Mini-workshop on "Jamming, rheology and granular matter"

Mean-field theory of vibrational density of states of jammed packing

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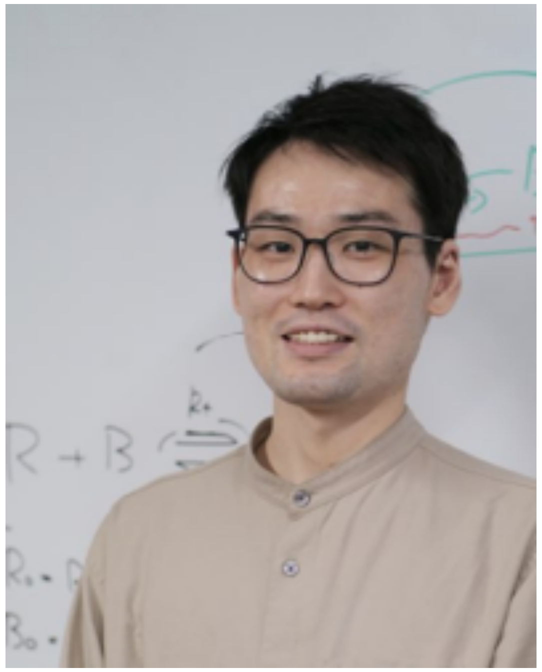

YITP
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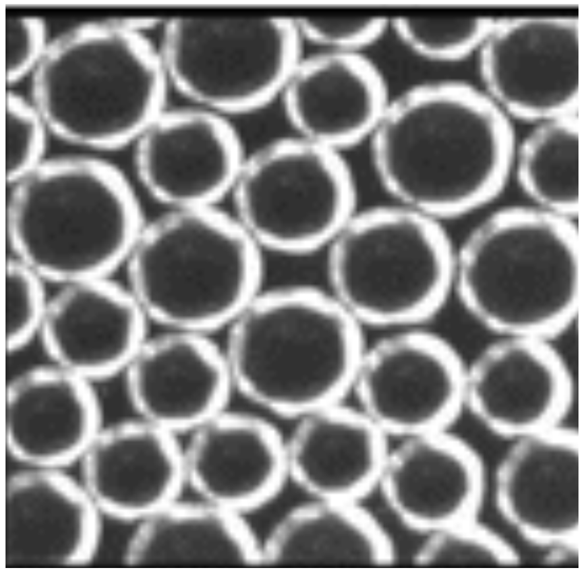
Introduction

What is granular matter?

Macroscopic particles where the thermal fluctuations are negligible.

M&M Candies



Forms

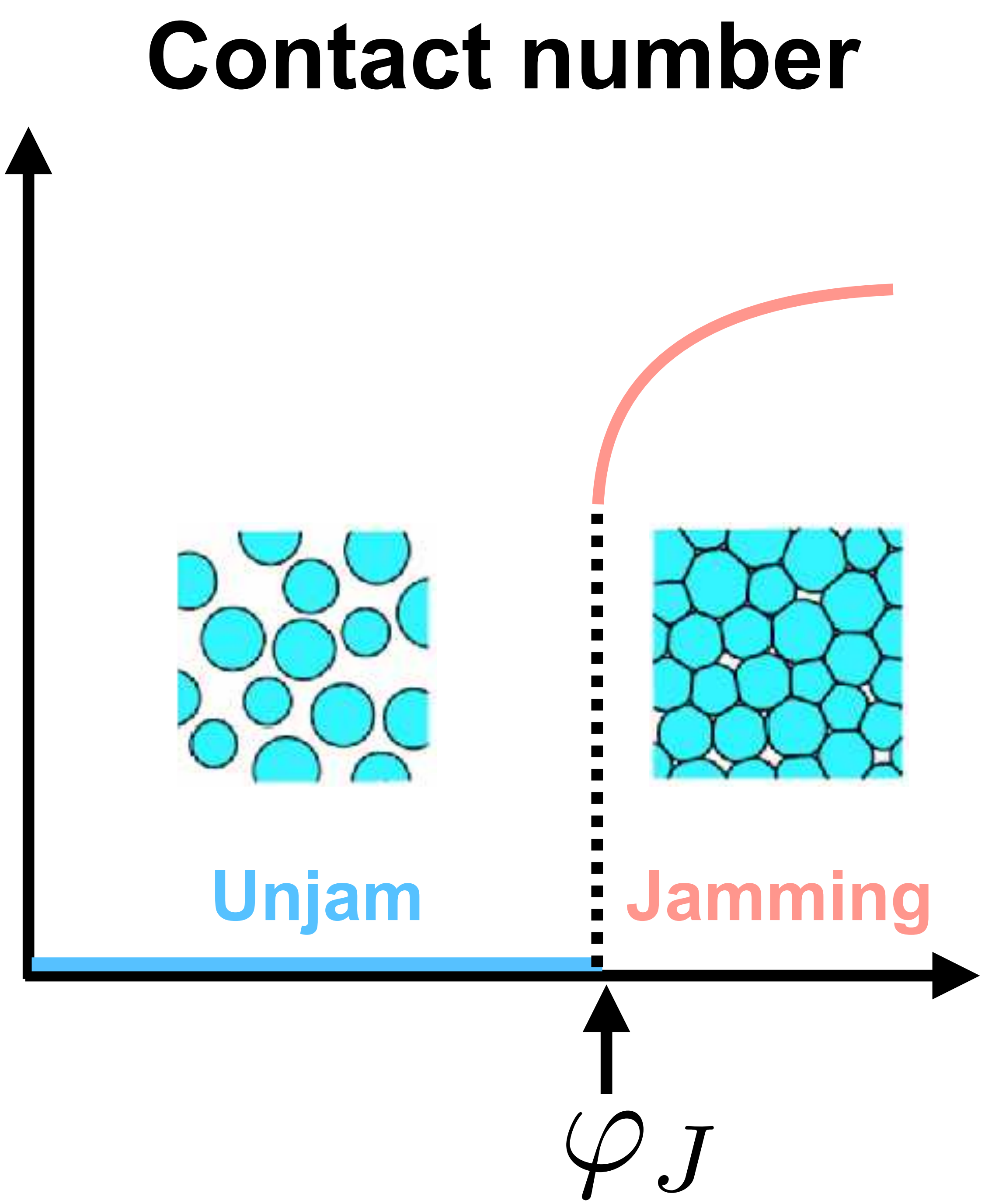
Sand & rock

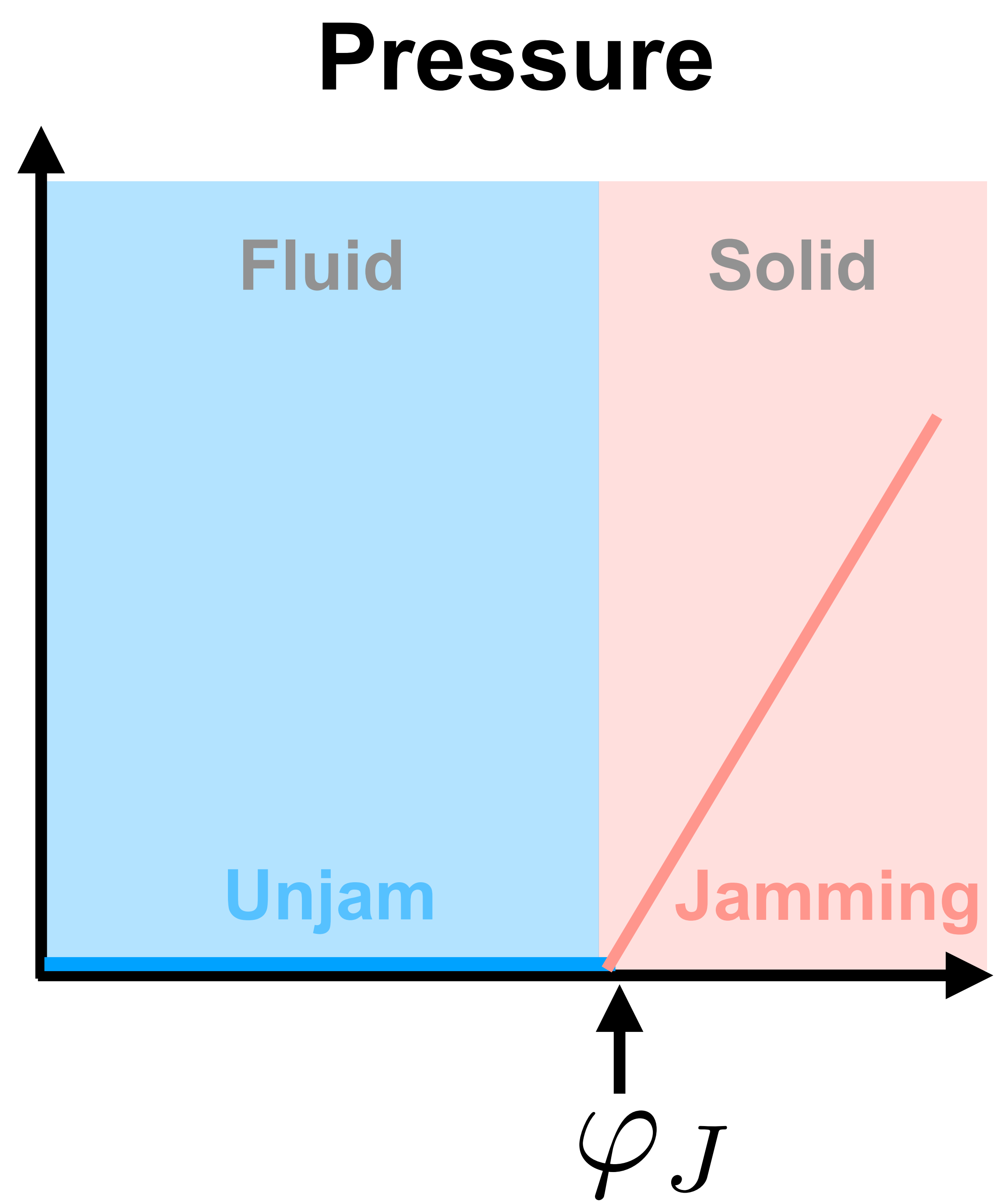
Grains

Snow powders

Introduction

What is the jamming transition?





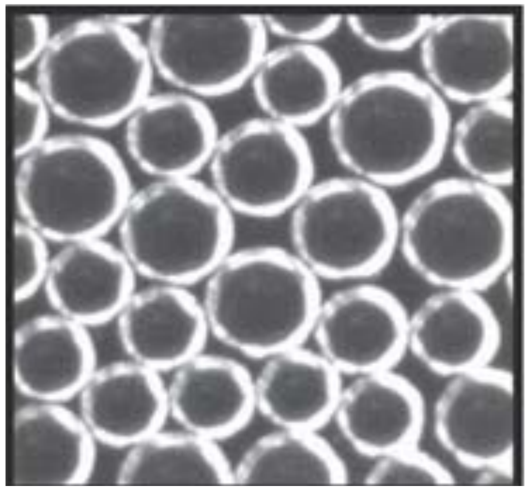
The jamming transition is a phase transition from fluid to solid at zero temperature

Introduction

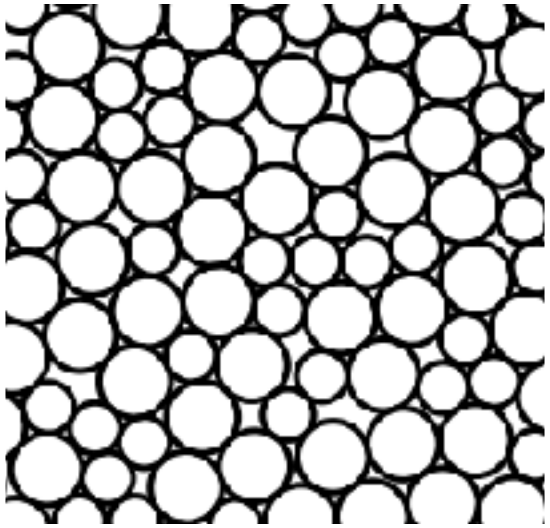
Minimal model to study jamming

Frictinless spherical particles

Metallic balls



Wet foams



Numerical simulation

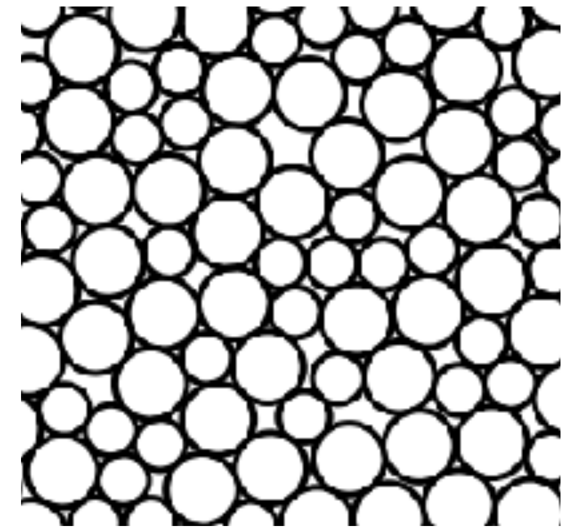
Introduction

Minimal model to study jamming

Frictinless spherical particles

Harmonic potential

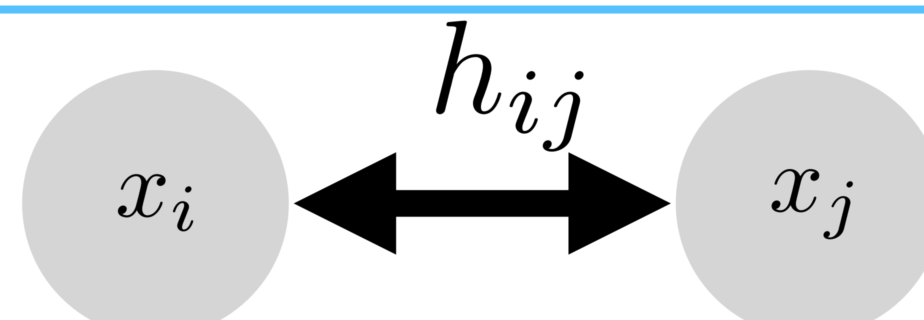
$$V_N = \sum_{i<j}^{N} v(h_{ij}), \quad v(h_{ij}^2) = \frac{h_{ij}^2}{2}\theta(-h_{ij})$$



Numerical simulation

Gap function

$$h_{ij} = |x_i - x_j| - R_i - R_j$$



Introduction

Contact number

J. C. Maxwell
1831-1879

Simple stability argument by Maxwell

\# of constraints > # of degrees of freedom

\# of constraints = # of contacts = $Nz/2$

\# of degrees of freedom = Nd

\# of contacts per particle

\# of particles

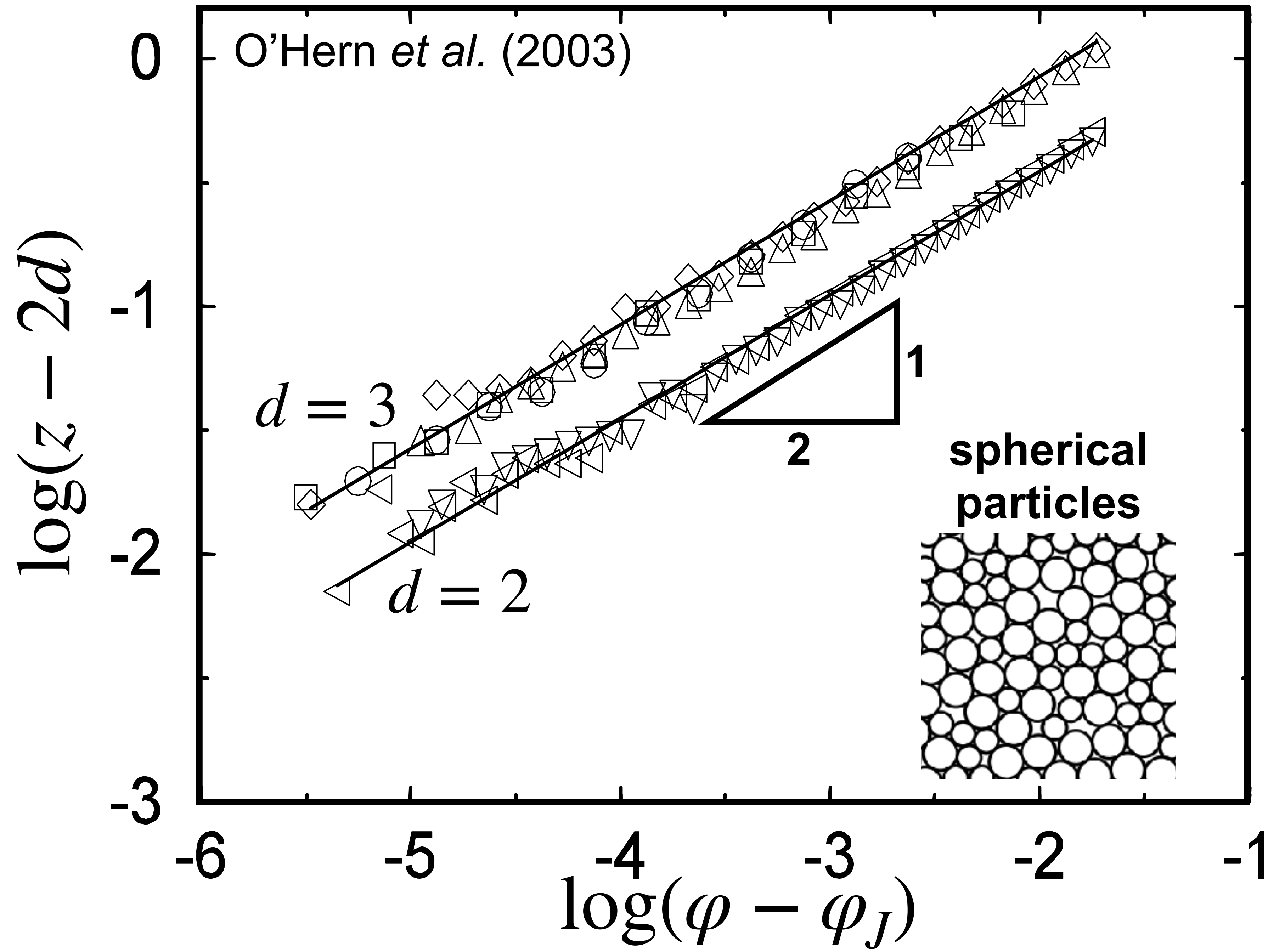
spatial dimension

$$z \geq 2d$$

Transition may occur at $z_J = 2d$ (isostatic)

Introduction

Contact number



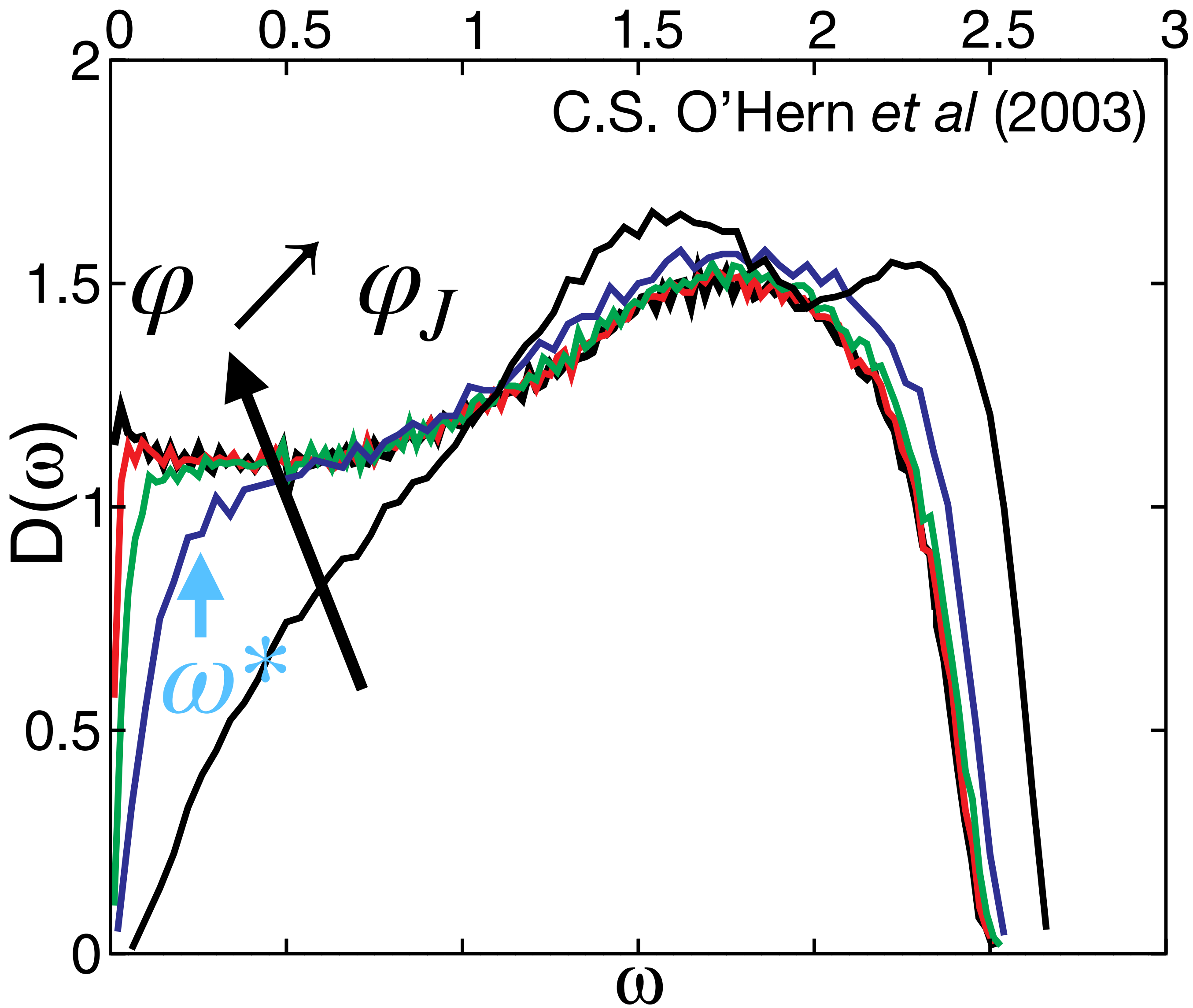
Scaling relation $z - 2d \propto (\varphi - \varphi_J)^{1/2}$

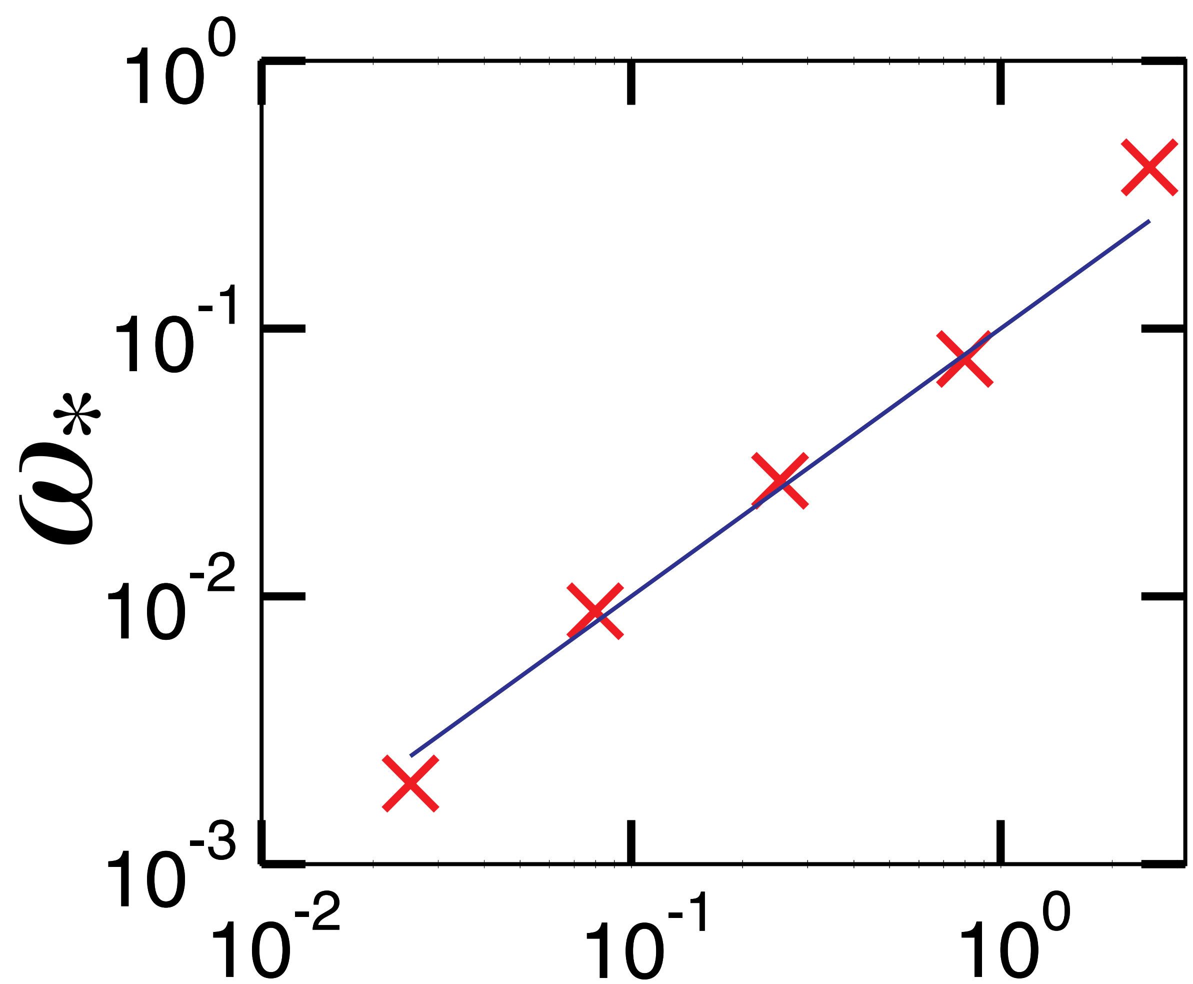
Power law = Critical phenomena!

Introduction

Vibrational density of states

Scaling of the vibrational density of states





$$\delta z = z - 2d$$

δz controls the onset of the soft-modes

Motivation

Previous theoretical studies (scaling)

Effective medium theory (lattice systems)

- M. Wyart (2010)
- E. DeGiuli et al. (2014)

$$\delta z \sim \delta\varphi^{1/2},\ \omega_* \sim \delta z$$

Replica liquid theory (particle systems)

- G. Parisi and F. Zamponi (2010)
- P. Charbonneau et al. (2014)

Exact results in $d \to \infty$

Current works (quantitative)

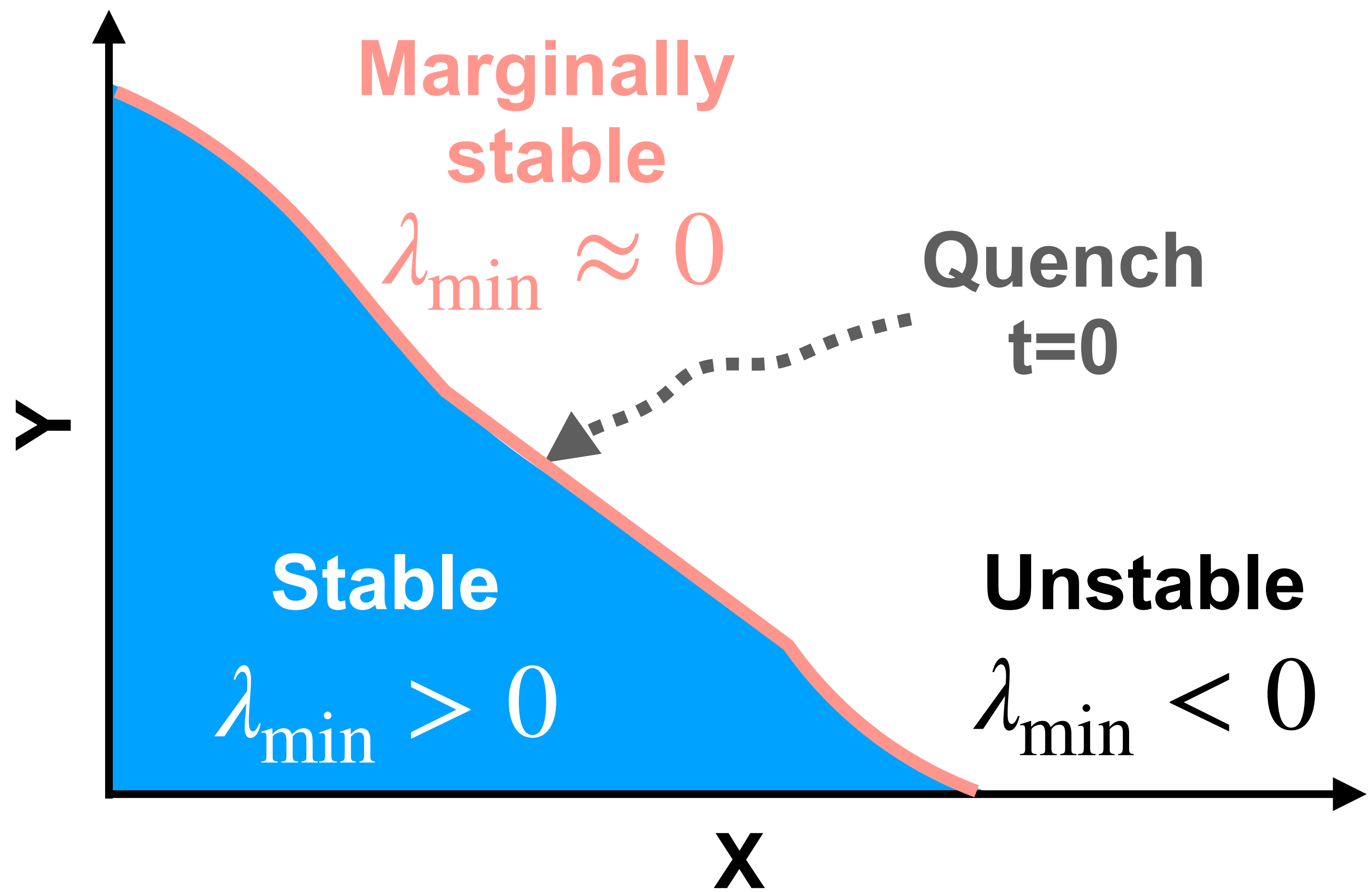
We aim to develop a quantitative theory for calculating physical quantities in finite dimensions.

Theory

Variational argument

M. Muller and M. Wyart (2014)

Assumption of the marginal stability



The aging will stop when the system becomes marginally stable

$$\lambda_{\min} \approx 0$$

Hessian

H. Ikeda and M. Shimada (2022)

Hessian of interaction potential

$$V_N = \sum_{\mu=1}^{N_c} v(h_\mu)$$

$$H_{ij}^{ab} = \nabla_i^a \nabla_j^b V_N = \underbrace{\boxed{\sum_{\mu=1}^{N_c} v''(h_\mu)\,\nabla_i^a h_\mu\,\nabla_j^b h_\mu}}_{H^{(1)}} + \underbrace{\boxed{\sum_{\mu=1}^{N_c} v'(h_\mu)\,\nabla_i^a \nabla_j^b h_\mu}}_{H^{(2)}}$$

Hessian

Calculation of $H^{(2)}$

Diagonalization

$$H^{(2)} \rightarrow (O^t H^{(2)} O)_{ij}^{ab} = \lambda_i^a \delta_{ij} \delta_{ab}$$

Mean-field approximation

$$\lambda_i^a \approx \langle \lambda \rangle = \frac{1}{Nd} \mathrm{Tr} H^{(2)} = \frac{ze}{d}$$

Pre-stress

$$e = -\frac{d-1}{N_c} \sum_{\mu=1}^{N_c} \frac{h_\mu}{r_\mu} = (d-1) \left\langle \frac{\sigma_\mu - r_\mu}{r_\mu} \right\rangle$$

Theory

Hessian

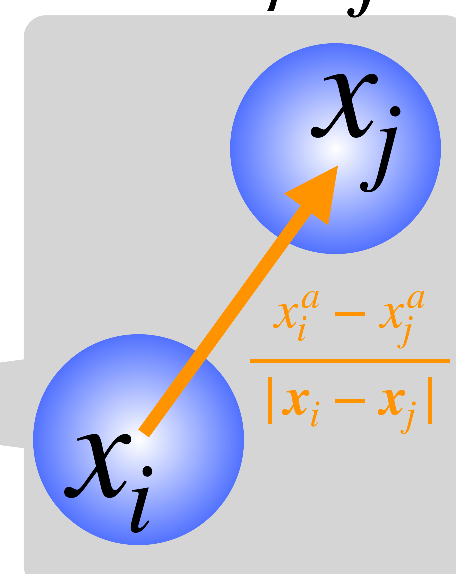
Calculation of $H^{(1)}$

Transformation

$$H^{(1)} \to (O^t H^{(1)} O)_{ij}^{ab} = \sum_{\mu} (O \nabla h_\mu)_i^a (O \nabla h_\mu)_j^b$$

Approximation by random variable

$$(\nabla h_{ij})_k^a = (\delta_{ki} - \delta_{kj}) \frac{x_i^a - x_j^a}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}$$



Random variable

$$(O \nabla h_\mu)_i^a \approx C \xi_i^a \leftarrow \boxed{\langle \xi_i^a \rangle = 0,\ \langle \xi_i^a \xi_j^b \rangle = \delta_{ij} \delta_{ab}}$$

$$|C\boldsymbol{\xi}|^2 = |O \nabla h_\mu|^2 = |\nabla h_\mu|^2 \to C = \sqrt{\frac{2}{Nd}}$$

Theory

Density of states

Calculation of minimal eigenvalue

$$H_{ij}^{ab} \approx \frac{2}{Nd} \sum_{\mu} \xi_{ia}^{\mu} \xi_{jb}^{\mu} - \frac{z}{2} e \delta_{ij} \delta_{ab}$$

Marchenko-Pastur Distribution

$$\rho(\lambda) = \frac{d}{z} \rho_{\mathrm{MP}}(d\lambda/z + e)$$

$$\rho_{\mathrm{MP}}(\lambda) = \frac{z}{2d} \frac{\sqrt{(\lambda_+ - \lambda)(\lambda - \lambda_-)}}{2\pi\lambda}, \quad \lambda_{\pm} = \left(1 \pm \sqrt{\frac{2d}{z}}\right)^2 .$$

Minimal eigenvalue

$$\lambda_{\min} = \frac{z}{d} \left(1 - \sqrt{\frac{2d}{z}}\right)^2 - \frac{z}{d} e$$

Theory

Contact number

Minimal eigenvalue

$$\lambda_{\min} = \frac{z}{d}\left(1 - \sqrt{\frac{2d}{z}}\right)^2 - \frac{z}{d}e$$

Maiginal stability

$$\lambda_{\min} = 0$$

Contact number

$$z(e) = \frac{2d}{(1 - e^{1/2})^2} \sim 2d(1 + e^{1/2})$$

H. Ikeda and M. Shimada (2022)

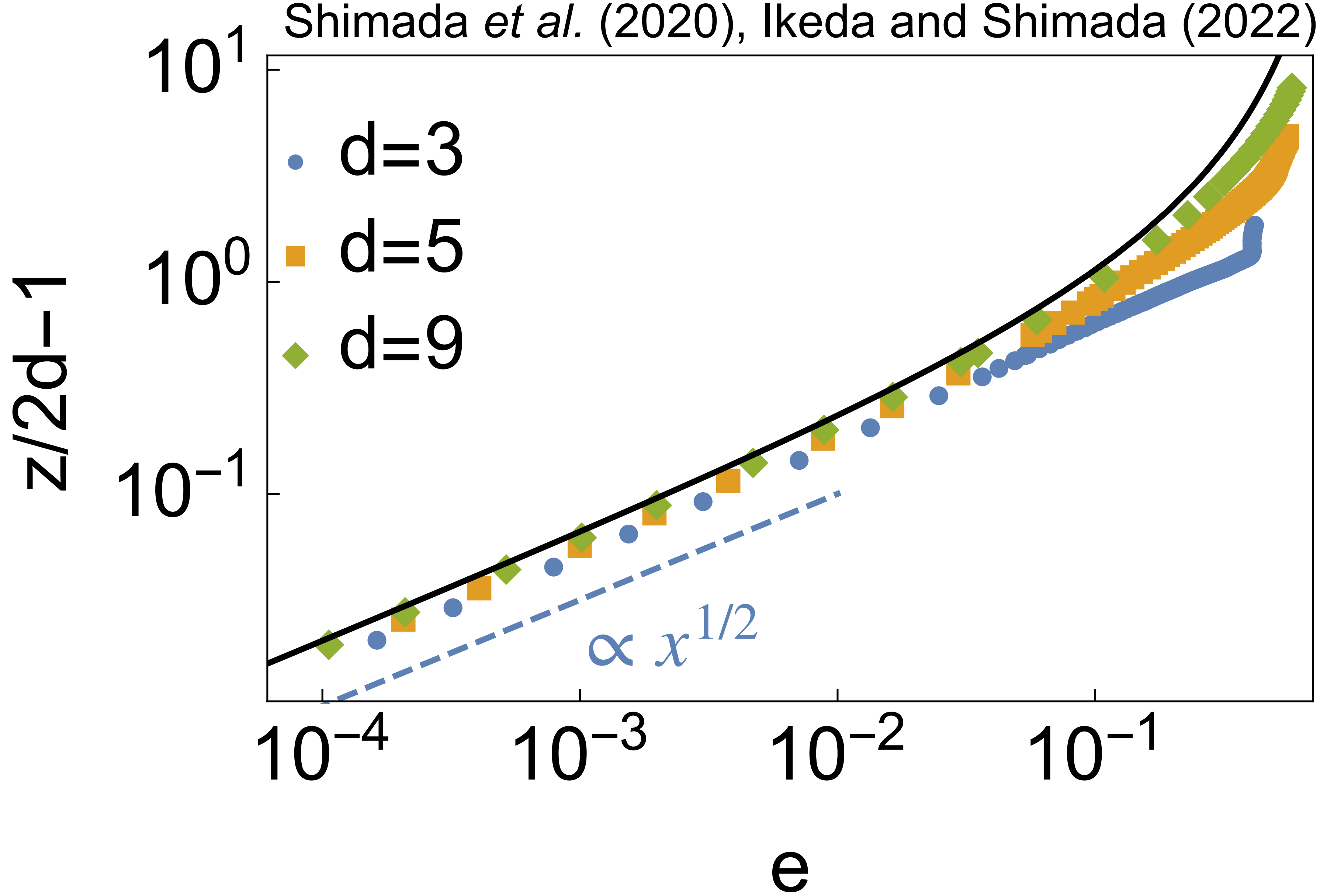
Result

Contact number

Theoretical prediction

$$z(e) = \frac{2d}{(1 - e^{1/2})^2}$$

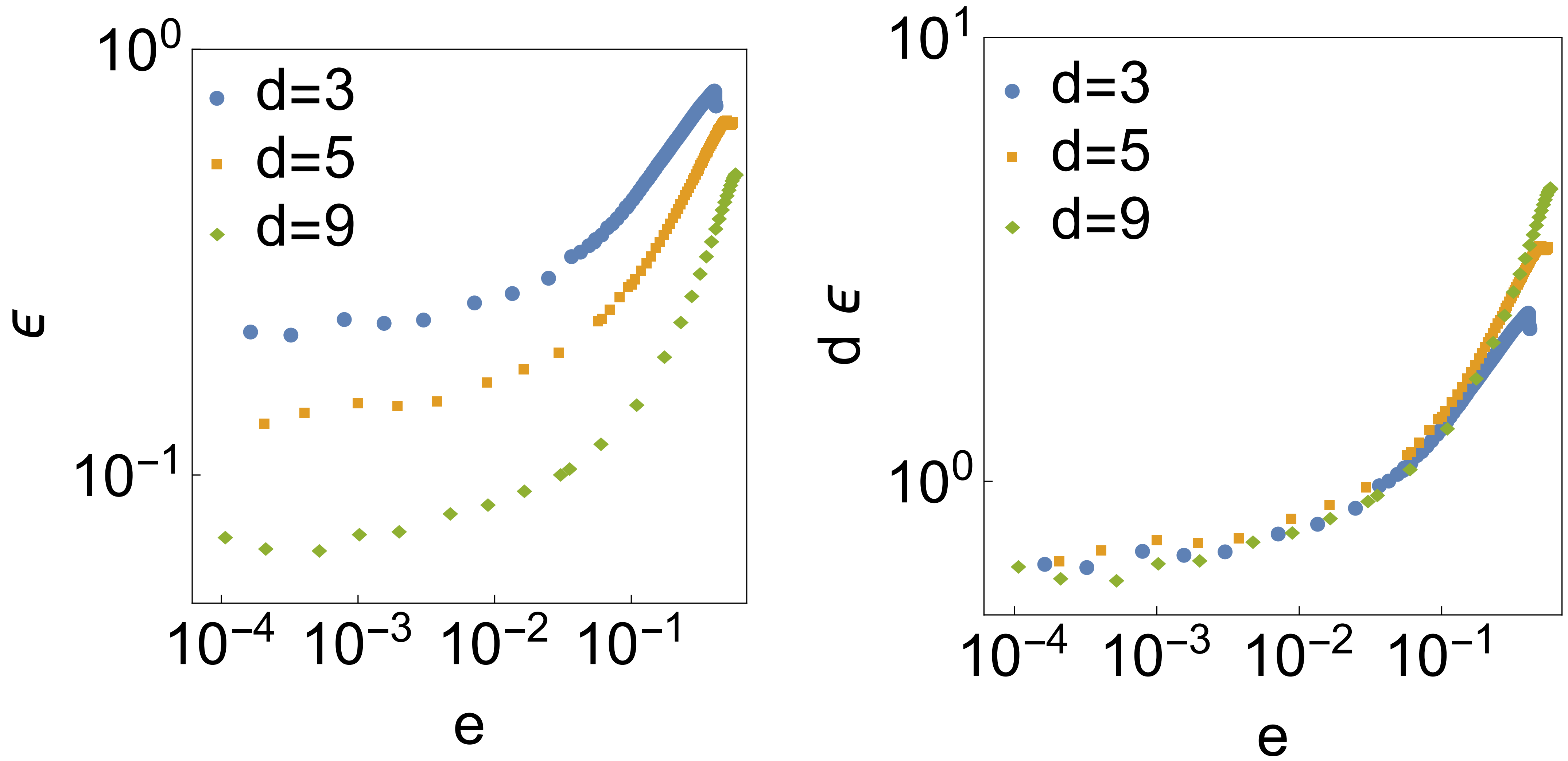
Shimada *et al.* (2020), Ikeda and Shimada (2022)



Result

Contact number

ε: Difference between theory and numerical results



$\varepsilon \sim 1/d \to 0$, **meaning that the theory become exact in the high dimensional limit.**

Result

Vibrational density of states

Linearization

$$\ddot{x} = -\nabla V \rightarrow \delta\ddot{x} = -\nabla^2 V \delta x$$

Eigenvalue expansion

$$\delta\ddot{x}_n = -\lambda_n \delta x_n \rightarrow \delta x_n(t) = e^{i\omega_n t}\delta x_n(0)$$

Eigenvalue of the Hessian

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

$$D(\omega) = \rho(\lambda)\frac{d\lambda}{d\omega} = 2\omega\rho(\lambda = \omega^2)$$

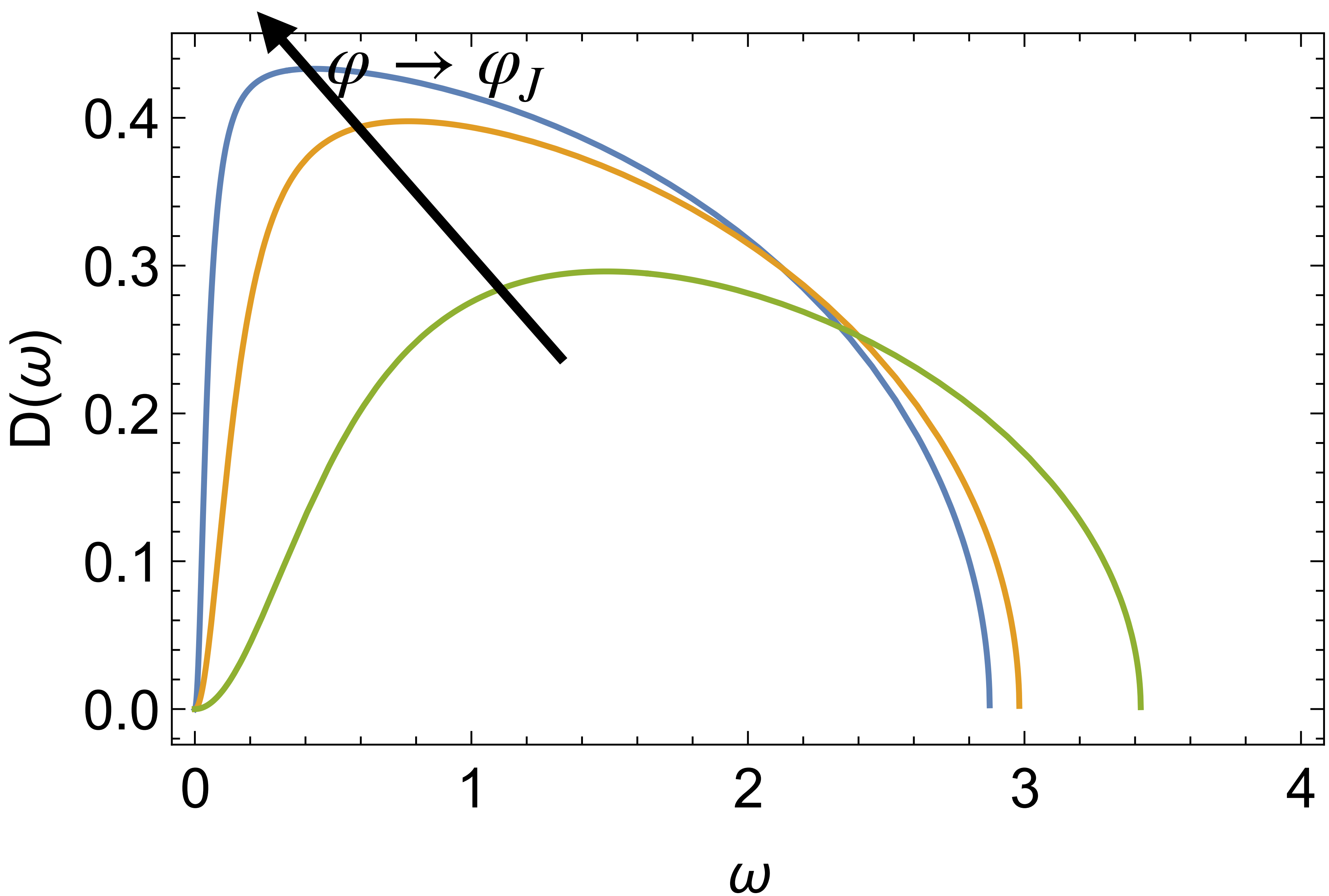
Eigenvalue distribution

Result

Vibrational density of states

Theoretical prediction

$$D(\omega) = \frac{\omega^2\sqrt{(1-e^{1/2})^3\left\{8-(1-e^{1/2})\omega^2\right\}}}{2\pi\left\{2e+(1-e^{1/2})^2\omega^2\right\}}.$$



Result

Vibrational density of states

Theoretical prediction

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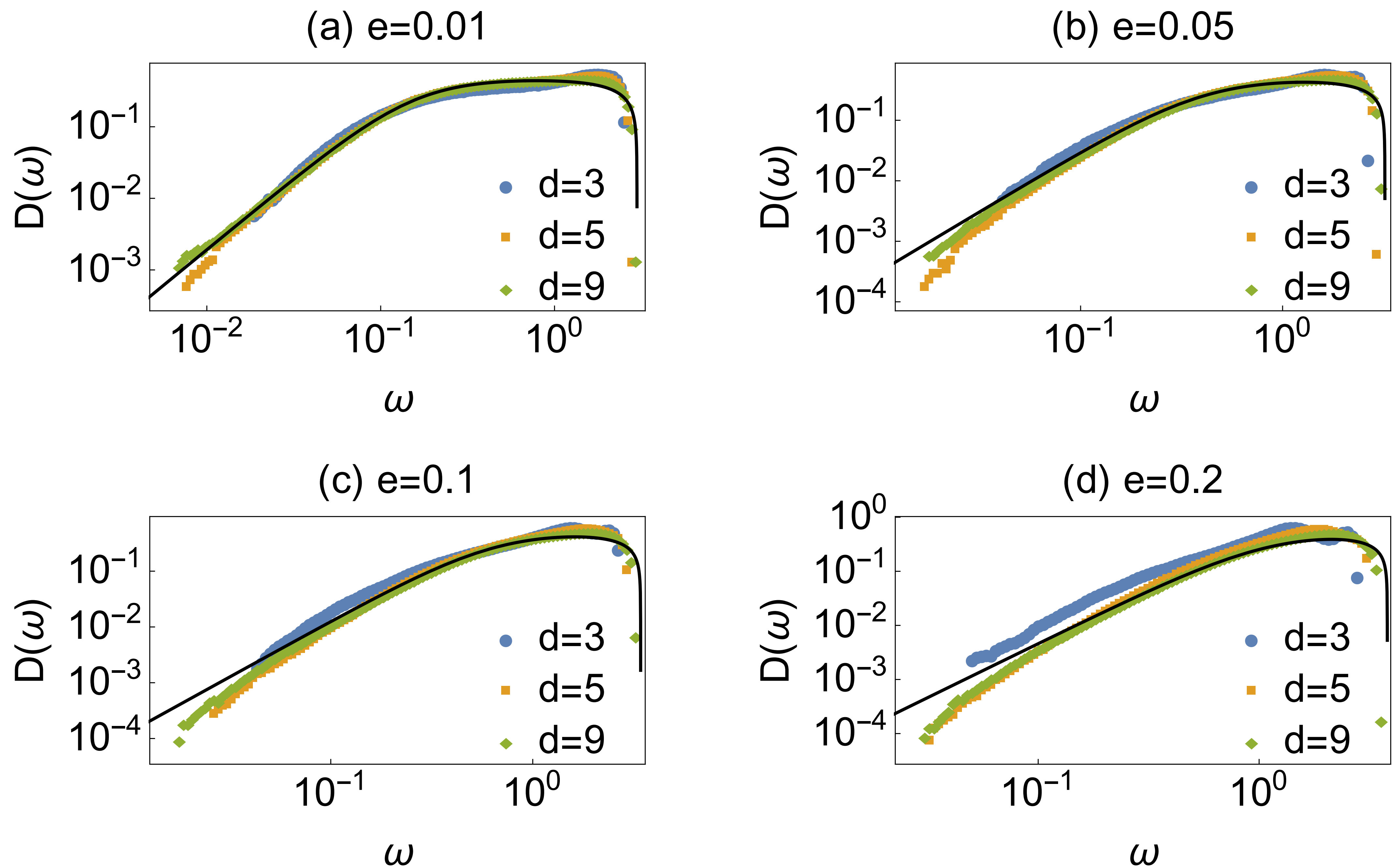

Conclusion

Summary

- We calculated the contact number and density of states above the jamming transition point.
- Our theoretical prediction agrees well with the numerical results near the jamming transition point.
- Some deviations are observed far from jamming.

Future work

- Can we extended the theory for more complex systems such as non-spherical particles, frictional particle, sticky particles, and so on?
- Quasi-localized mode