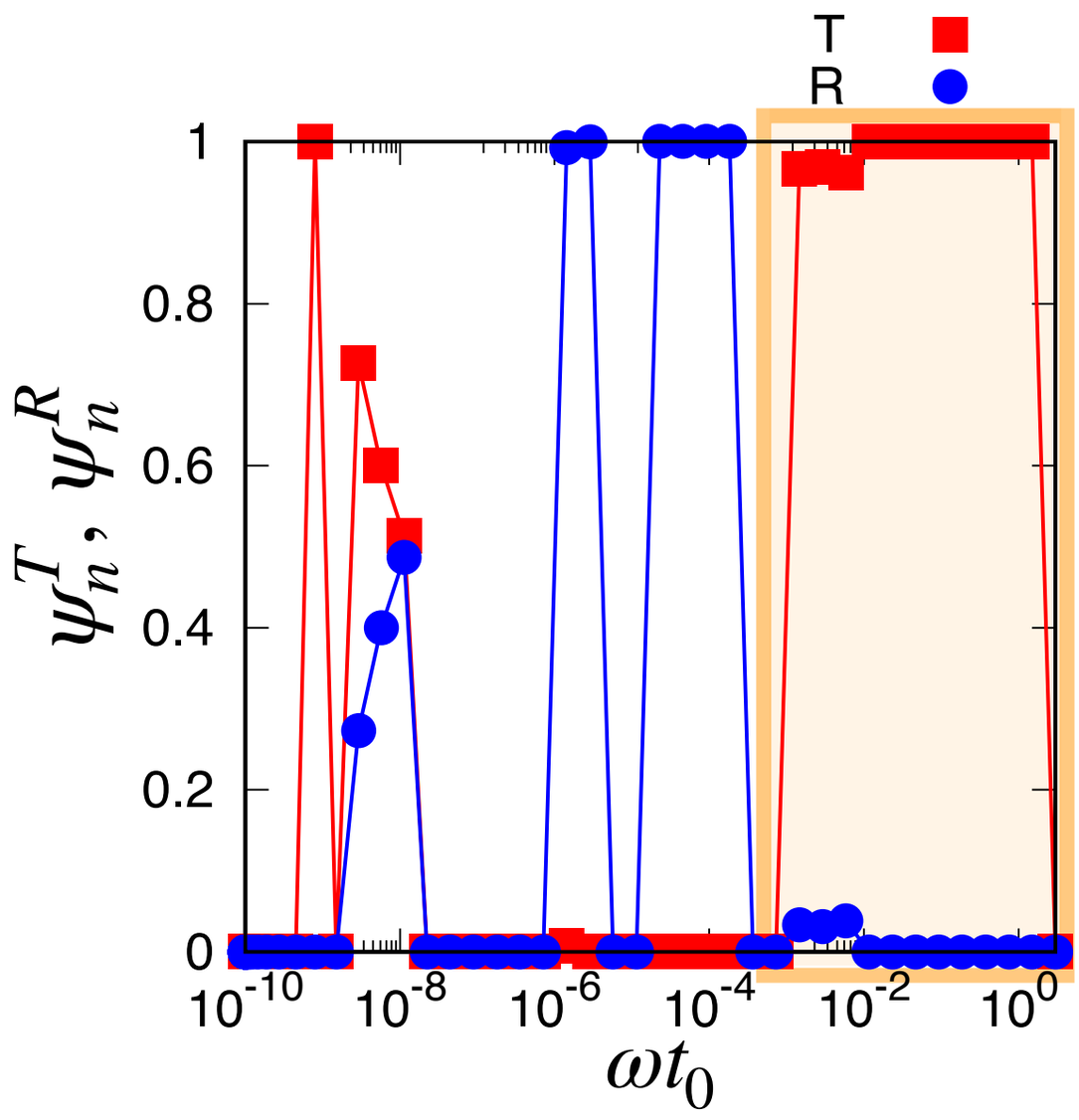
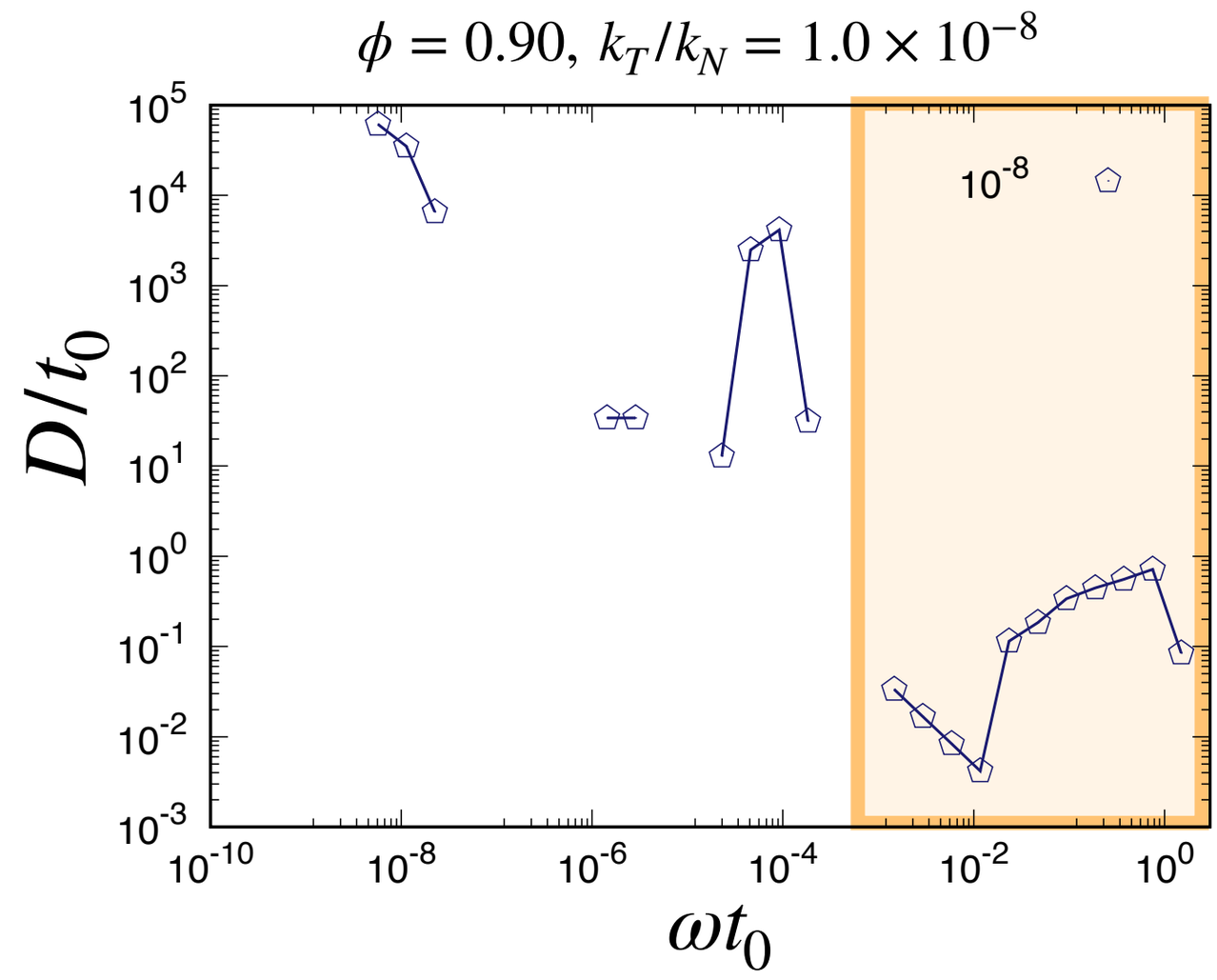




Transnational modes is dominant for Region III.

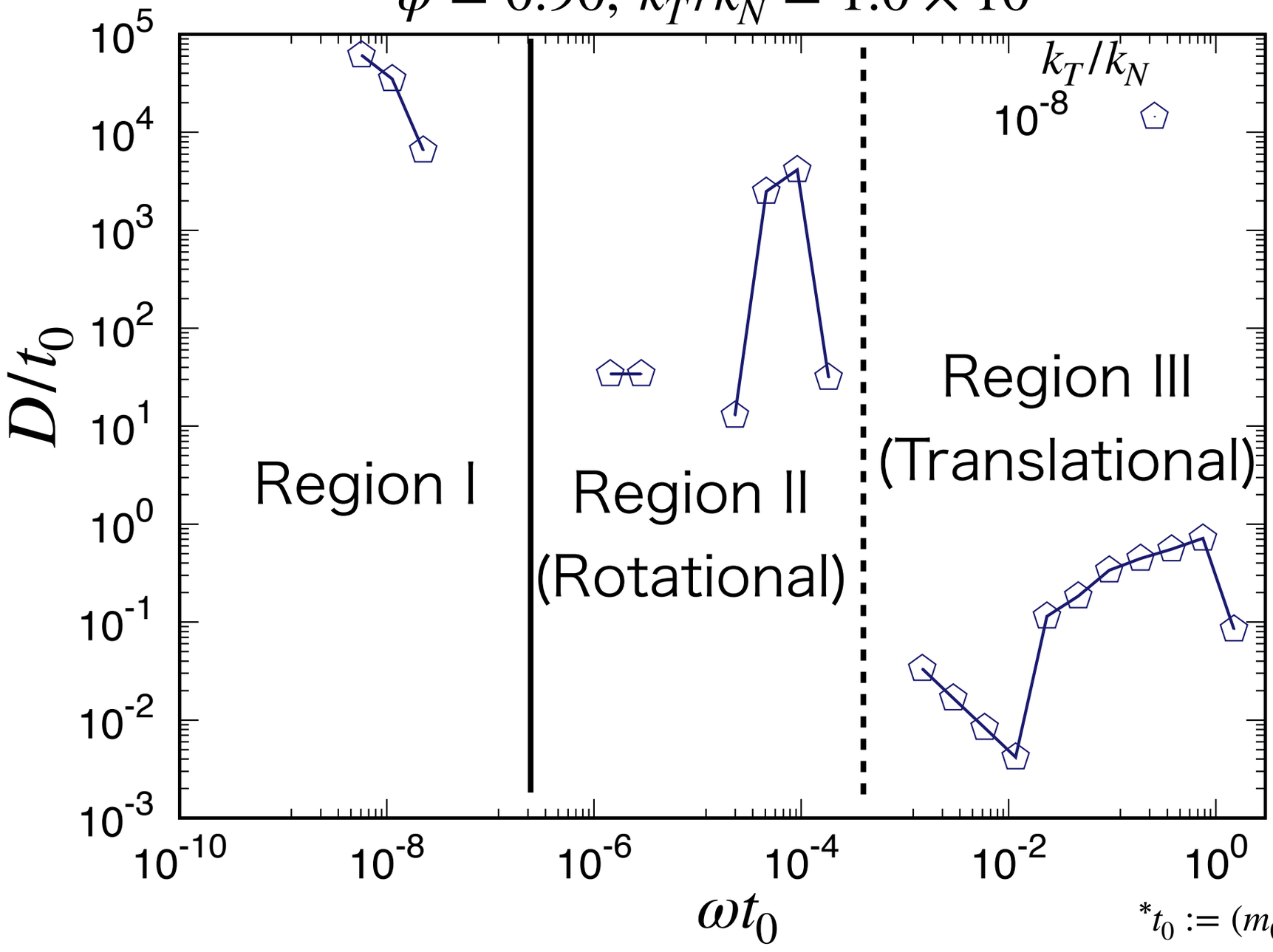
Density of State

$$J|R_n\rangle = \lambda_n |R_n\rangle, \quad J_{ij}^{\alpha\beta} := -\frac{\partial \tilde{F}_i^\alpha}{\partial q_j^\beta} \quad \text{(Jacobian*)}$$

$$\omega_n^2 = \lambda_n .$$

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

$$\phi = 0.90,\ k_T/k_N = 1.0 \times 10^{-8}$$



*$t_0 := (m_0/k_N)^{1/2} d_0^{1/4}$ (unit of time)

DOS is divided into 3 parts for $k_T/k_N \leq 1.0 \times 10^{-8}$.

Density of State

$$J|R_n\rangle = \lambda_n |R_n\rangle, \quad J_{ij}^{\alpha\beta} := -\frac{\partial \tilde{F}_i^\alpha}{\partial q_j^\beta} \quad \text{(Jacobian*)}$$

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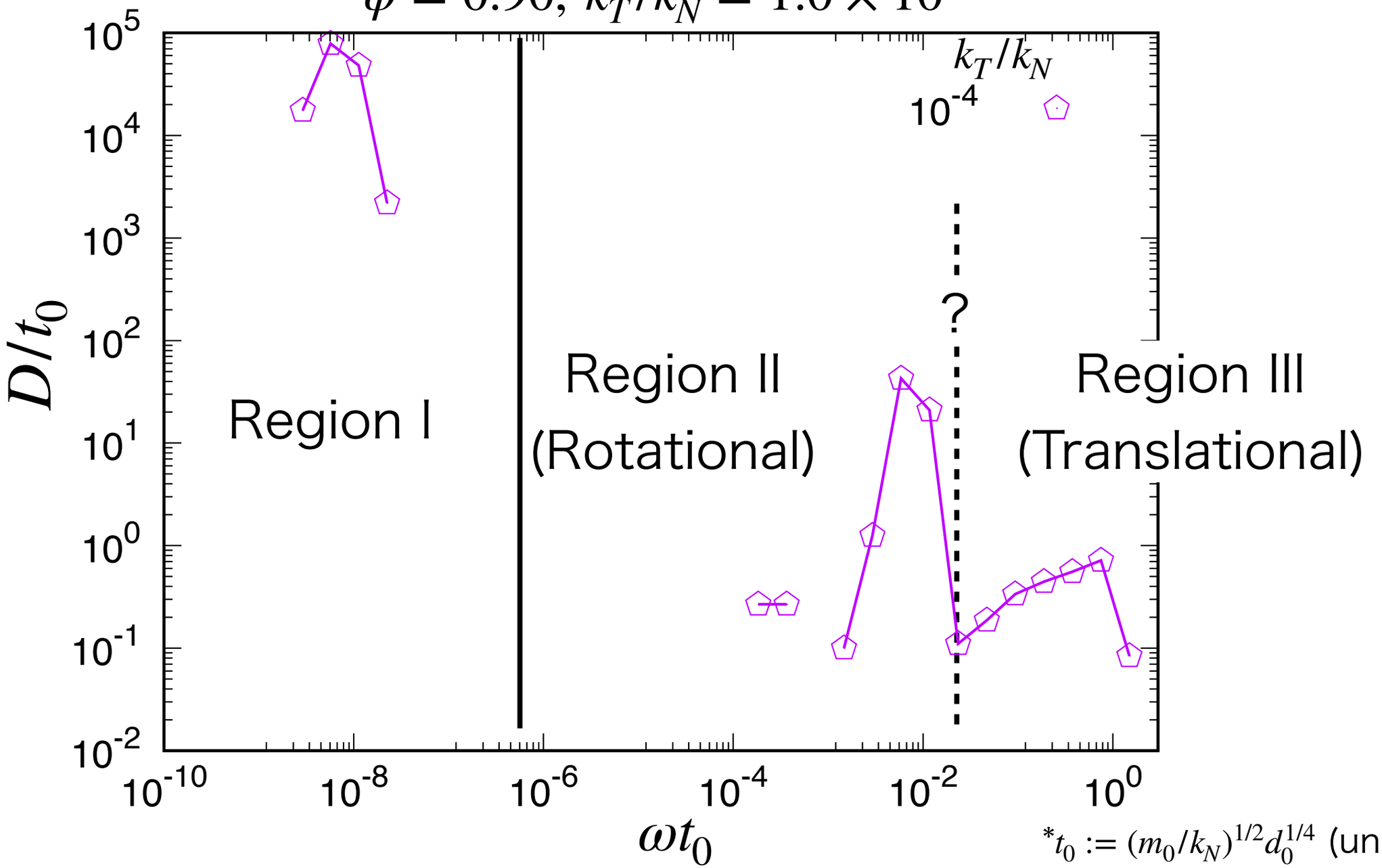


$^*t_0 := (m_0/k_N)^{1/2} d_0^{1/4}$ (unit of time)

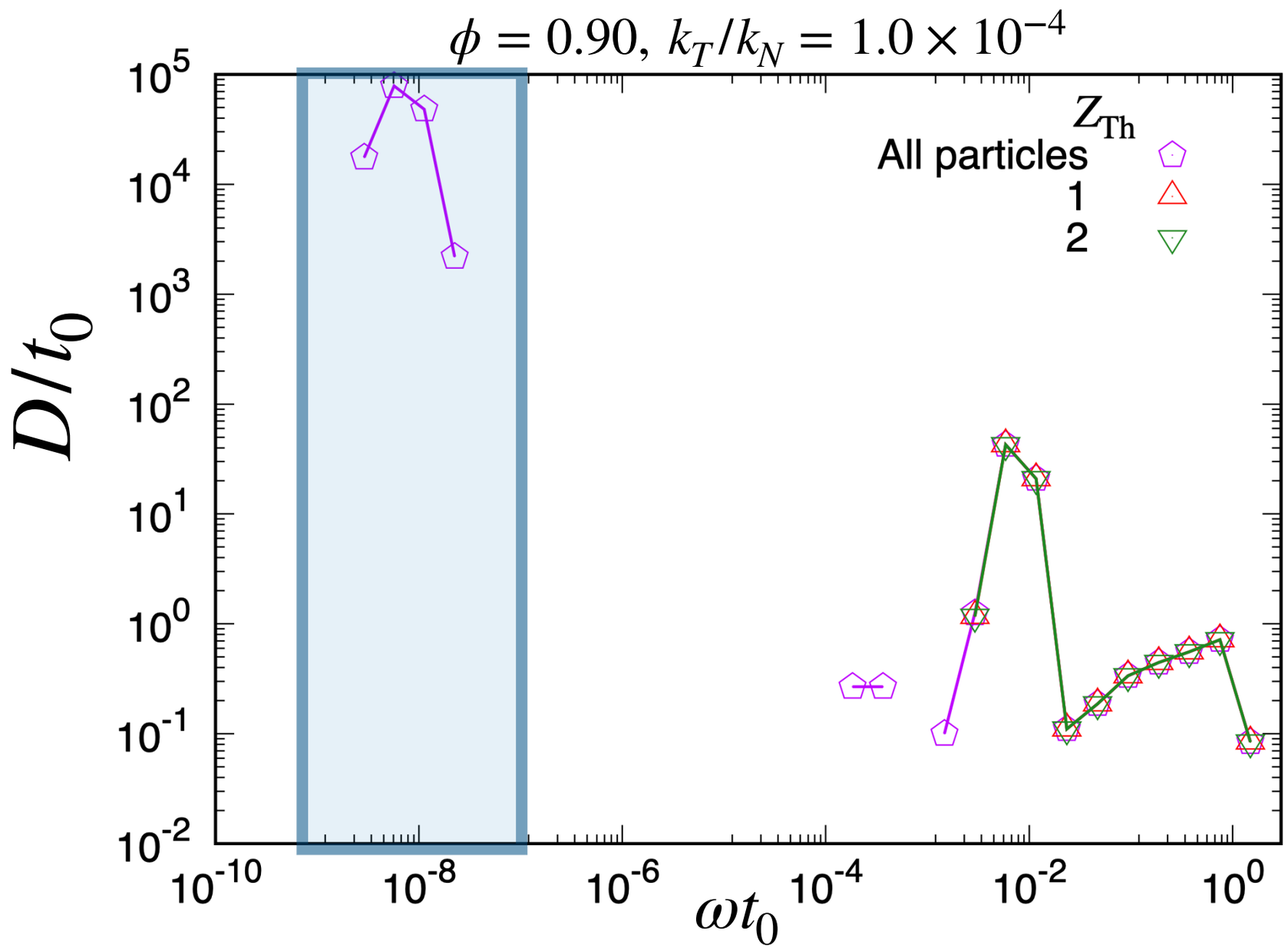
DOS is divided into 3 parts for $k_T/k_N \leq 1.0 \times 10^{-8}$.

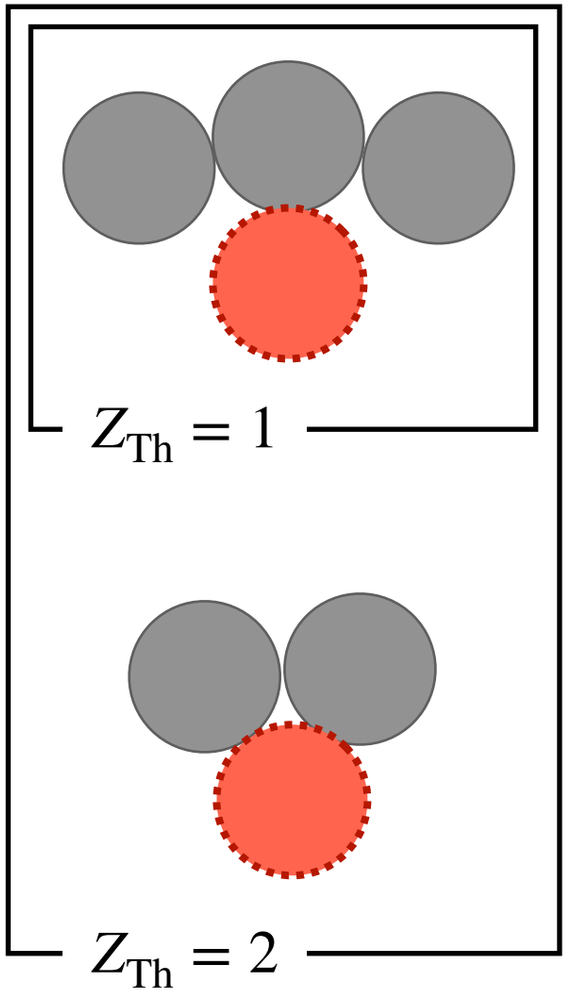
Density of State: Region I

DOS without rattlers which is defined by $Z_i \leq Z_{\mathrm{Th}}$

Z_i: coordination number of i particle,

Z_{Th}: Threshold value of coordination number





Region I disappears for $Z_{\mathrm{Th}} \geq 1$.

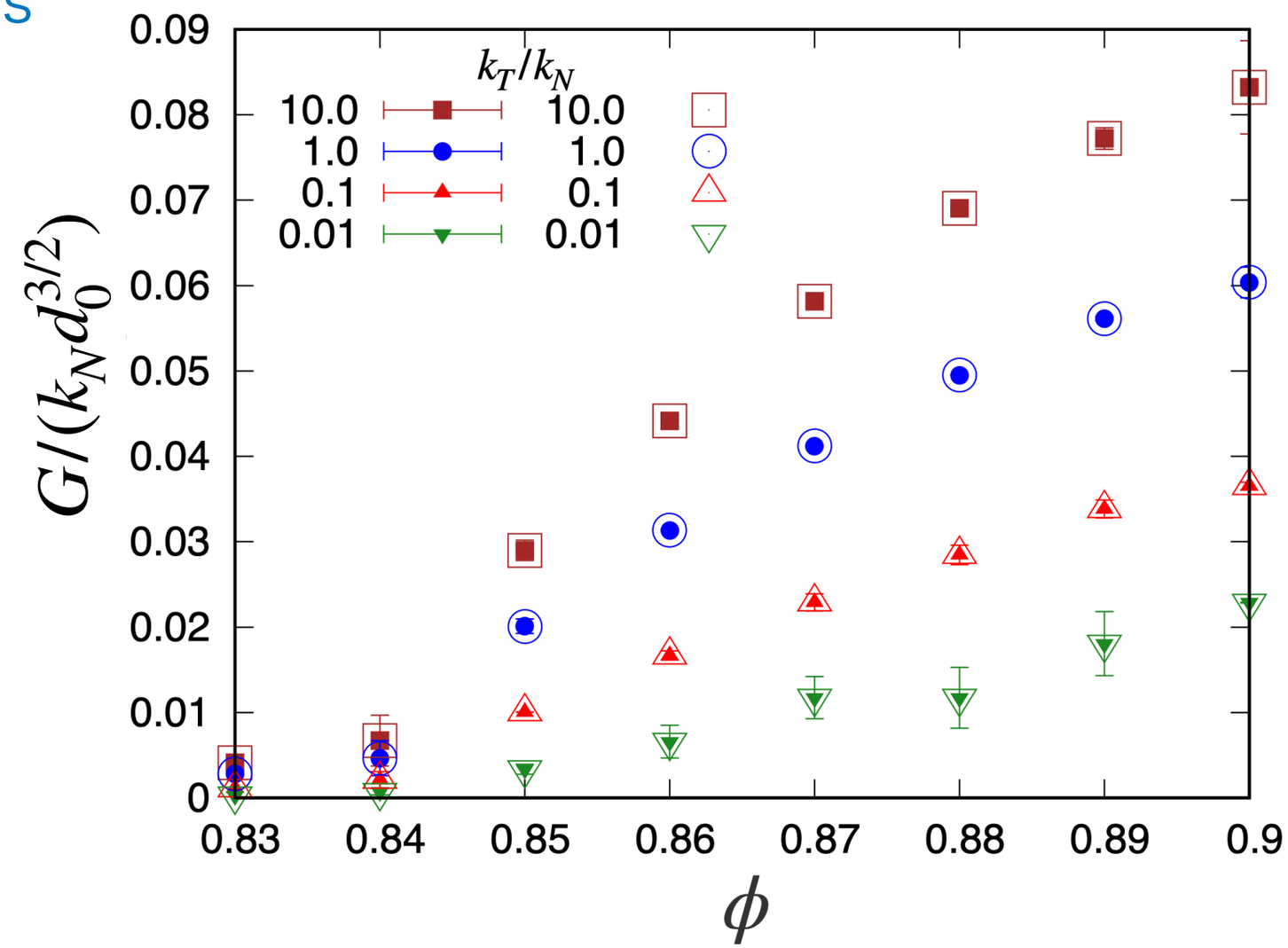
->Region I consists of rattlers.

[11]

Expression of G by J

We obtain shear modulus G by J:

$$G = \underbrace{\frac{1}{2L^2}\sum_{i,j(i\neq j)}\left[y_{ij}^2 J_{N,ij}^{xx}\right]}_{\text{Affine shear modulus } (=:\, G_{\mathrm{A}})} + \underbrace{\frac{1}{L^2}\sum_n{}' \frac{\langle \tilde{L}_n|\Xi\rangle\langle\Theta|\tilde{R}_n\rangle}{\tilde{\lambda}_n}}_{\text{Non affine shear modulus } (=:\, G_{\mathrm{NA}})} \quad \cdots \quad (1)$$



Eq. (1) reproduces ϕ & k_T dependence.

[12]

ϕ-dependence

We obtain shear modulus G by J:

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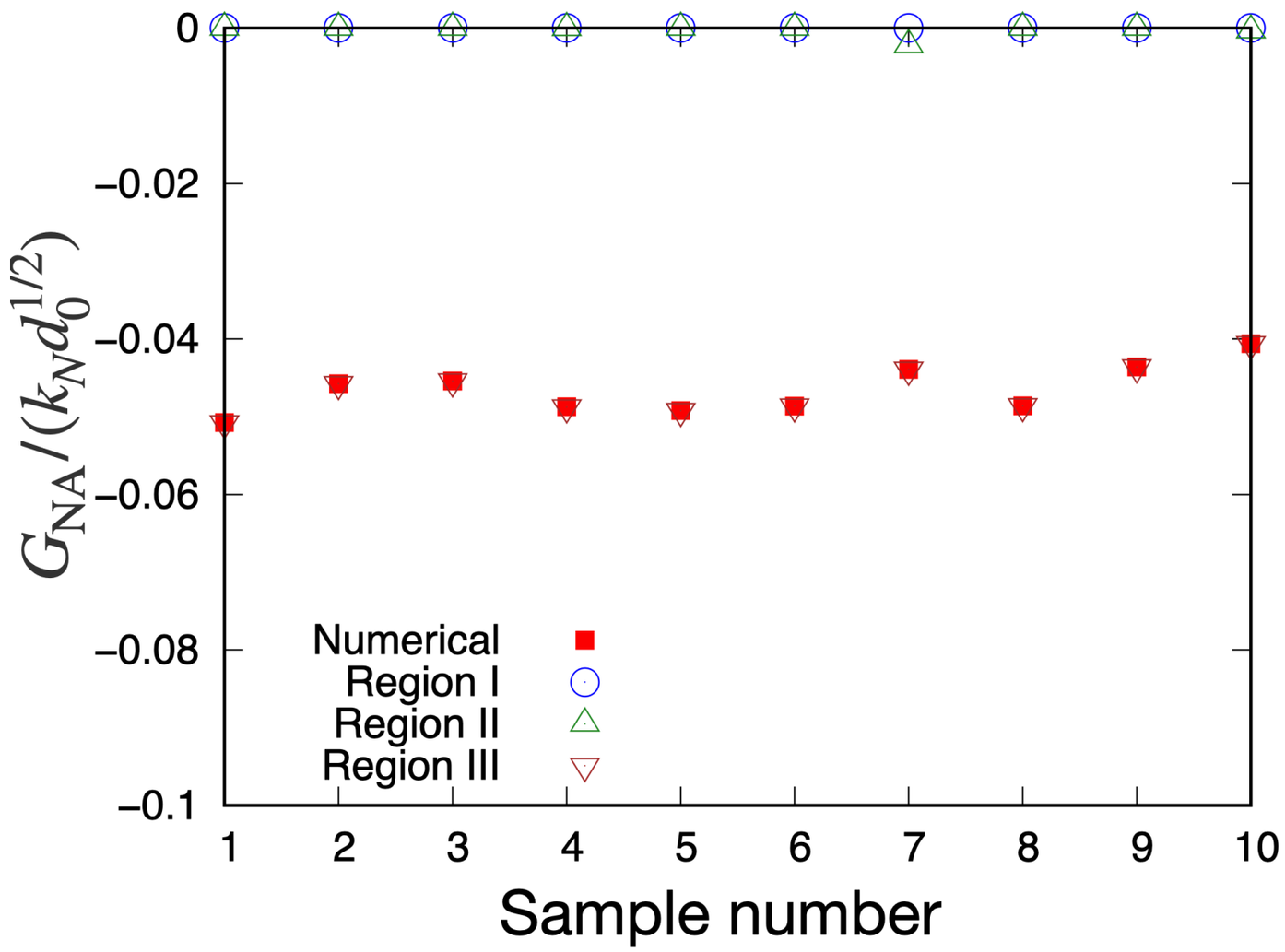

Region III (translational modes) only contributes shear modulus.

[13]

Summary

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

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

- **DOS consists of 3 region for $k_T/k_N \leq 1.0 \times 10^{-8}$**
  Region I consists of rattlers.
  Region II consists of rotational modes.
  Translational modes is dominant for region III.

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

- **Jacobain's representation can reproduce G.**
- **Region III only contributes G.**

Future work

- Expanding our theory to apply to finite sheared system

Density of State

$$J|R_n\rangle = \lambda_n |R_n\rangle, \quad J_{ij}^{\alpha\beta} := -\frac{\partial \tilde{F}_i^\alpha}{\partial q_j^\beta} \quad \text{(Jacobian*)}$$

$$\omega_n^2 = \lambda_n \,.$$

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

$$\phi = 0.90, k_T/k_N = 1.0 \times 10^{-4}$$