Jamming transition of non-spherical particles

[EPJE, 44, 120 (2021) or arXiv:2012.07294]

Harukuni Ikeda
Department of Physics, Gakushuin University

Outline

- **Introduction**

- **Jamming of spherical particles**

- **Jamming of non-spherical particles**

Outline

- Introduction
- Jamming of spherical particles
- Jamming of non-spherical particles

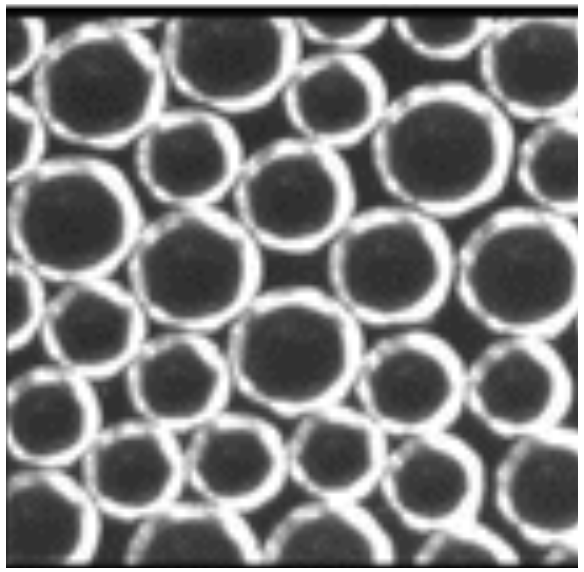
Introduction

Granular matters are ubiquitous in our daily life!

Assembly of macroscopic particles (0.1mm~)
Thermal fluctuations are completely negligible = Non equilibrium

M&M Candies

Grains



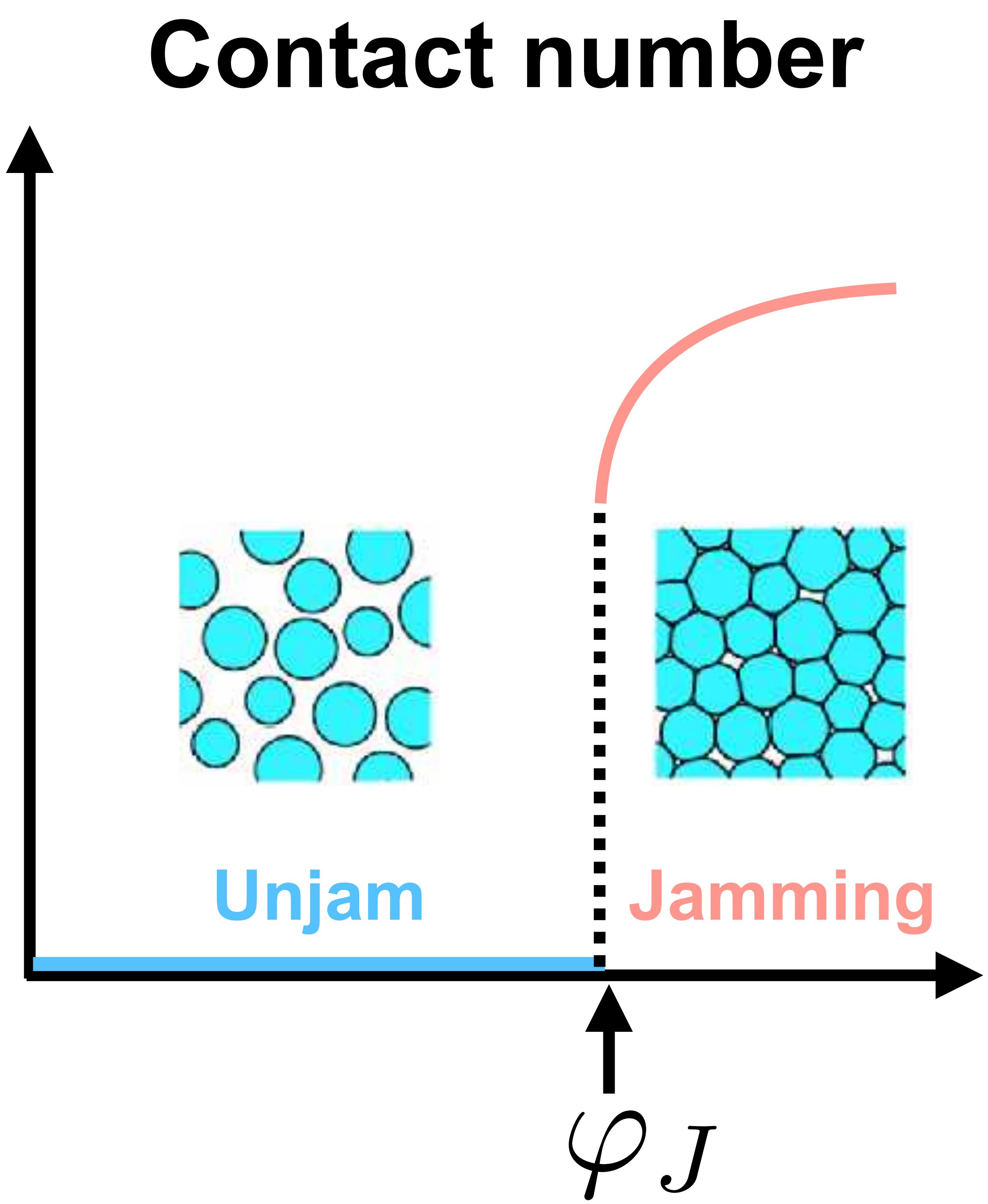
Forms

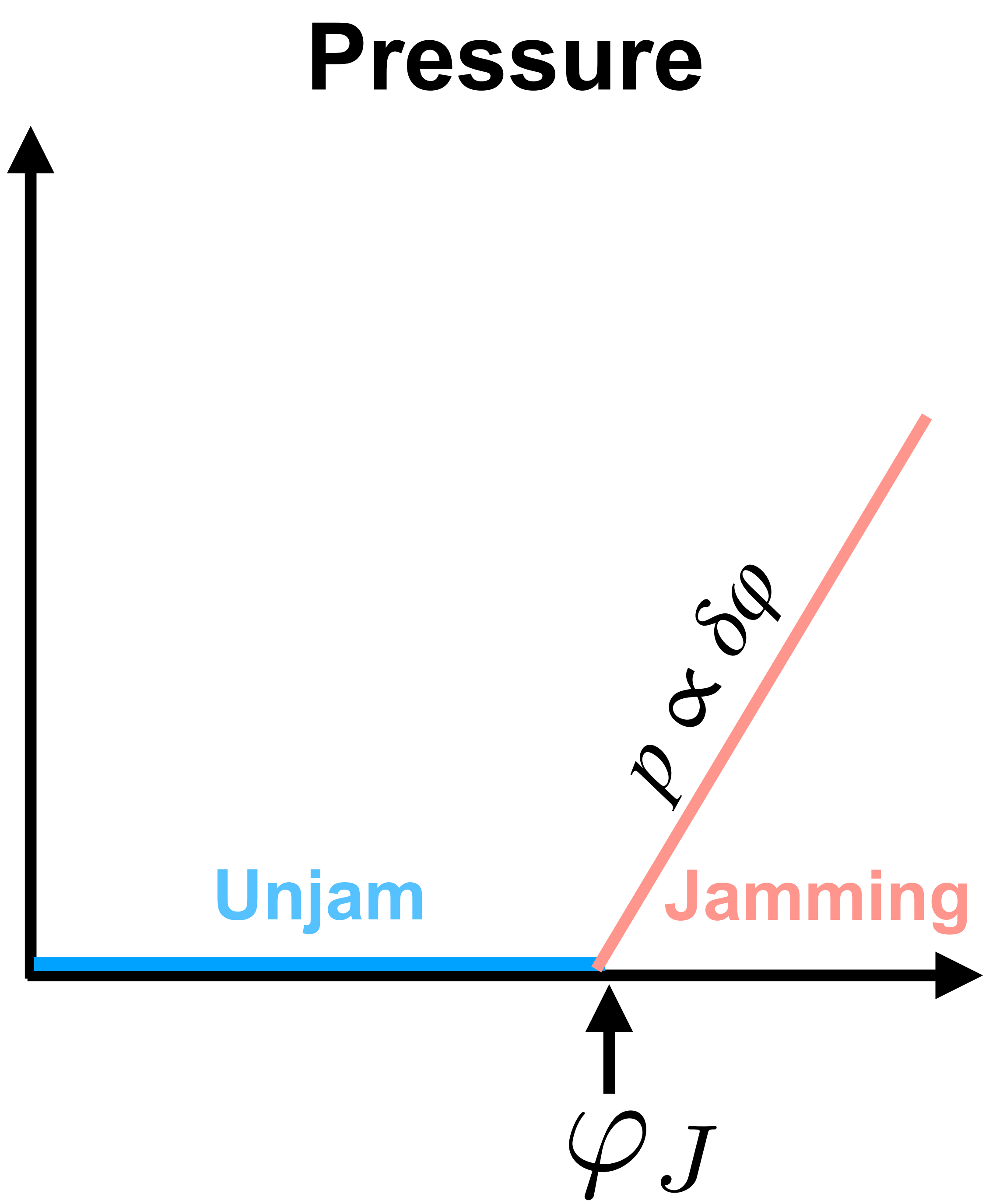
Sand & rock

Snow powders

Introduction

What is the jamming transition?



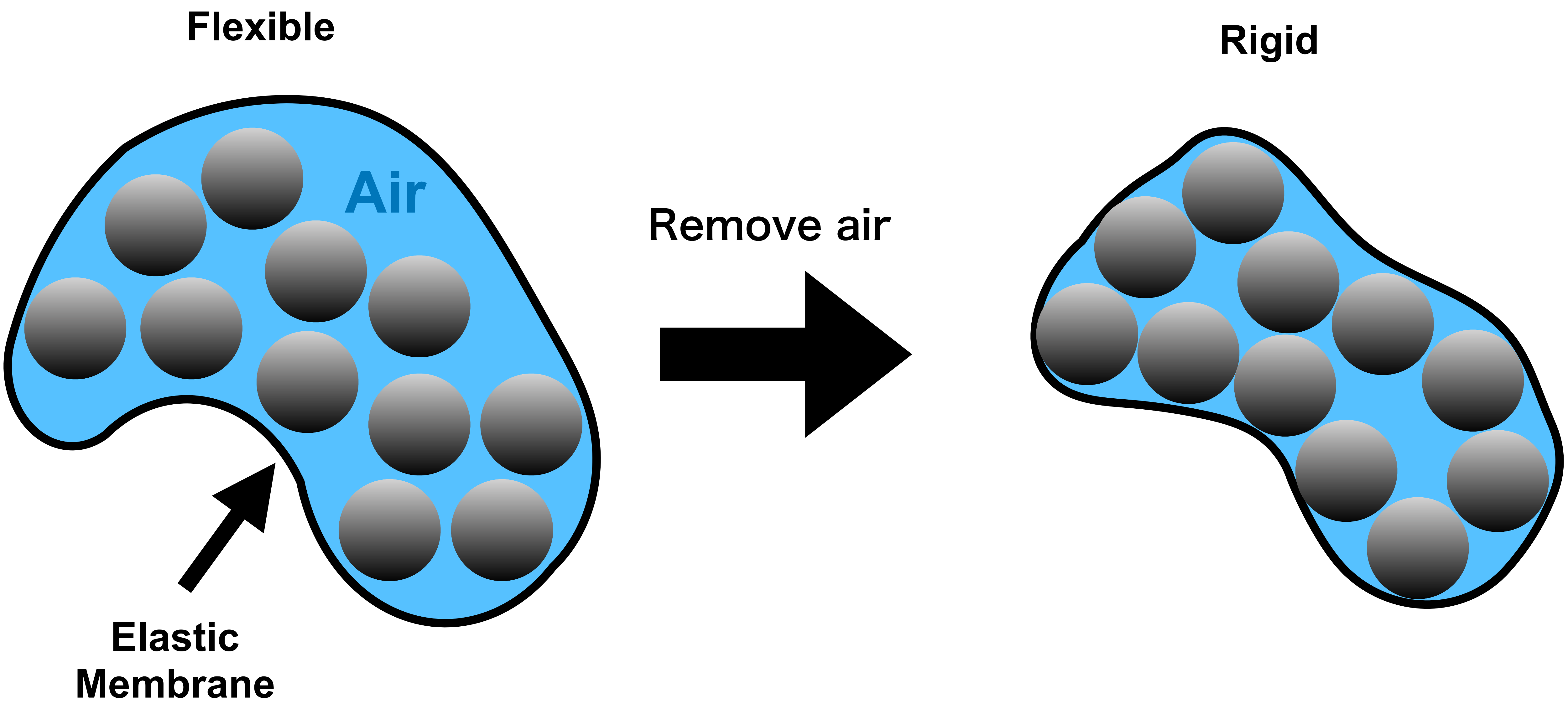


The jamming transition is a phase transition from solid to liquid at zero temperature

Introduction

Related phenomena

“Soft” robot



Introduction

Related phenomena

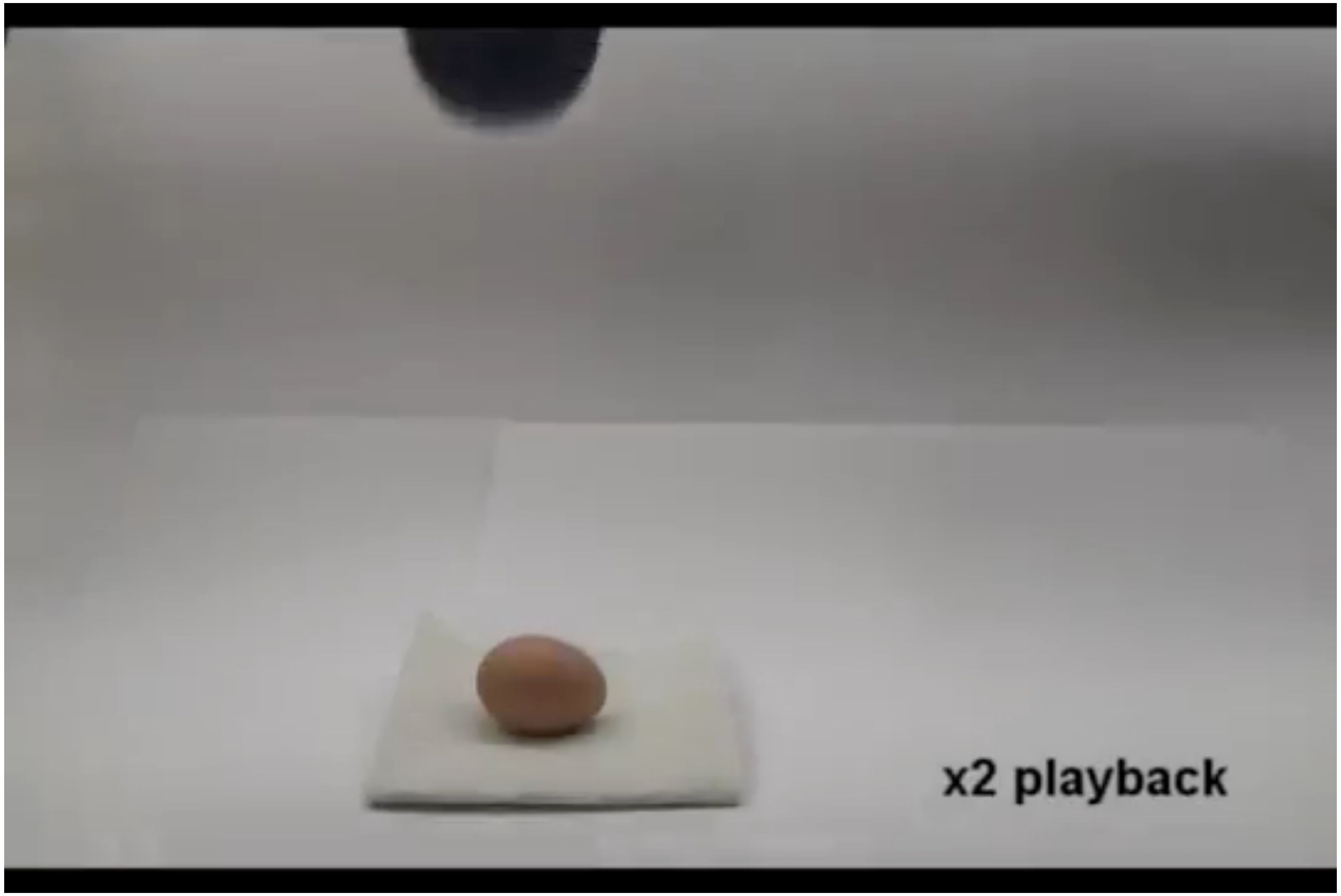
“Soft” robot

Cornell Creative Machines Lab: http://creativemachines.cornell.edu/

Introduction

Related phenomena

"Soft" robot



Cornell Creative Machines Lab: http://creativemachines.cornell.edu/

Introduction

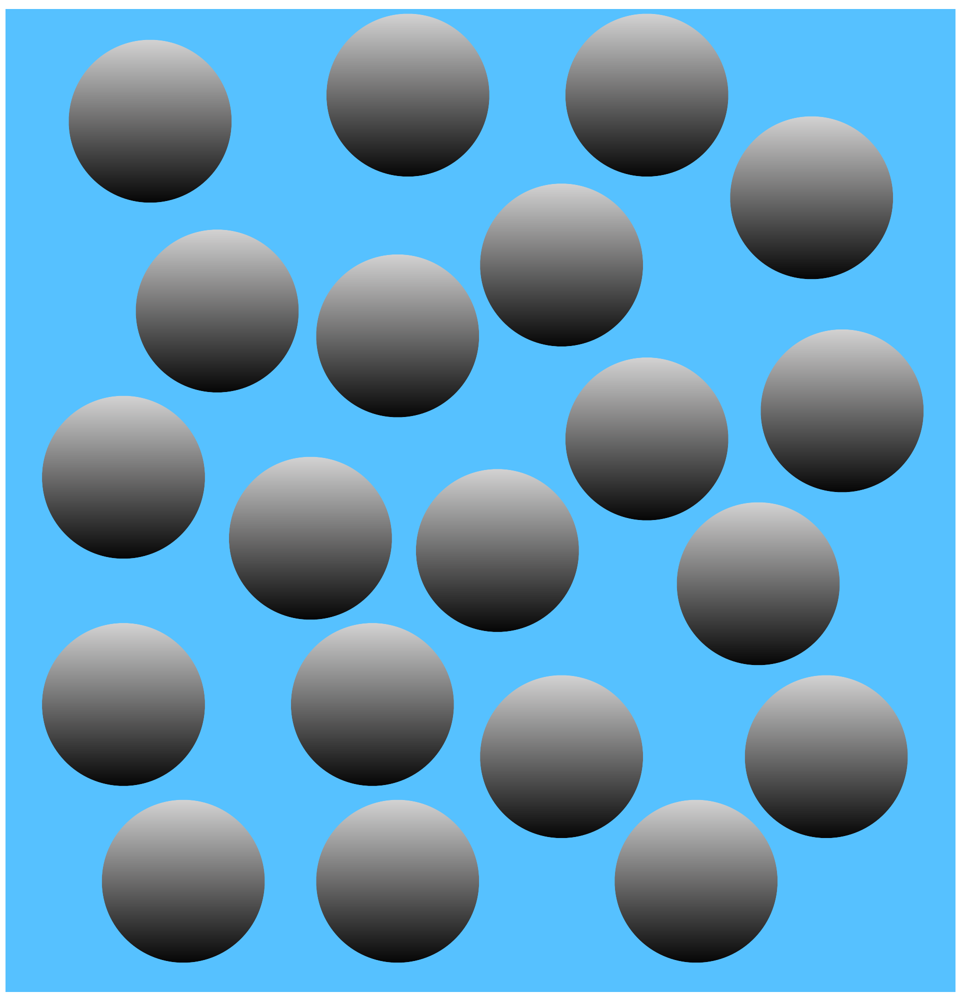
Related phenomena

Dilatancy (shear thickening)

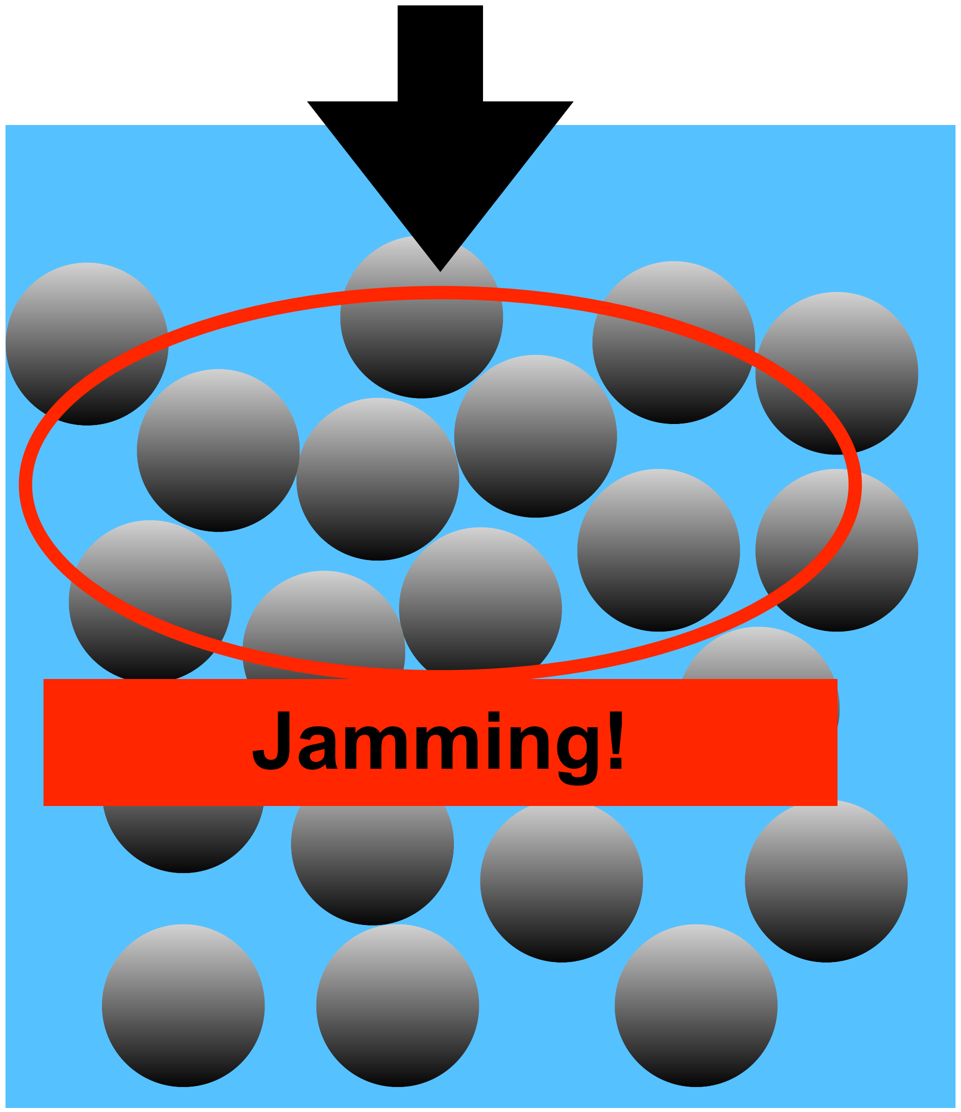
Introduction

Related phenomena

Dilatancy (shear thickening)



Without external force



External force induces the jamming transition

Outline

- Introduction
- Jamming of spherical particles
- Jamming of non-spherical particles

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Spherical particles

Motivation

Granular particles have complex shapes.

M&M Candies

Sand & rock

Grains

Snow powders

Spherical particles

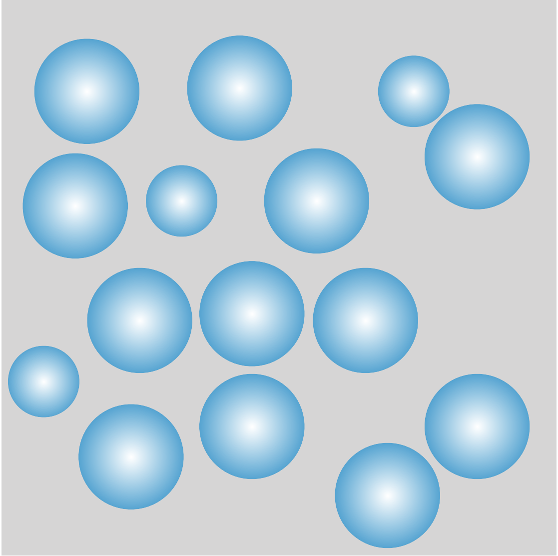
Motivation

To simplify the problem, we consider spherical particles

M&M Candies

Sand & rock

Grains

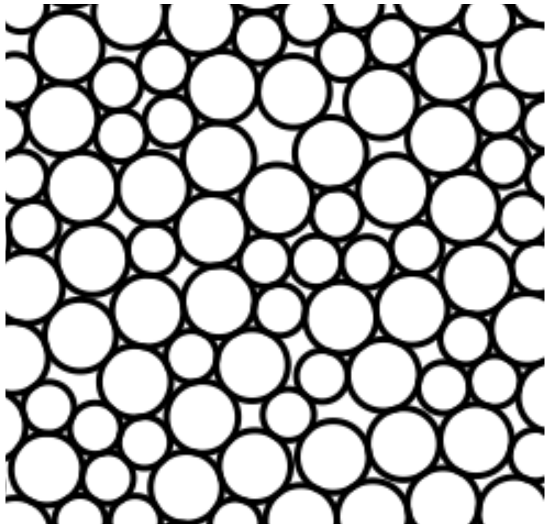


spherical particles

Spherical particles

Motivation

metallic balls



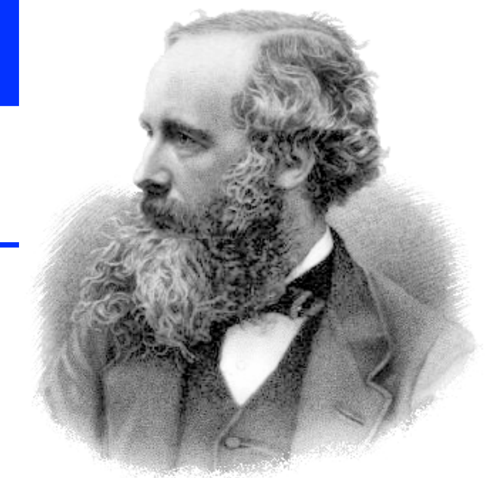
hard spheres (simulation)

Mables

For frictionless spherical particle
The jamming occurs at $\varphi_J \sim 0.64$

Spherical particles

Contact number



J. C. Maxwell
1831-1879

Simple stability argument by Maxwell

\# of constraints > # of degree of freedom

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

\# of degree of freedom = Nd

N: # of particles
z: # of contacts per particle
d: spatial dimensions

$$z > 2d$$

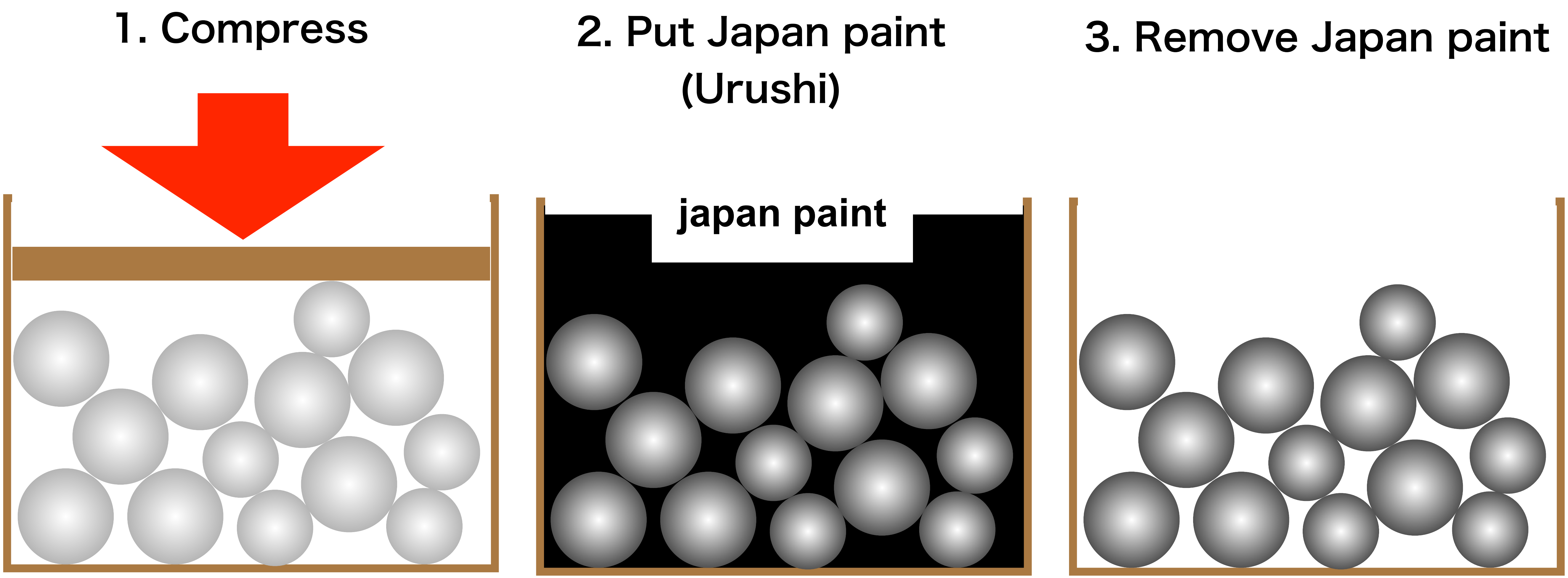
Transition may occur at $z_J = 2d$

Spherical particles

Contact number

J. Bernal and J. Mason (1960)

Experiment

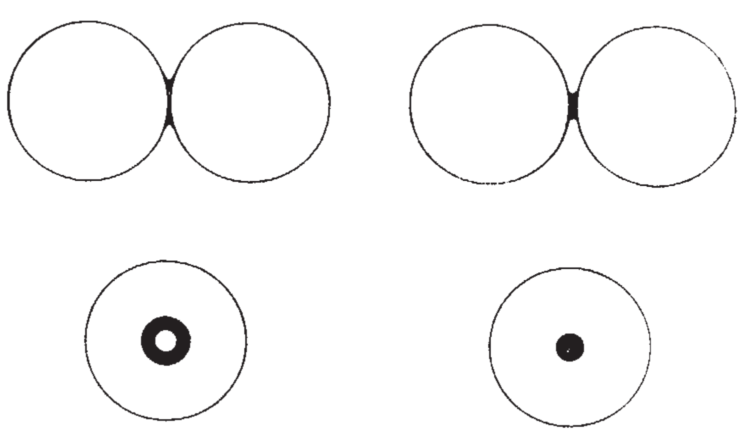


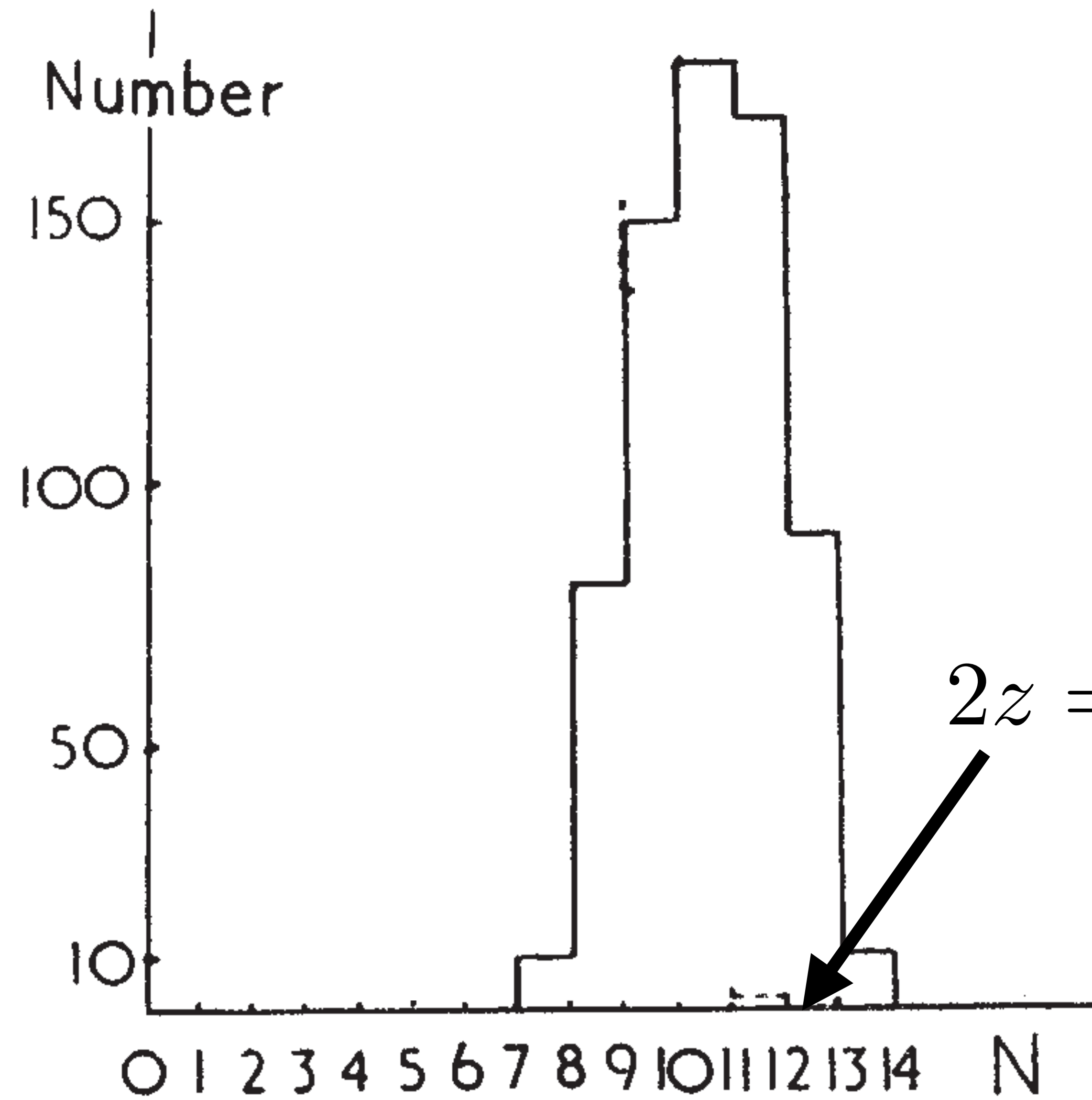
Spherical particles

Contact number

J. Bernal and J. Mason (1960)

N= 500
metallic balls painted
with black japan paint





$$2z = 4d = 12$$

$$2z$$

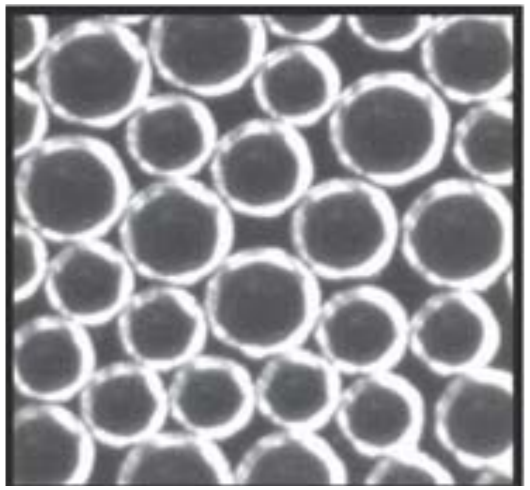
Spherical particles

Contact number

Simulation

Harmonic potential

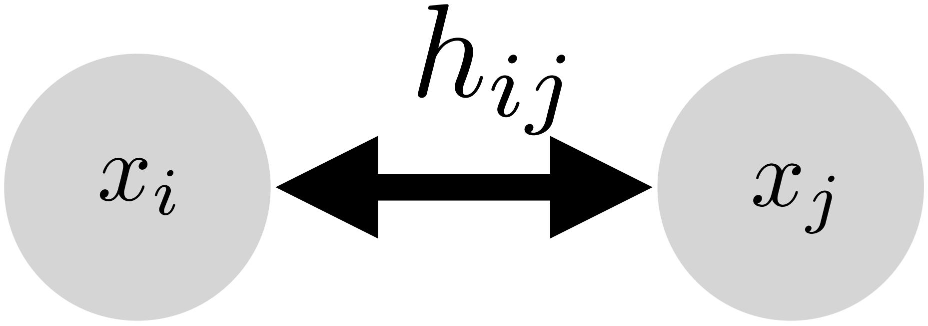
$$E = \sum_{i<j} v(h_{ij}) = \frac{\varepsilon}{2} \sum_{i<j} h_{ij}^2 \theta(-h_{ij})$$



Wet foams

Gap function

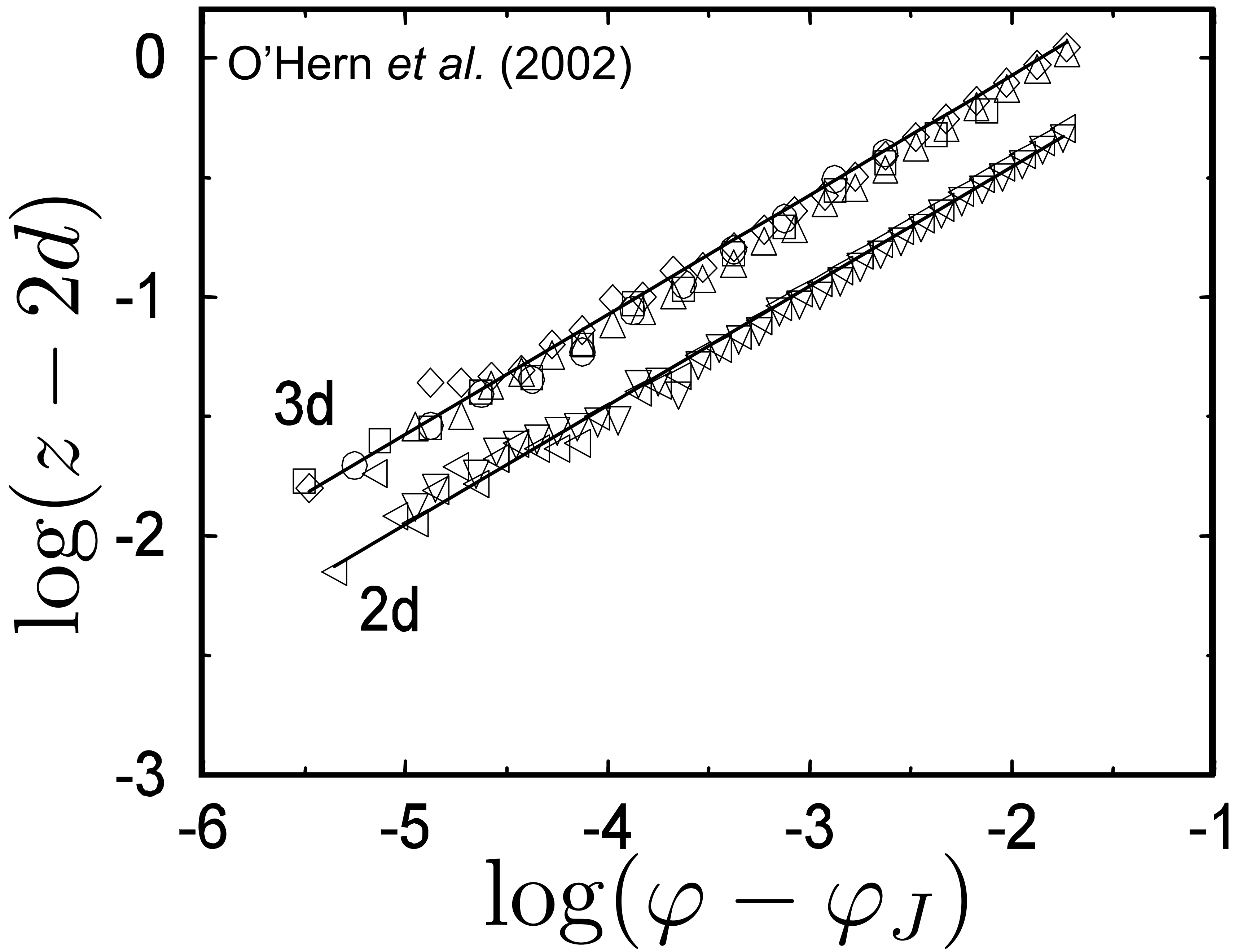
$$h_{ij} = |x_i - x_j| - \sigma_{ij}$$



Spherical particles

Power-law

Contact number of hard spheres

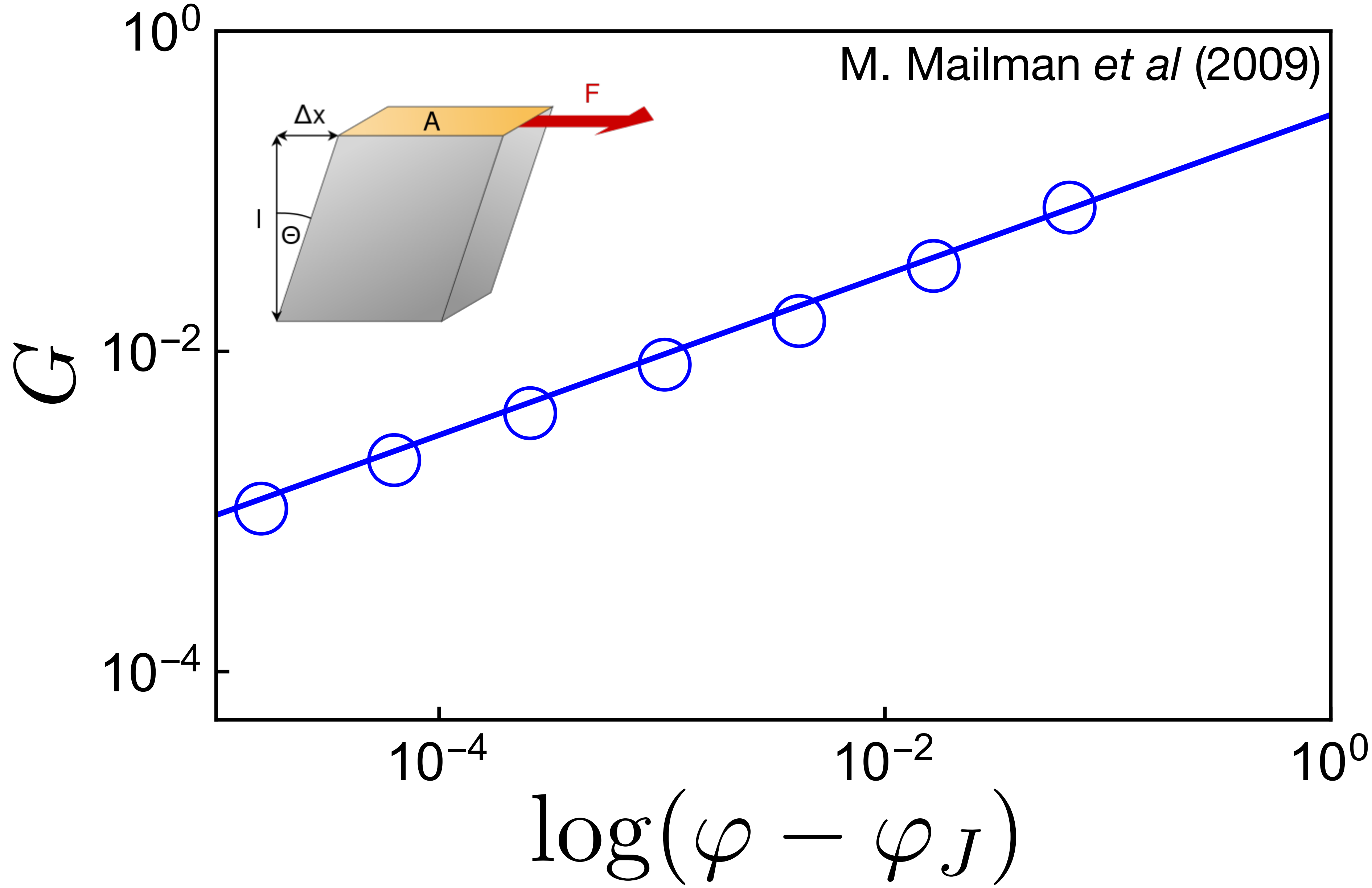


Scaling $z - 2d \sim (\varphi - \varphi_J)^{1/2}$

Spherical particles

Power-law

Shear modulus of harmonic spheres

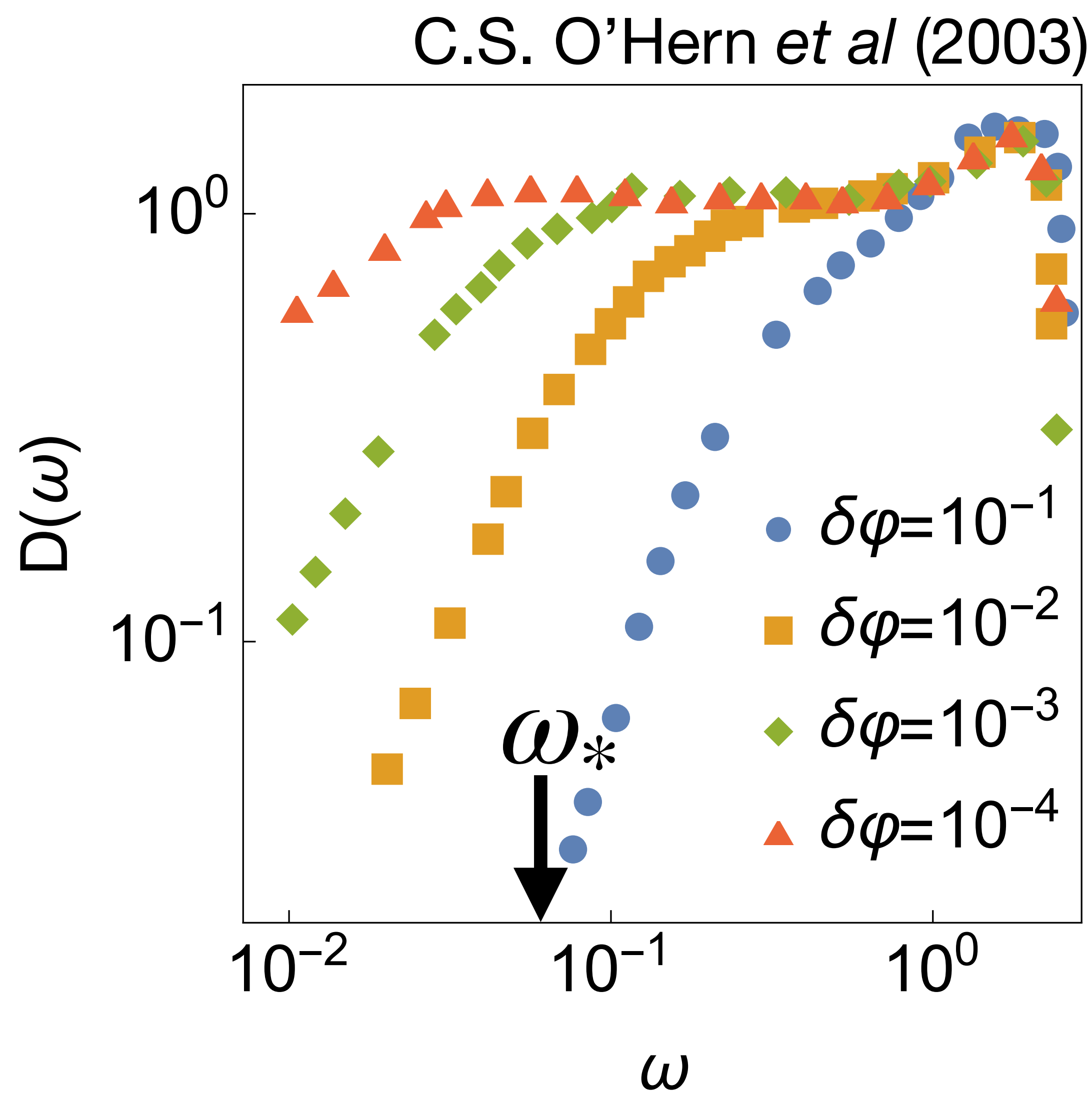


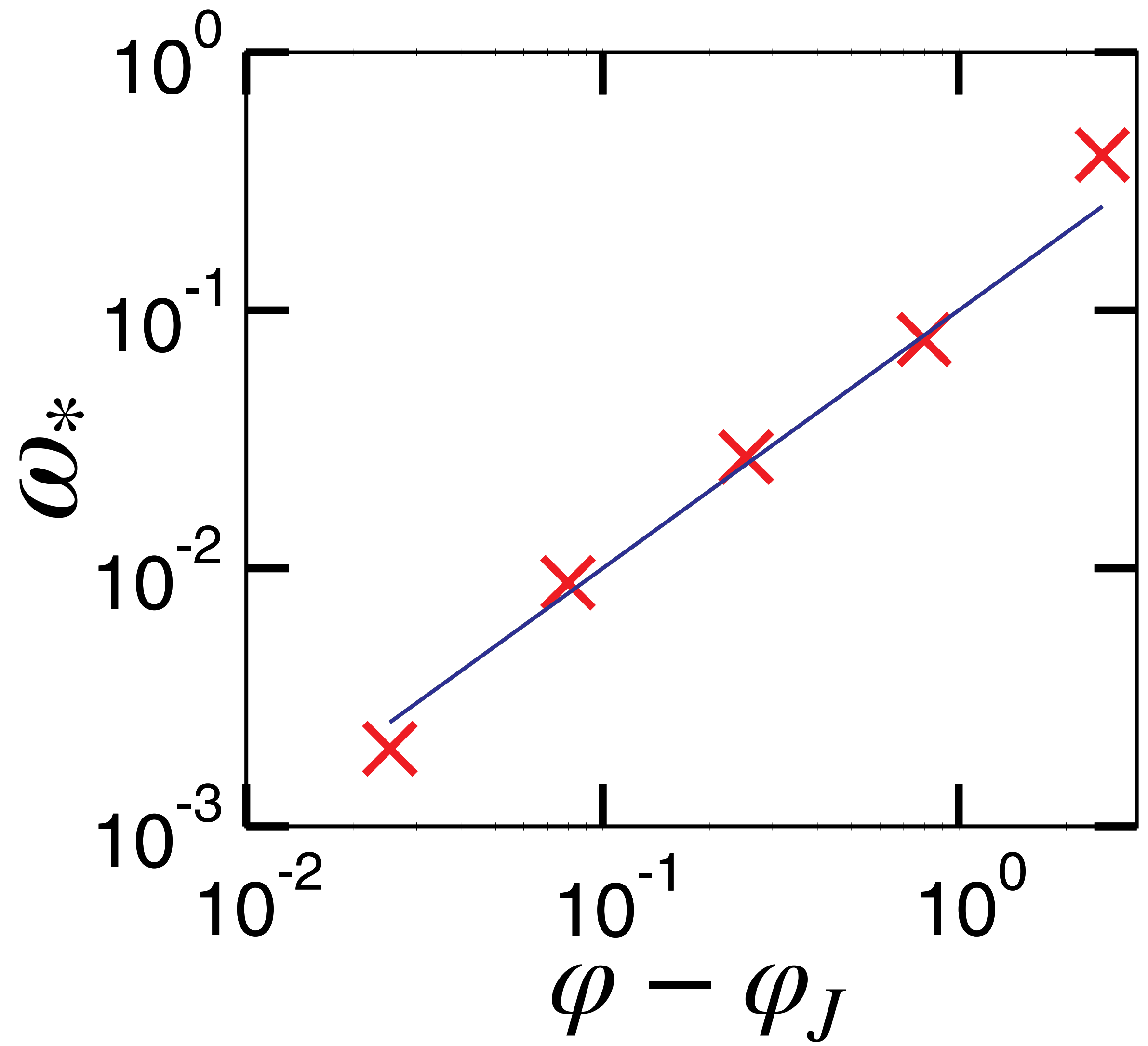
Scaling $G \sim (\varphi - \varphi_J)^{1/2}$

Spherical particles

Power-law

Scaling of the vibrational density of states





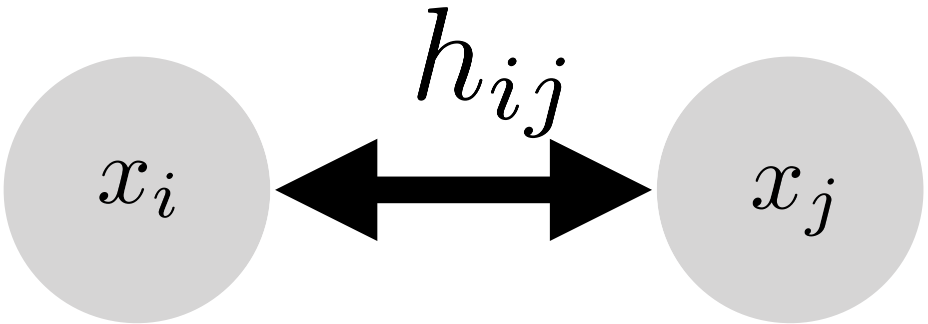
Scaling $\omega_* \sim (\varphi - \varphi_J)^{1/2}$

Spherical particles

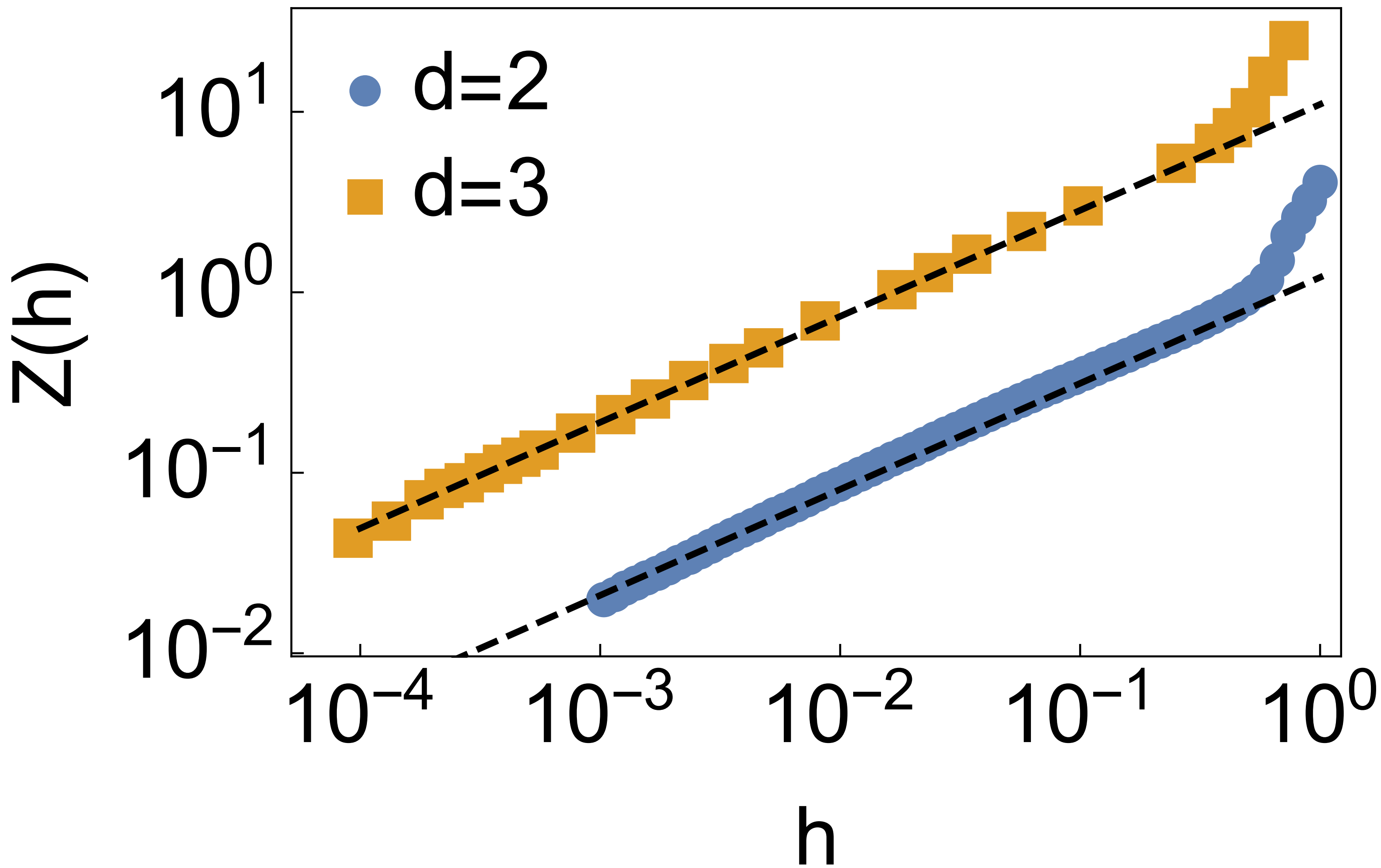
Power-law

Gap distribution function

$$g(h) = \frac{1}{N_c} \sum_{i<j} \delta(h_{ij} - h),\ Z(h) = \int_0^h dh' g(h')$$



P. Charbonneau *et al.* (2014)



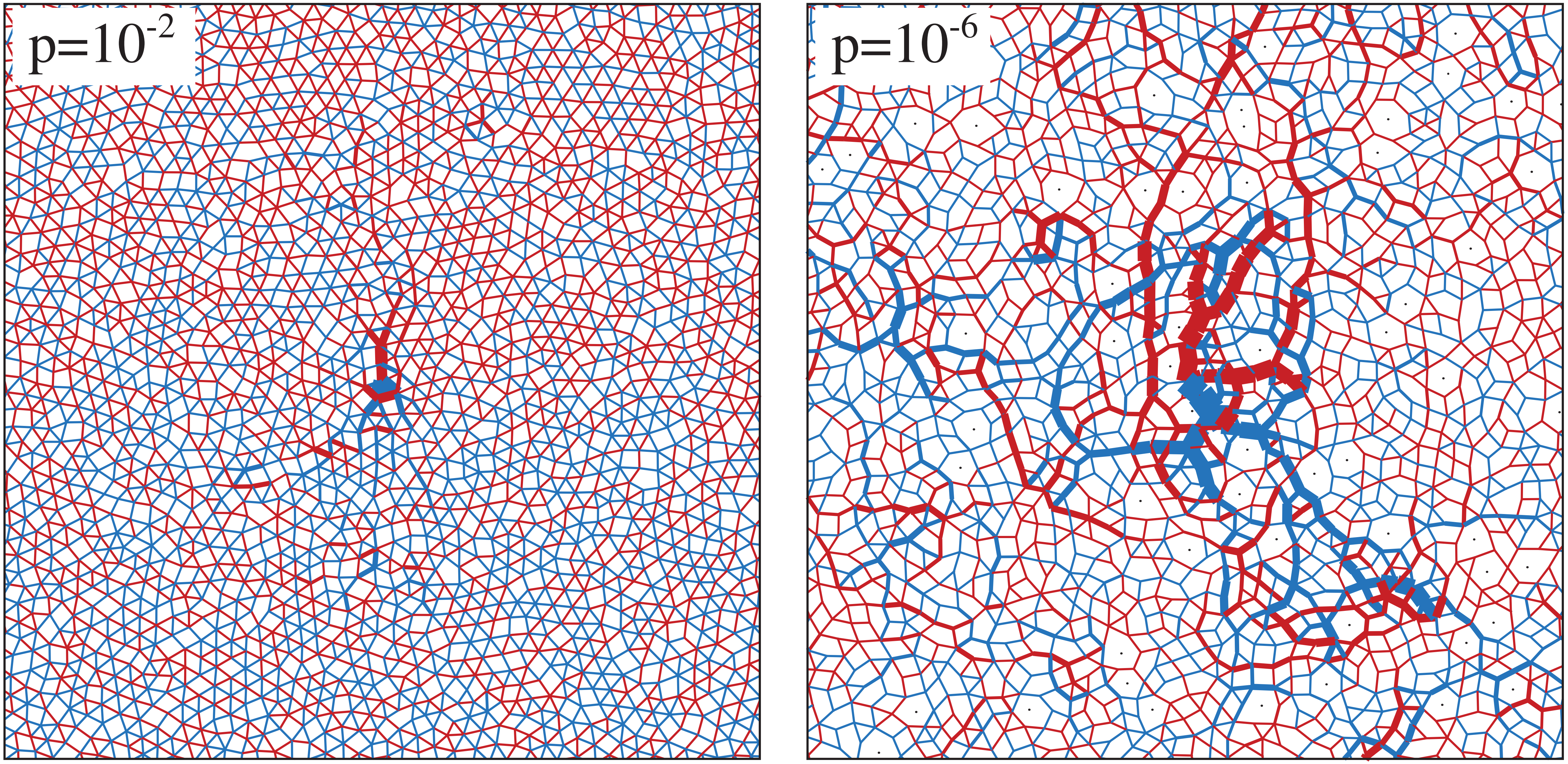
Scaling $g(h) \sim h^{-\gamma},\ \gamma = 0.41$

Spherical particles

Power-law

W. G. Ellenbroek *et al.* (2006)

Far from the jamming transition point **Near the jamming transition point**



Correlation length $\xi \sim (\varphi - \varphi_J)^{-1/4}$

E. Lernar *et al.* (2015), M. Shimada *et al.* (2019)

Spherical particles

Summary

Several physical quantities exhibit the power-low behavior

Contact number	$z - 2d \sim \delta\varphi^{1/2}$
Shear modulus	$G \sim \delta\varphi^{1/2}$
Correlation length	$\xi \sim \delta\varphi^{-1/4}$
Pair correlation	$\gamma = 0.41,\ \mu = \dfrac{1}{1-\gamma}$ $g(h) \sim \begin{cases} \delta\varphi^{-\mu\gamma}(h \ll \delta\varphi^{\mu}) \\ h^{-\gamma} \quad (h \gg \delta\varphi^{\mu}) \end{cases}$

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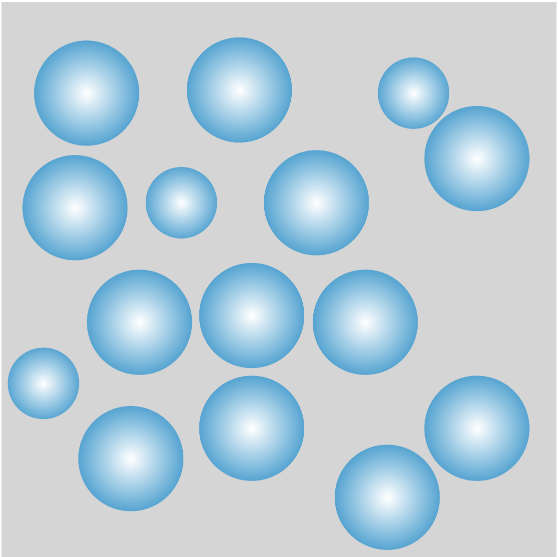
Non-spherical particles

Motivation



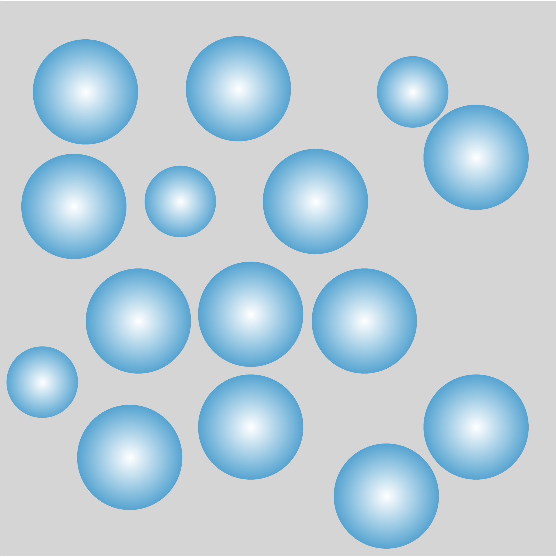
Spherical particles

Non-spherical particles

Motivation

Sand & rock

Snow powders



Spherical particles

Grains

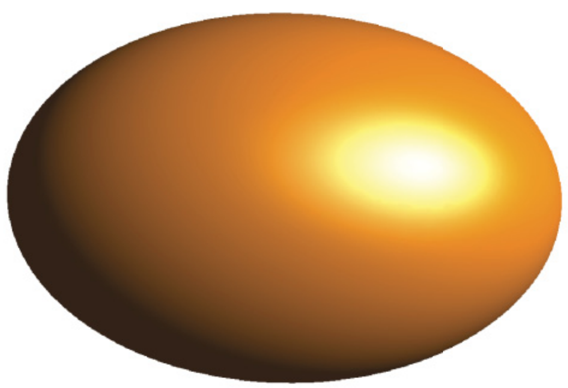
M&M Candies

However, in most cases, the constituent particles are **non-spherical**.

Non-spherical particles

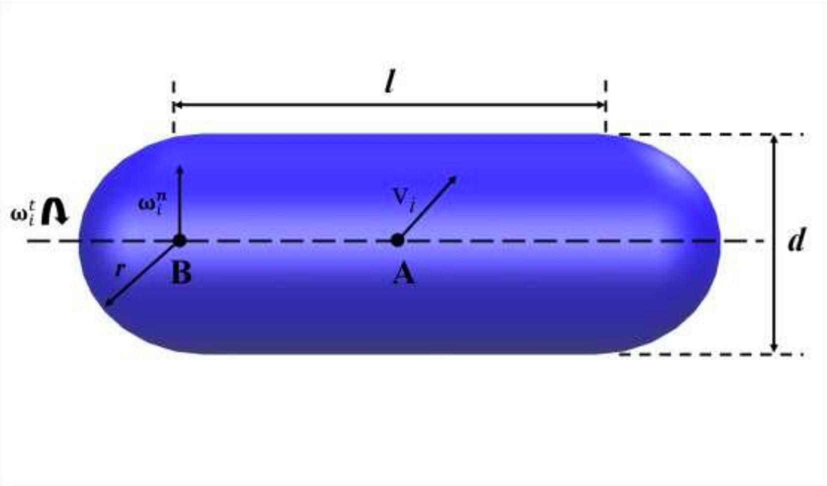
Previous numerical studies

Ellipsoid



A. Donev *et al* (2007)
M. Mailman *et al* (2009)
C. F. Schreck et al. (2010, 2012)

Sphero-cylinder



T. Marschall and S. Teitel (2018)

Other shapes

???

Purpose of this study

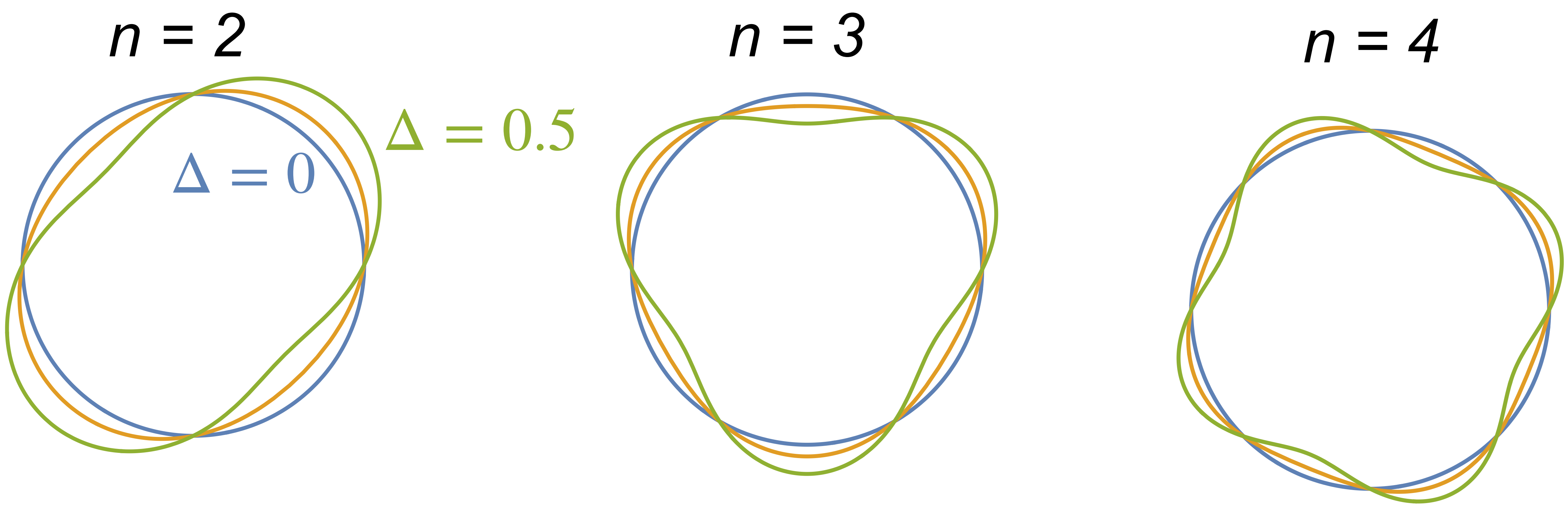
Systematic investigation of various shapers of particles

Non-spherical particles

Model

Radius of a particle

$$R_i(\theta) = R_i^0\left(1 + F_n(\theta)\right),\ F_n(\theta) = \frac{\Delta}{n}\sin(n\theta)$$



We investigate the jamming transitions of various shapes by changing n and Δ systematically.

Non-spherical particles

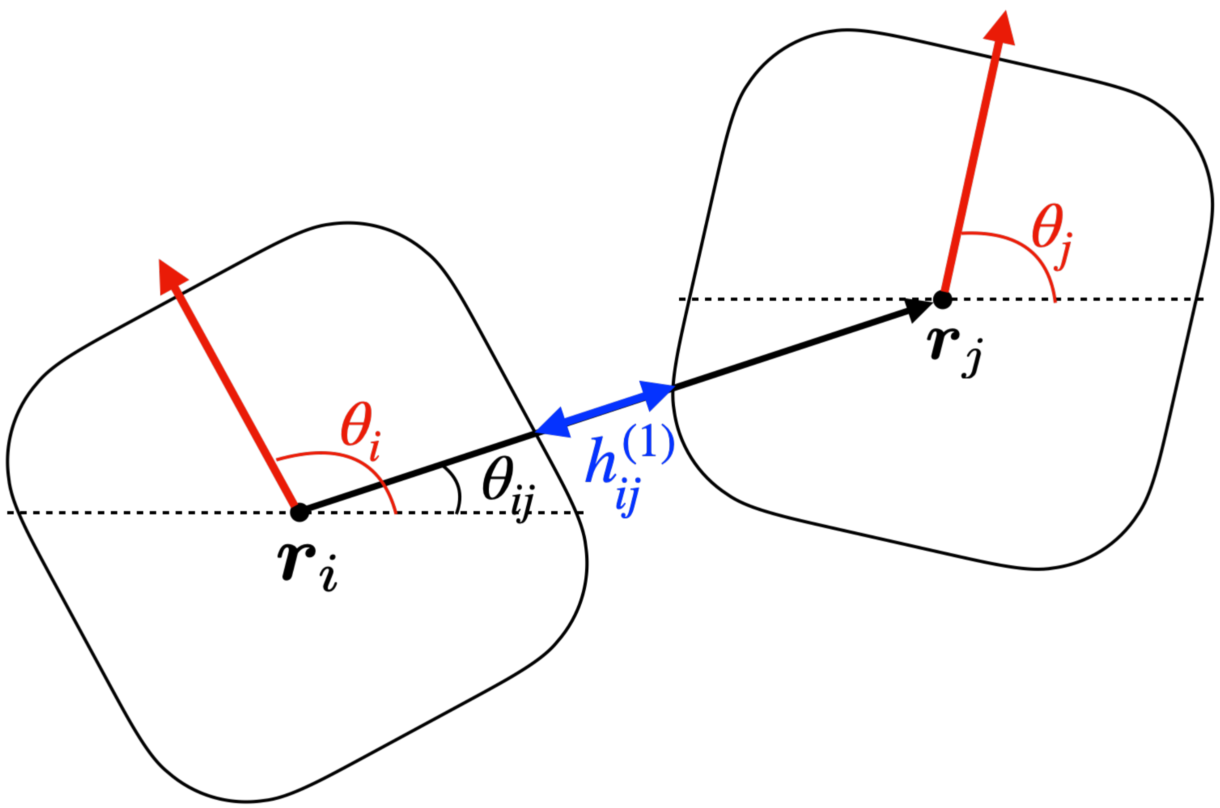
Model

Harmonic potential

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

Gap function: the minimal distance between two particles

For nearly spherical particles, we can derive an analytic form by using a perturbation w.r.t Δ.



Small Δ expansion

$$h_{ij} = h_{ij}^{(1)} + O(\Delta^2),$$

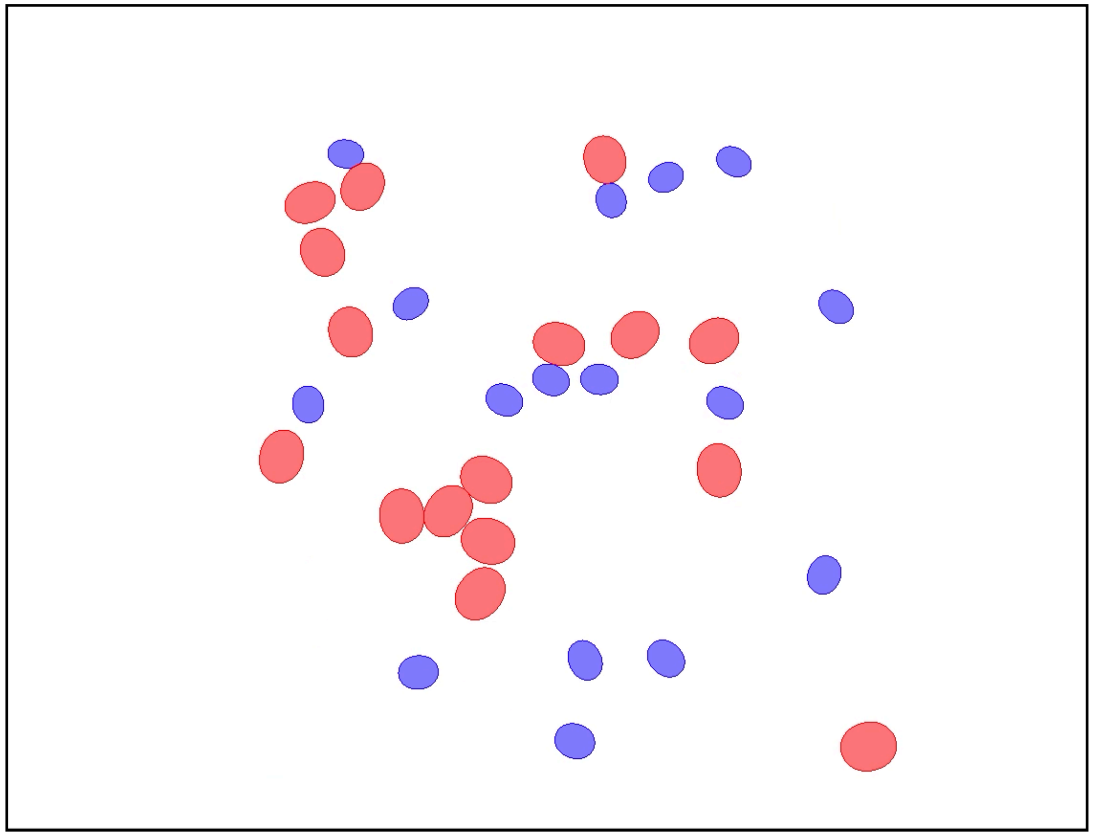
$$h_{ij}^{(1)} = |\boldsymbol{r}_i - \boldsymbol{r}_j| - R_i^0 - R_j^0$$
$$- \Delta\left[R_i^0 F_n(\theta_i - \theta_{ij}) + R_j^0 F_n(\theta_j - \theta_{ji})\right]$$

Non-spherical particles

Numerics

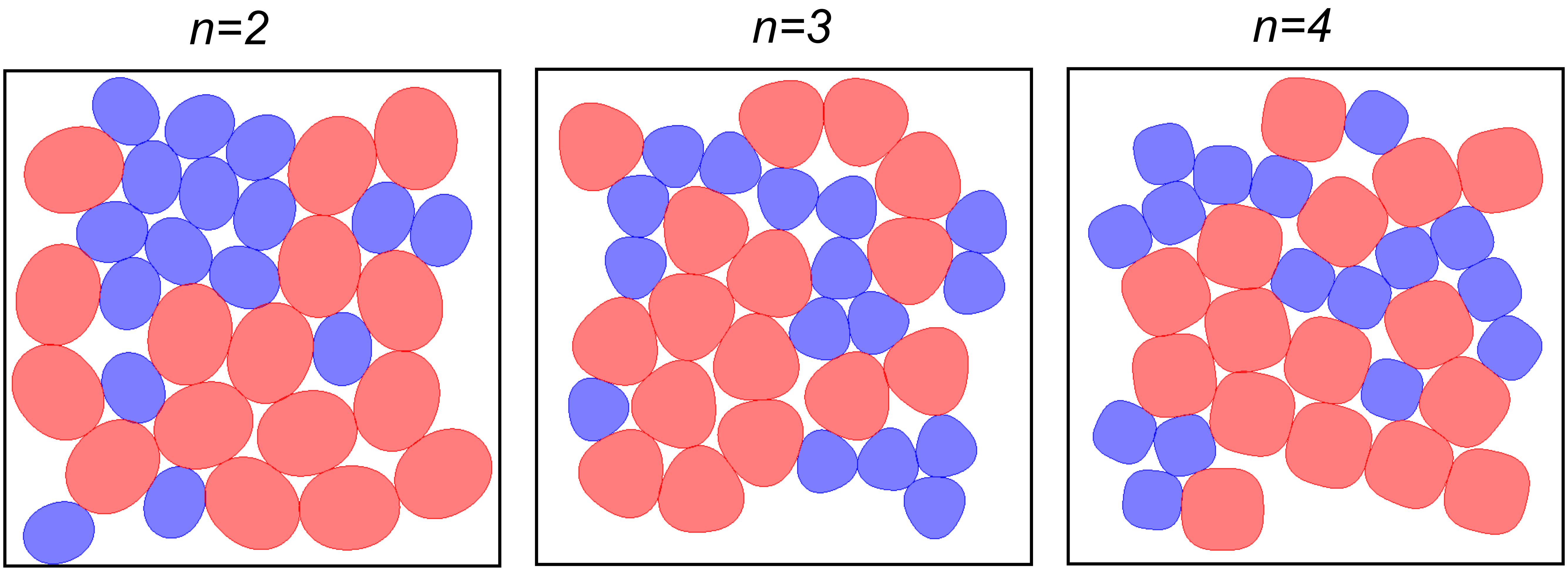
Algorithm

1. Start from a random configuration.
2. Increase the packing fraction $\varphi \rightarrow \varphi+\delta\varphi$.
3. Remove contact by the energy minimization.
4. Repeat 2 and 3 until the jamming transition point.



Non-spherical particles

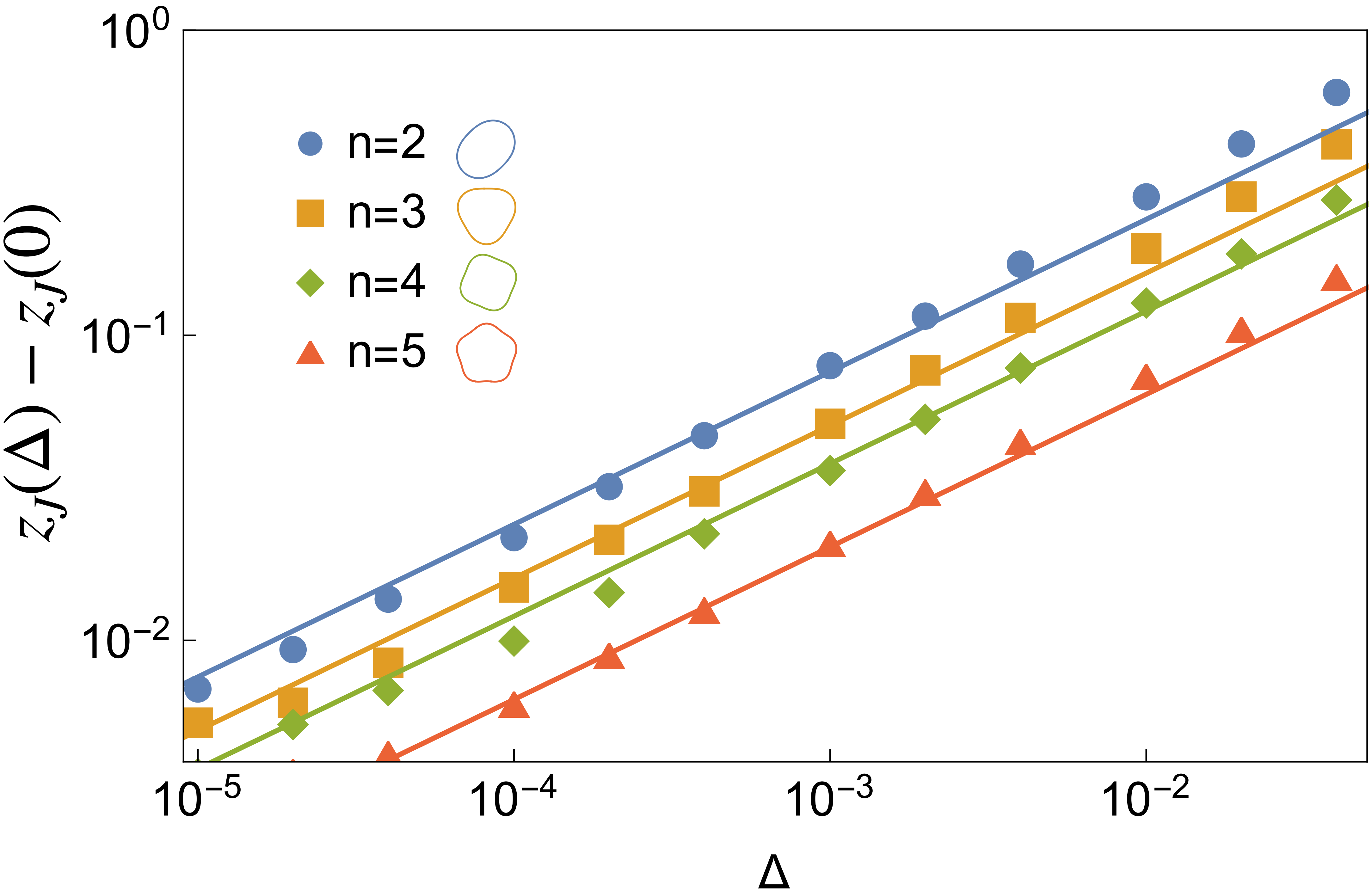
Numerics



We focus on the configurations at the jamming transition point.

Non-spherical particles

Contact number

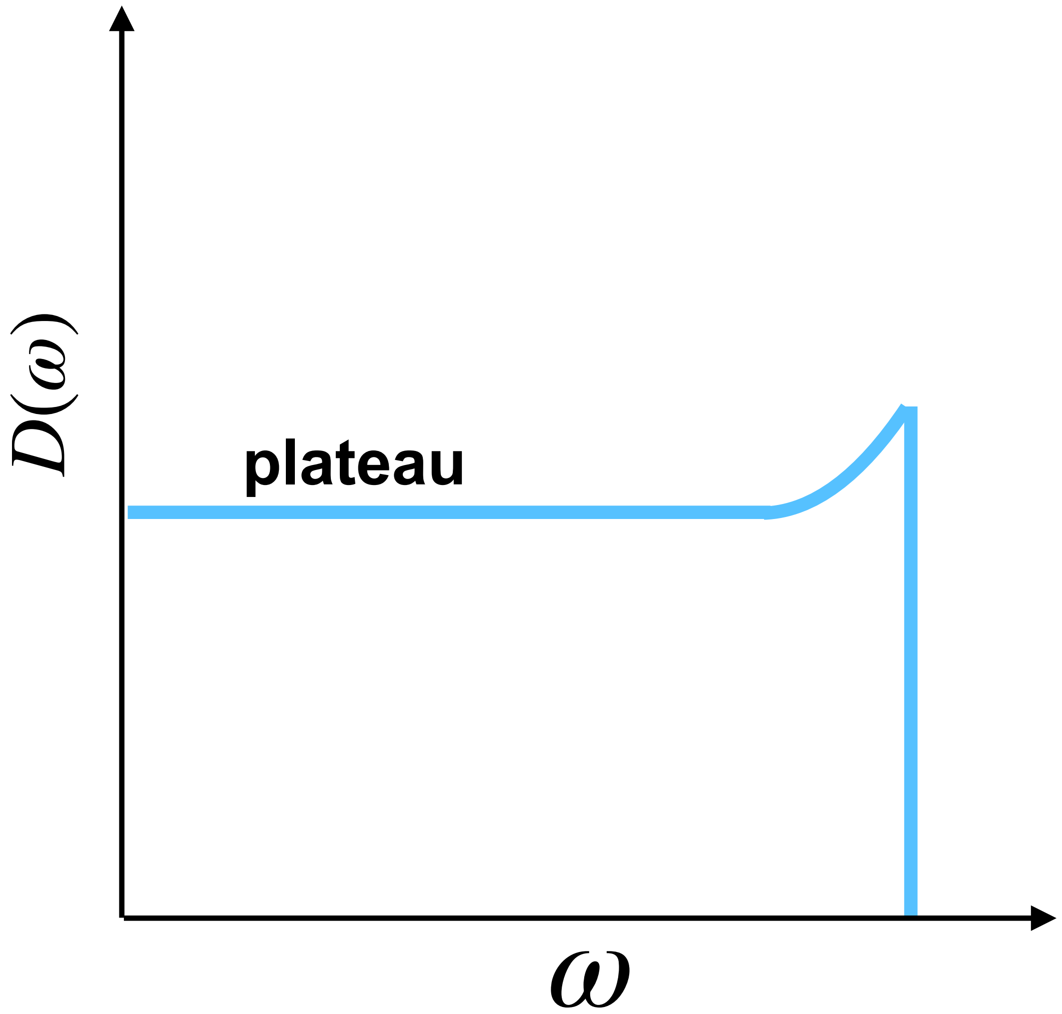


The contact number increases with the aspect ratio as
$$z_J(\Delta) - z_J(0) \sim \Delta^{1/2}$$

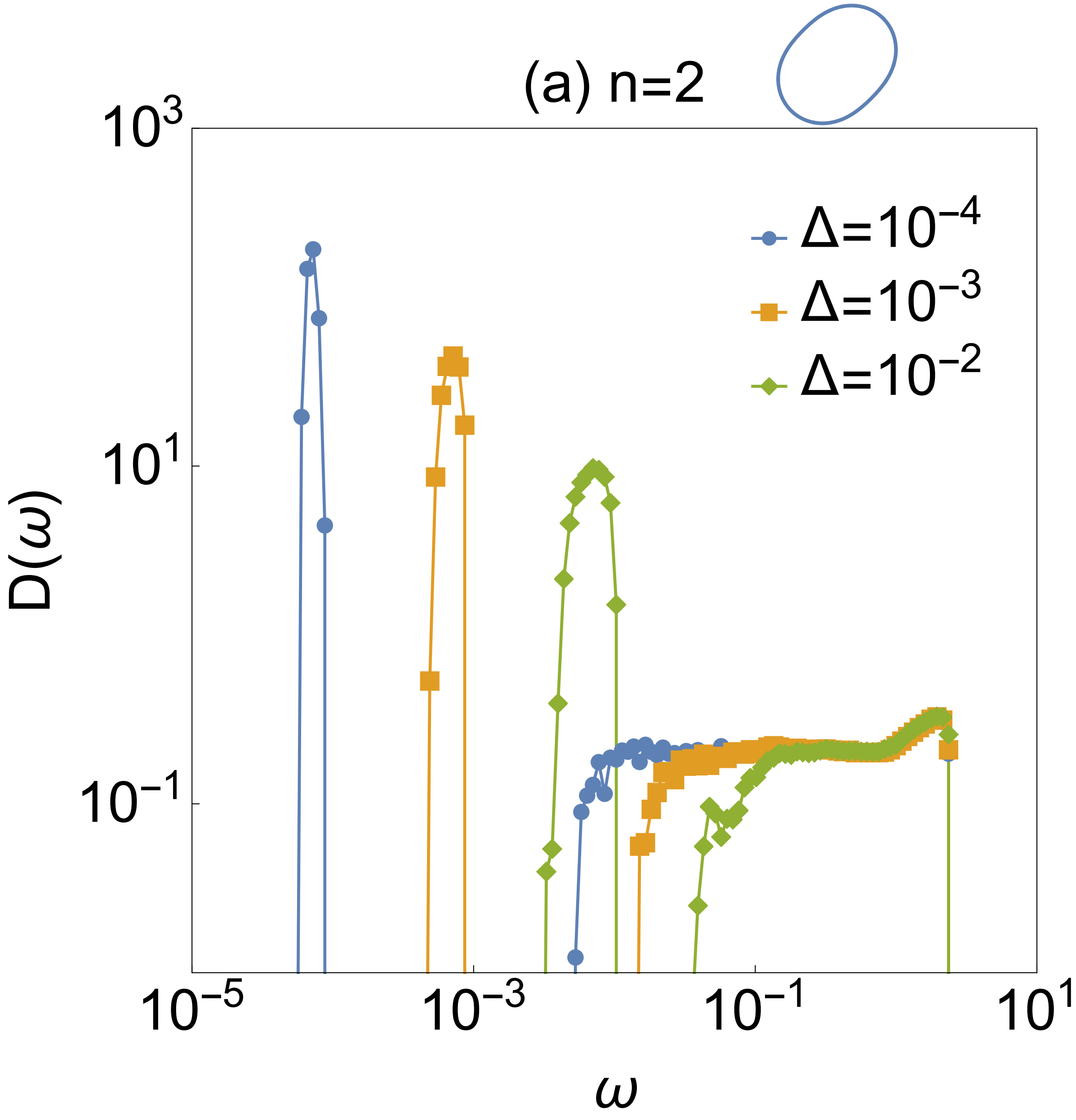
Non-spherical particles

Vibrational density of states

Spherical (at jamming)



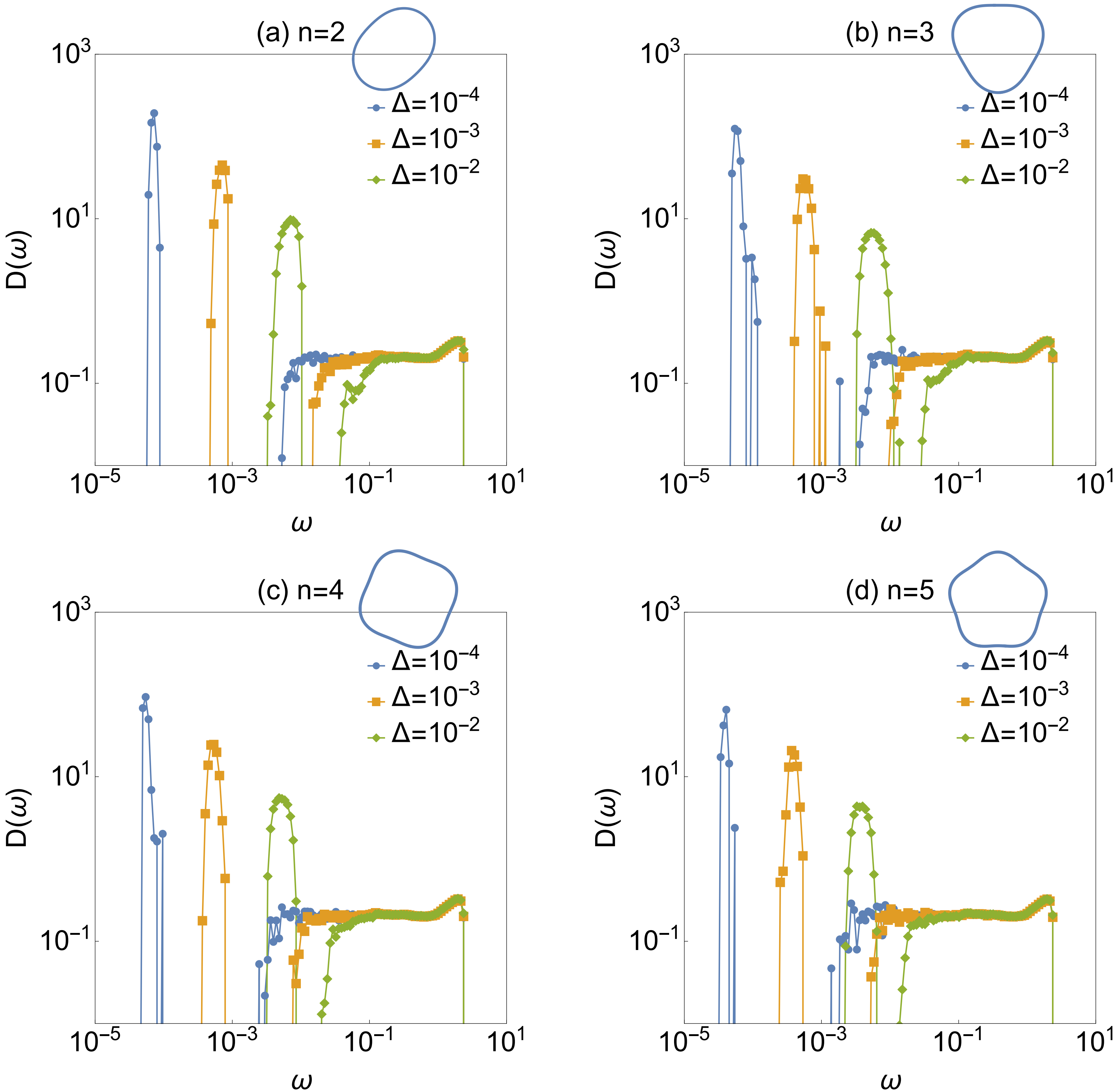
Non-spherical



vDOS of non-spherical particles is gapped!

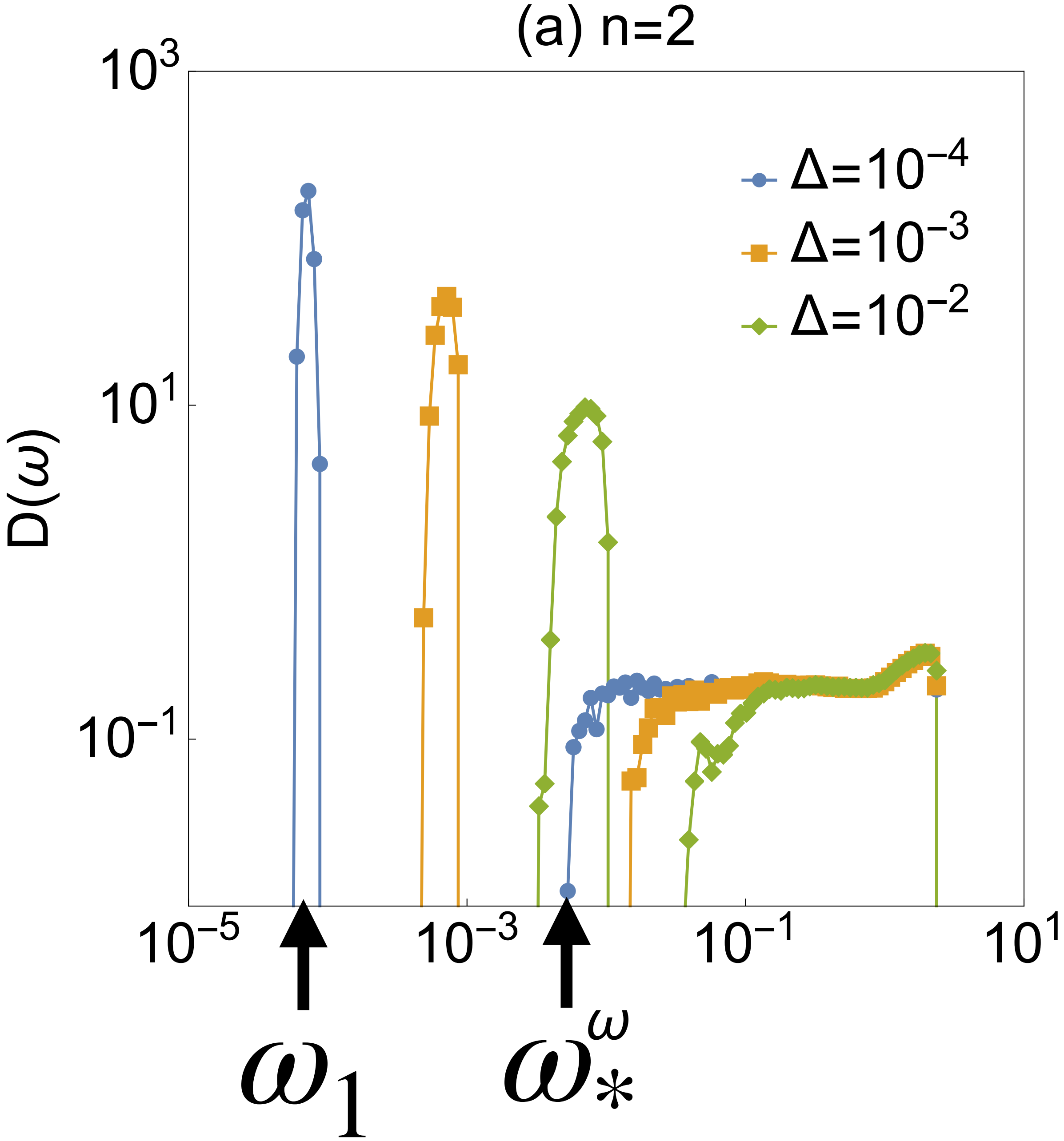
Non-spherical particles

Vibrational density of states

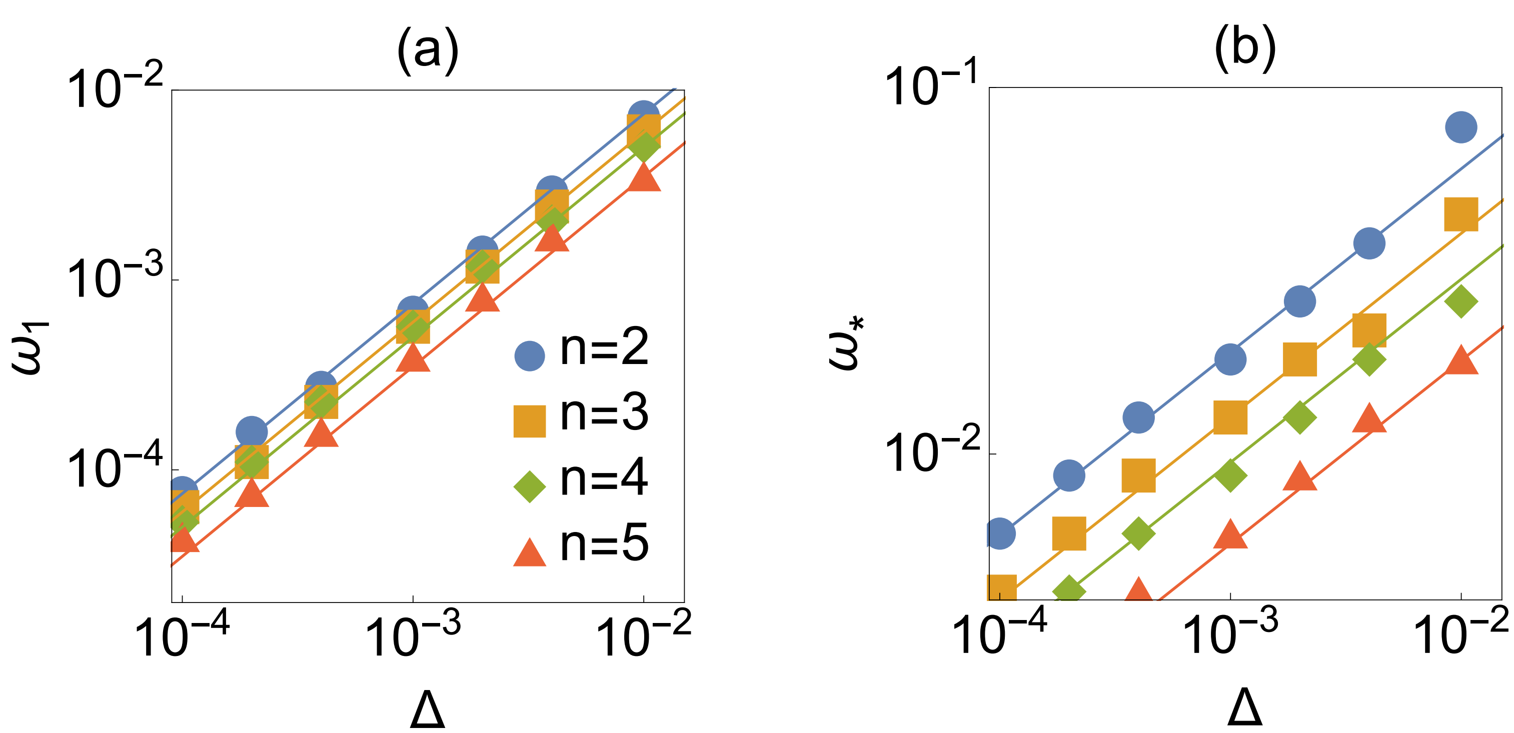


Non-spherical particles

Vibrational density of states



Scalings of characteristic frequencies



Scalings of characteristic frequencies

$$\omega_1 \sim \Delta,\ \omega_* \sim \Delta^{1/2}$$

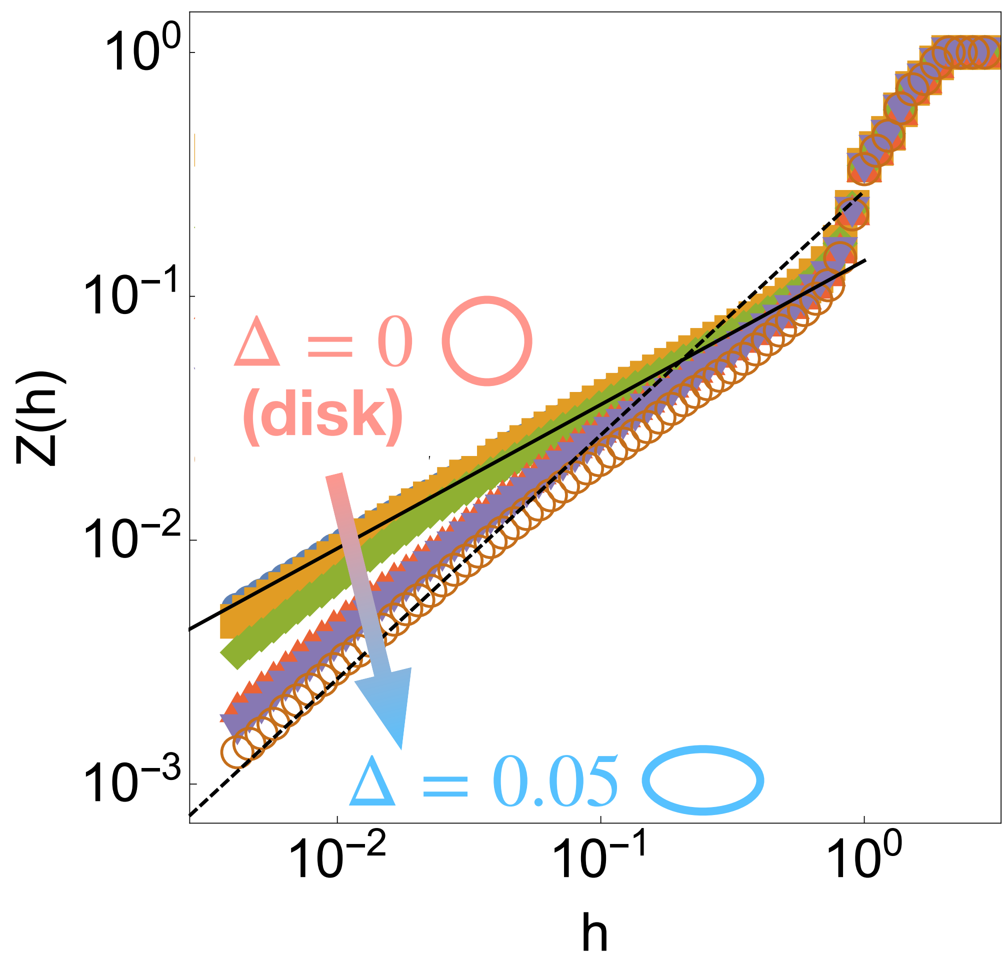
Non-spherical particles

Gap distribution

Cumulative distribution function

$$Z(h) = \int_0^h dh g(h), \; (g(h) \sim h^{-\gamma} \rightarrow Z(h) \sim h^{1-\gamma})$$

n=2

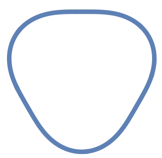
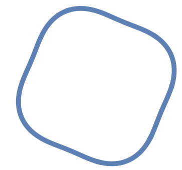
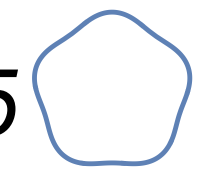


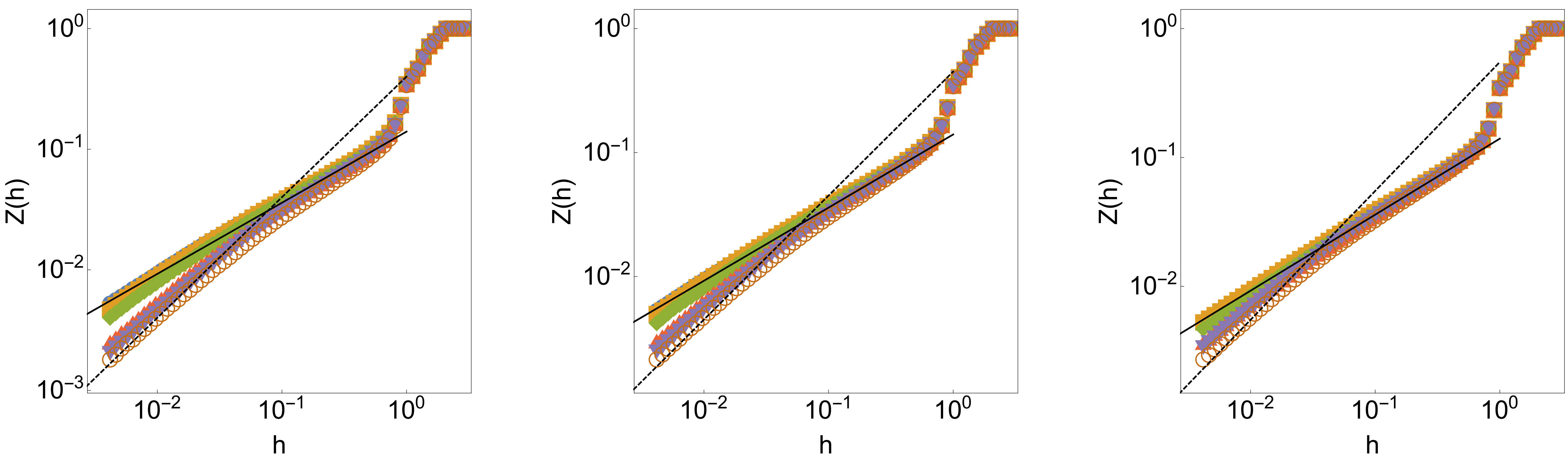
Gap distribution function is finite and regular

$$Z(h) \sim h \rightarrow g(h) \sim const\,.$$

Non-spherical particles

Gap distribution

n=3  *n=4*  *n=5* 



Gap distribution function is finite and regular

$$Z(h) \sim h \rightarrow g(h) \sim const\,.$$

Discussion

Spherical vs non-spherical

Spherical particles (near jamming)

$$z(\varphi) - 2d \sim \delta\varphi^{1/2}$$

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

$$g(h) \sim \begin{cases} \delta\varphi^{-\mu\gamma} (h \ll \delta\varphi^{\mu}) \\ h^{-\gamma} \quad (h \gg \delta\varphi^{\mu}) \end{cases}$$

Non-spherical (at jamming)

$$z_J - 2d \sim \Delta^{1/2}$$

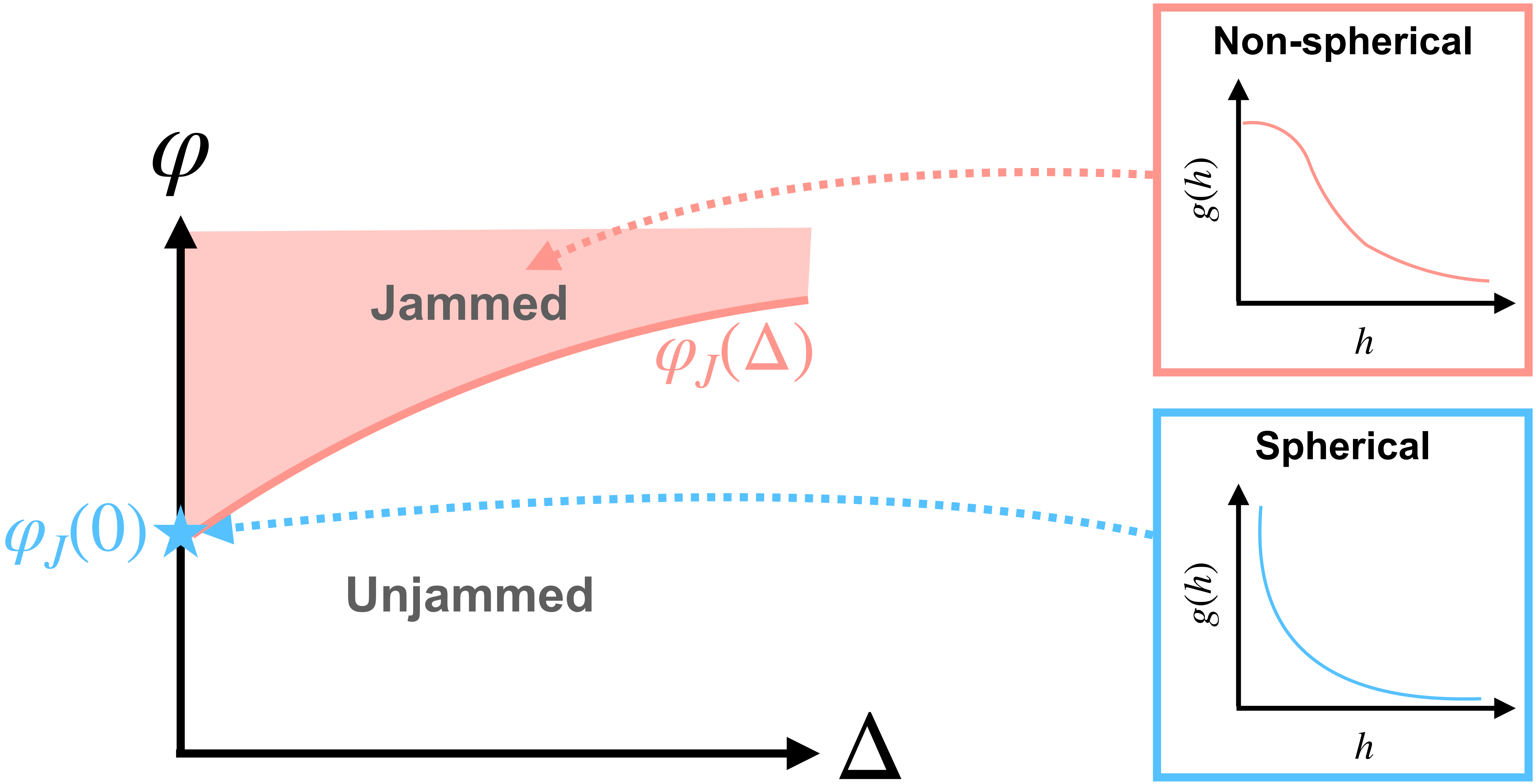
$$\omega_* \sim \Delta^{1/2}$$

$$g(h) \sim \begin{cases} \Delta^{-\mu\gamma} (h \ll \Delta^{\mu}) \\ h^{-\gamma} \quad (h \gg \Delta^{\mu}) \end{cases}$$

Δ plays the same role as δφ !

Discussion

Phase diagram



The jamming transition point of non-spherical particles is not critical in terms of g(r)!!!

Discussion

Summary and Future works

Summary

Deformation = compression

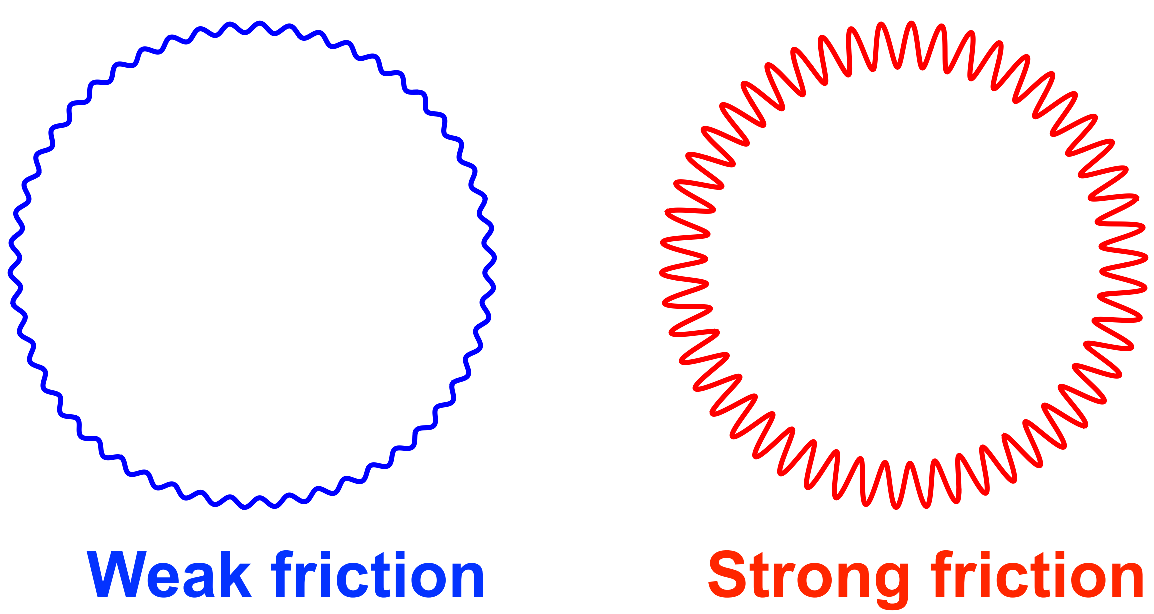
Future works

- Does the correlation length diverge at the jamming transition point of non-spherical particles?
- Investigate scalings above jamming

cf: ellipsoids $G \sim (\varphi - \varphi_J)^1$ $z - z_J \sim (\varphi - \varphi_J)^1$ M. Mailman *et al* (2009), C. F. Schreck et al. (2012)

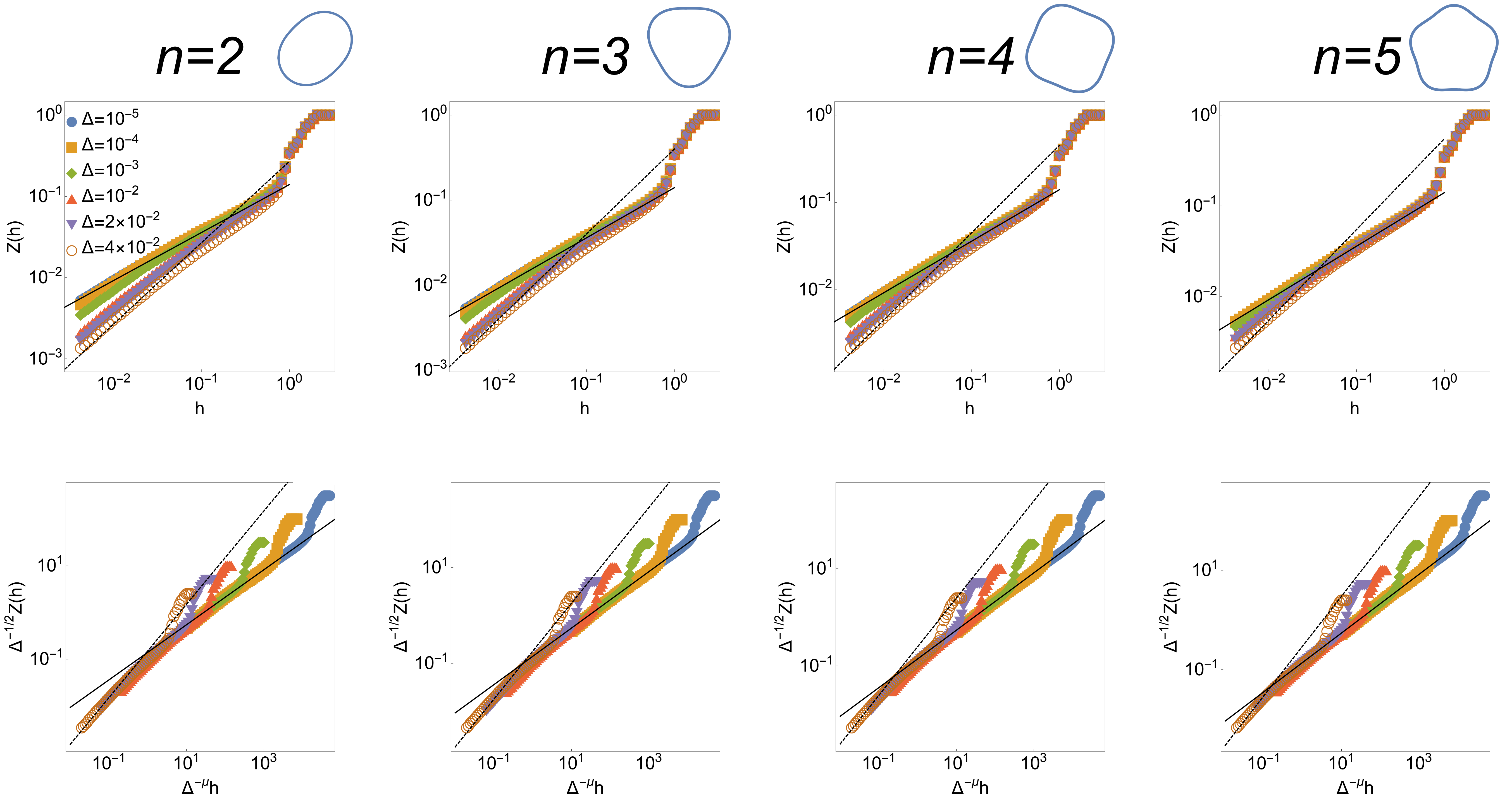
- Investigate scalings below jamming (rheology)
- Geometric friction

H. Ikeda et al. PRL **124**, 208001 (2020)



Non-spherical particles

Gap distribution



Gap distribution function is finite and regular

$$Z(h) \sim h \rightarrow g(h) \sim const\,.$$

Discussion

Spherical vs non-spherical

Spherical particles (near jamming)

$$z(\varphi) - 2d \sim \delta\varphi^{1/2}$$

$$g(h) \sim \begin{cases} \delta\varphi^{-\mu\gamma} (h \ll \delta\varphi^{\mu}) \\ h^{-\gamma} \quad (h \gg \delta\varphi^{\mu}) \end{cases}$$

Non-spherical (at jamming)

$$z_J - 2d \sim \Delta^{1/2}$$

$$g(h) \sim \begin{cases} \Delta^{-\mu\gamma} (h \ll \Delta^{\mu}) \\ h^{-\gamma} \quad (h \gg \Delta^{\mu}) \end{cases}$$

Both the distance from the jamming transition point and deviation from spheres controls the scaling behaviors.

Non-spherical particles

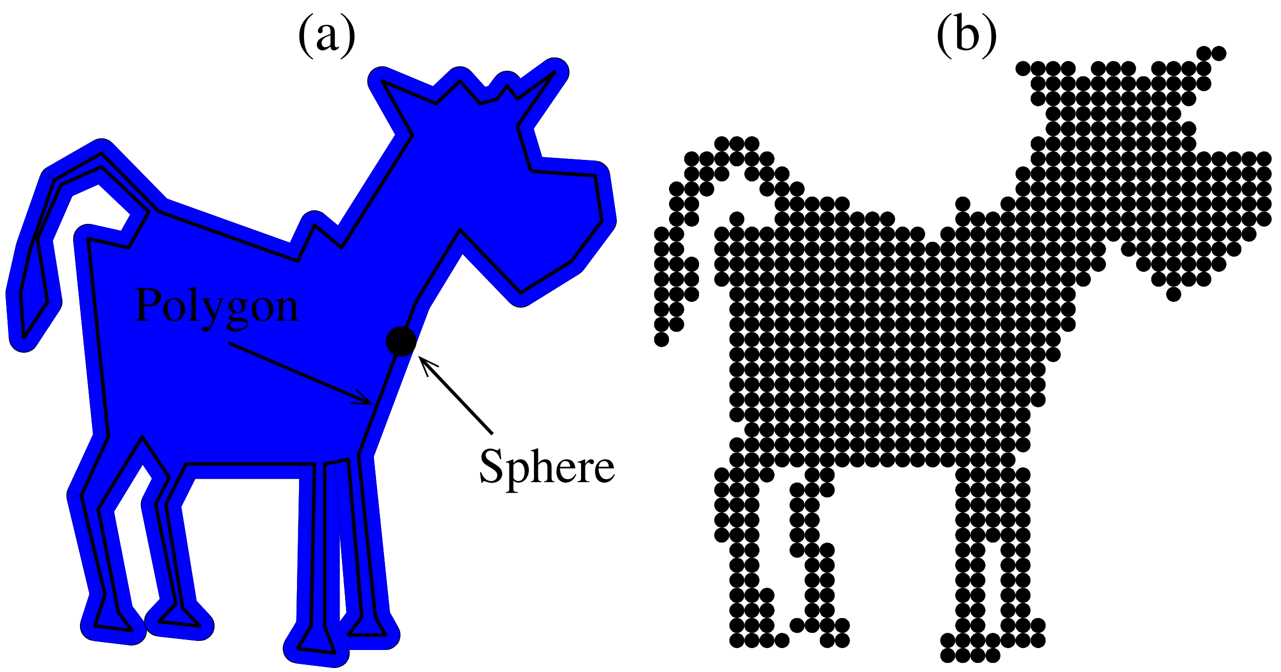
Model

Harmonic potential

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

Gap function: the minimal distance between two particles

For general shapes of non-spherical particles, the calculation of the gap function is not so easy.



F. Alonso-Marroquin (2008)

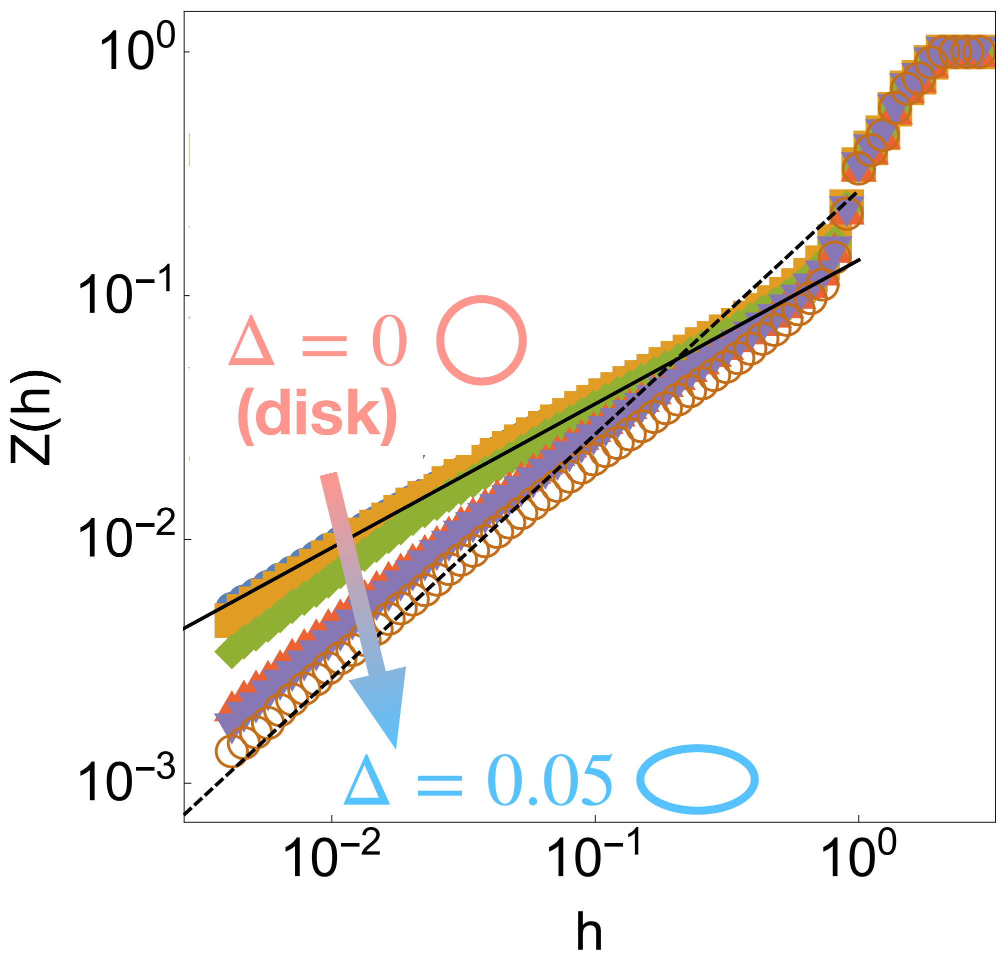
Non-spherical particles

Gap distribution

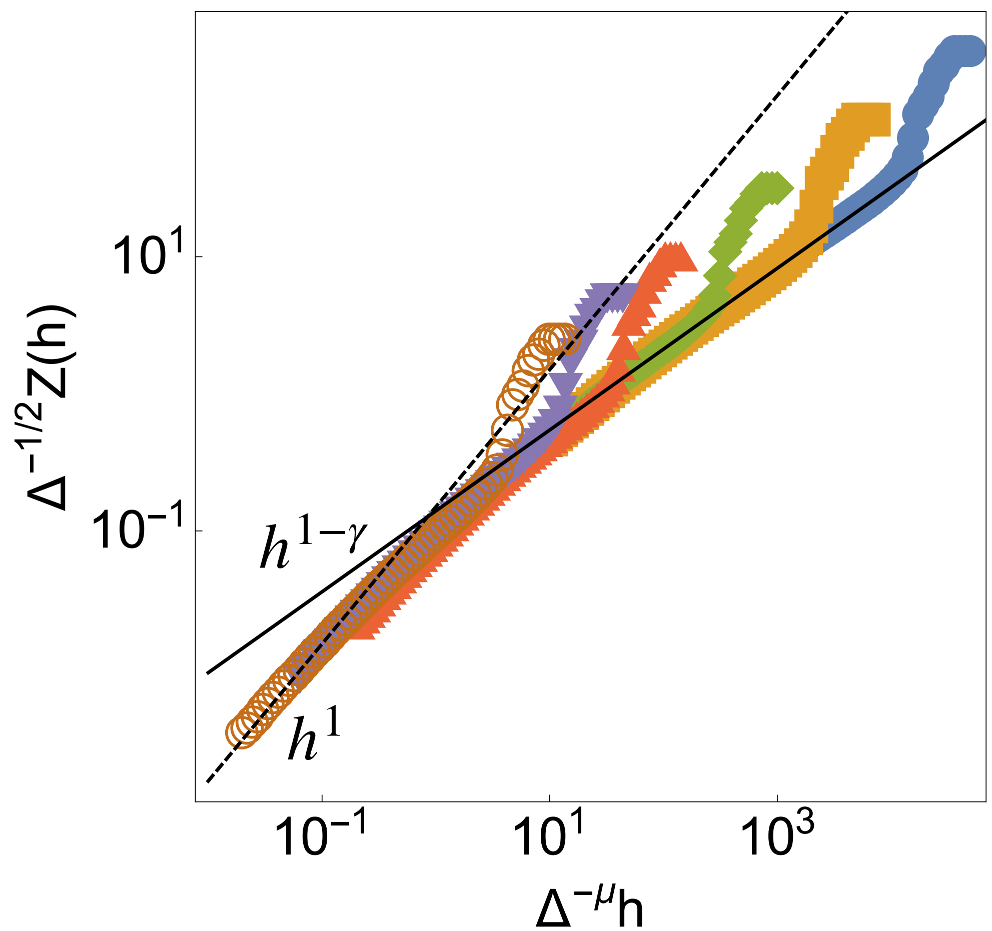
Cumulative distribution function

$$Z(h) = \int_0^h dh g(h),\ (g(h) \sim h^{-\gamma} \to Z(h) \sim h^{1-\gamma})$$

n=2



n=2 (scaling plot)

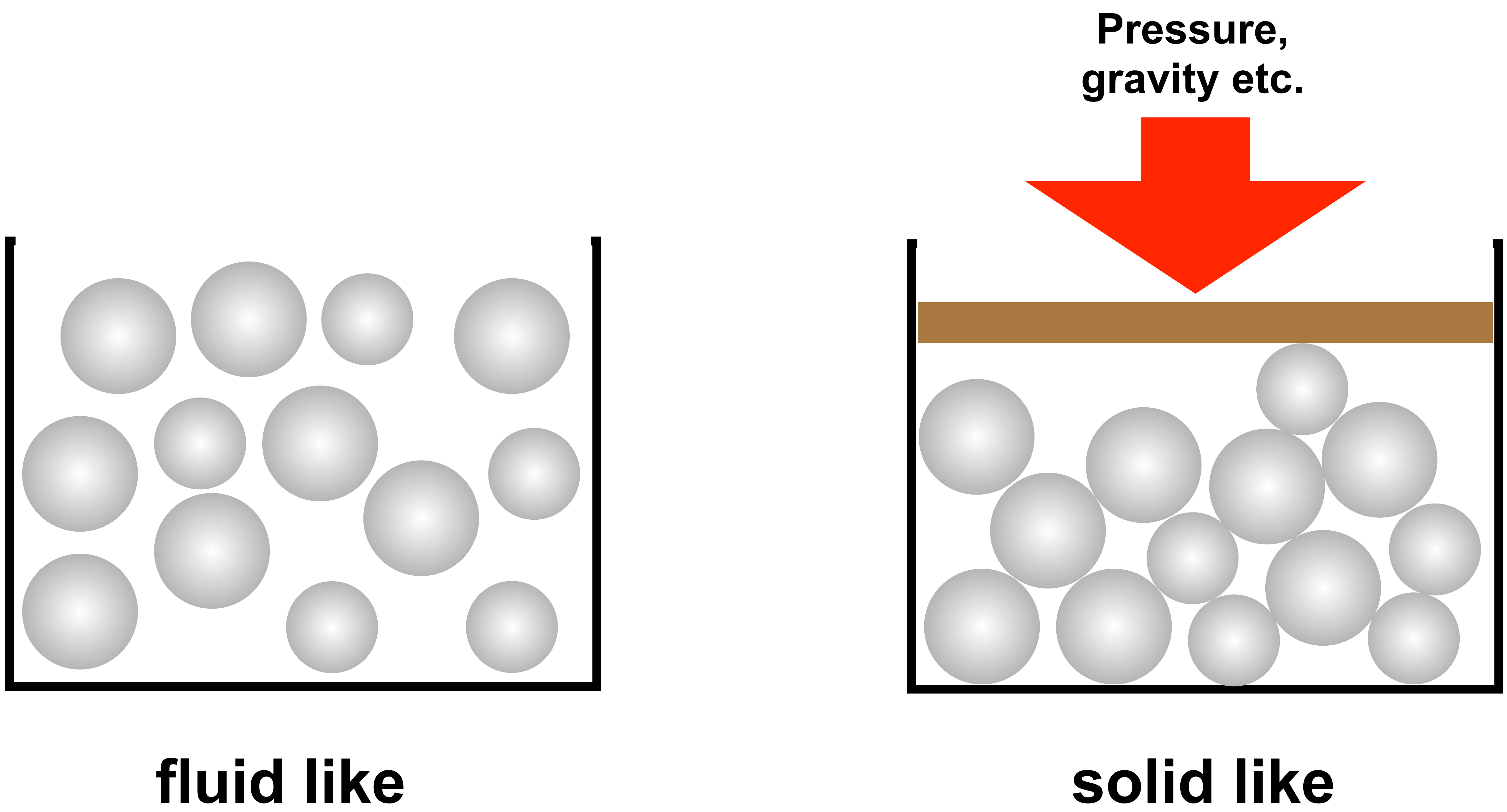


Gap distribution function is finite and regular

$$Z(h) \sim h \to g(h) \sim const\,.$$

Introduction

What is the jamming transition?

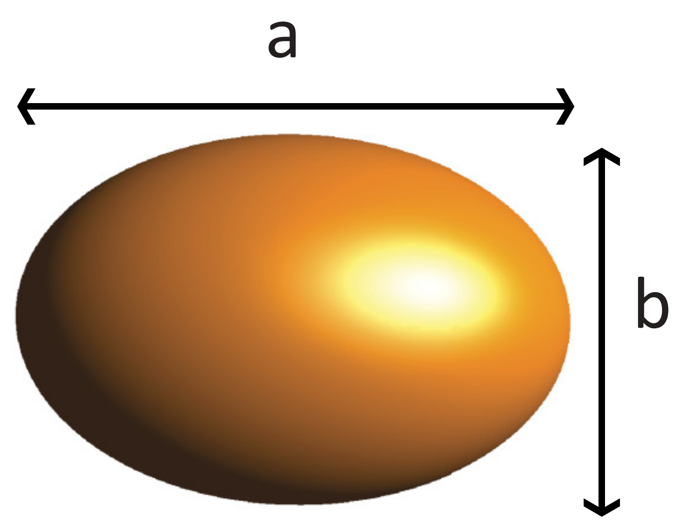


Jamming transition = fluid-solid phase transition
at zero temperature

Non-spherical particles

Previous numerical studies

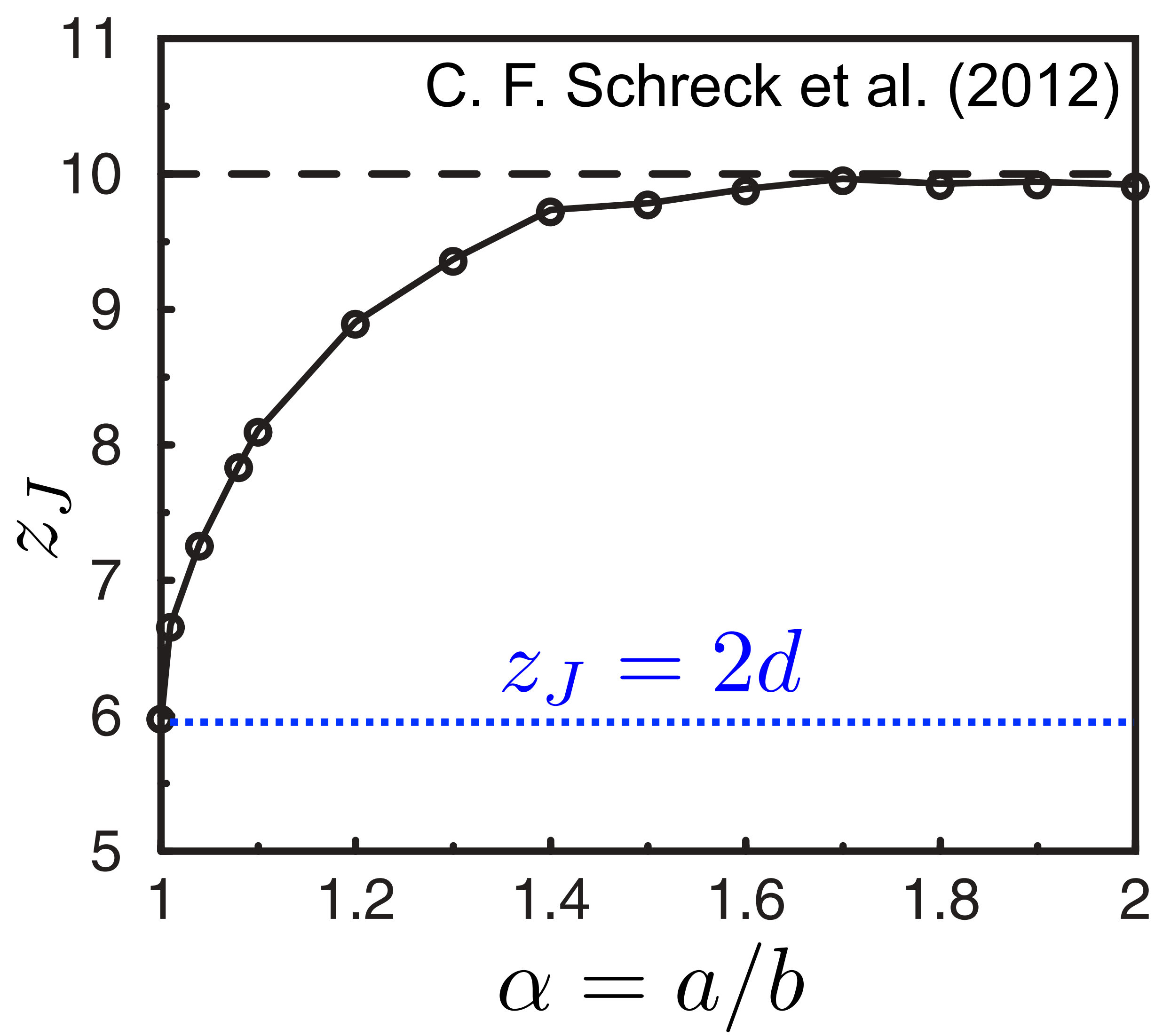
Ellipsoid



Control parameter

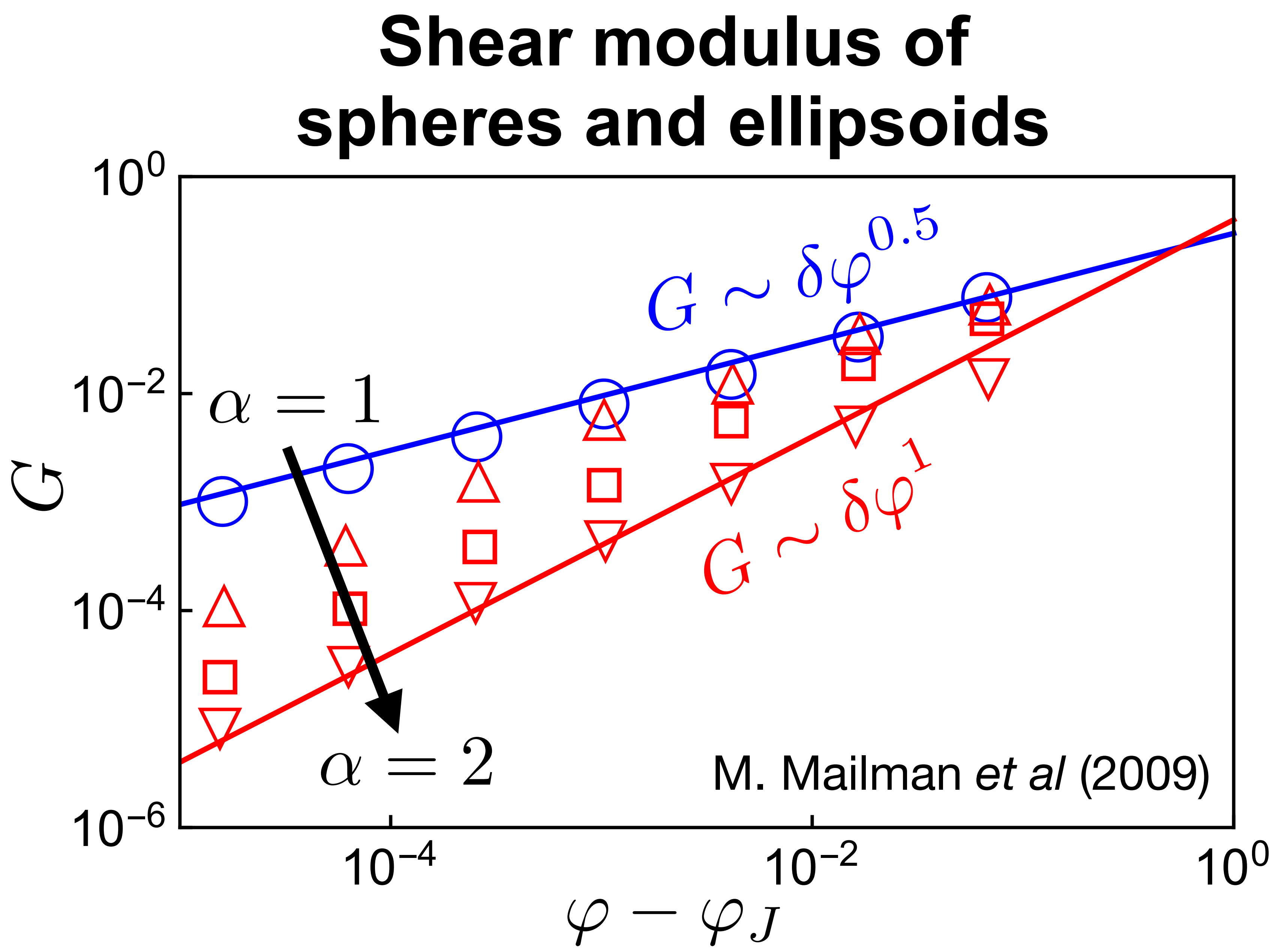
$$\alpha = a/b$$

Contact number at the jamming point



Non-spherical particles

Previous numerical studies

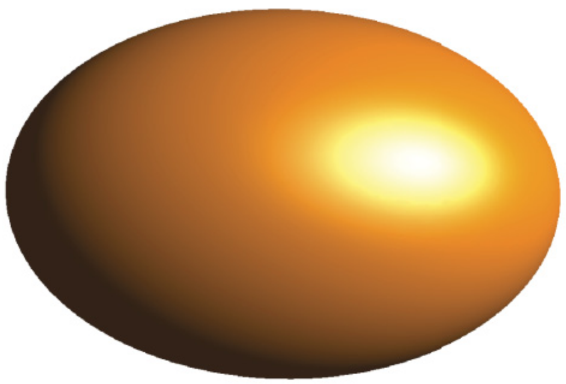


Spheres : $G \sim \delta\varphi^{1/2}$ Ellipsoids : $G \sim \delta\varphi^{1}$

Non-spherical particles

Previous numerical studies

Ellipsoid



M. Mailman *et al* (2009)

$$G \sim (\varphi - \varphi_J)^1$$

C. F. Schreck et al. (2012)

$$z - z_J \sim (\varphi - \varphi_J)^1$$

$$g(r) = ???$$

Other shapes

???

Purpose of this study

Systematic investigation of various shapers of particles

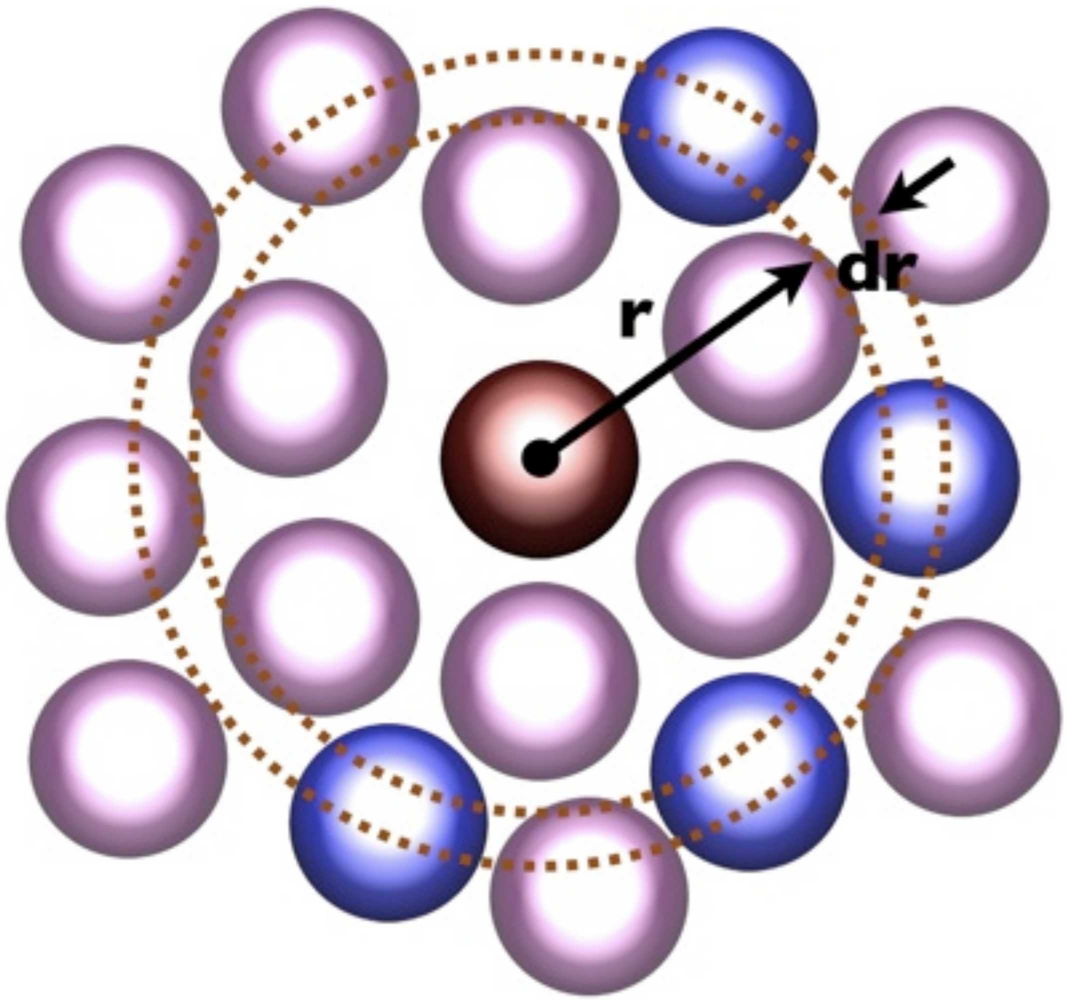
Spherical particles

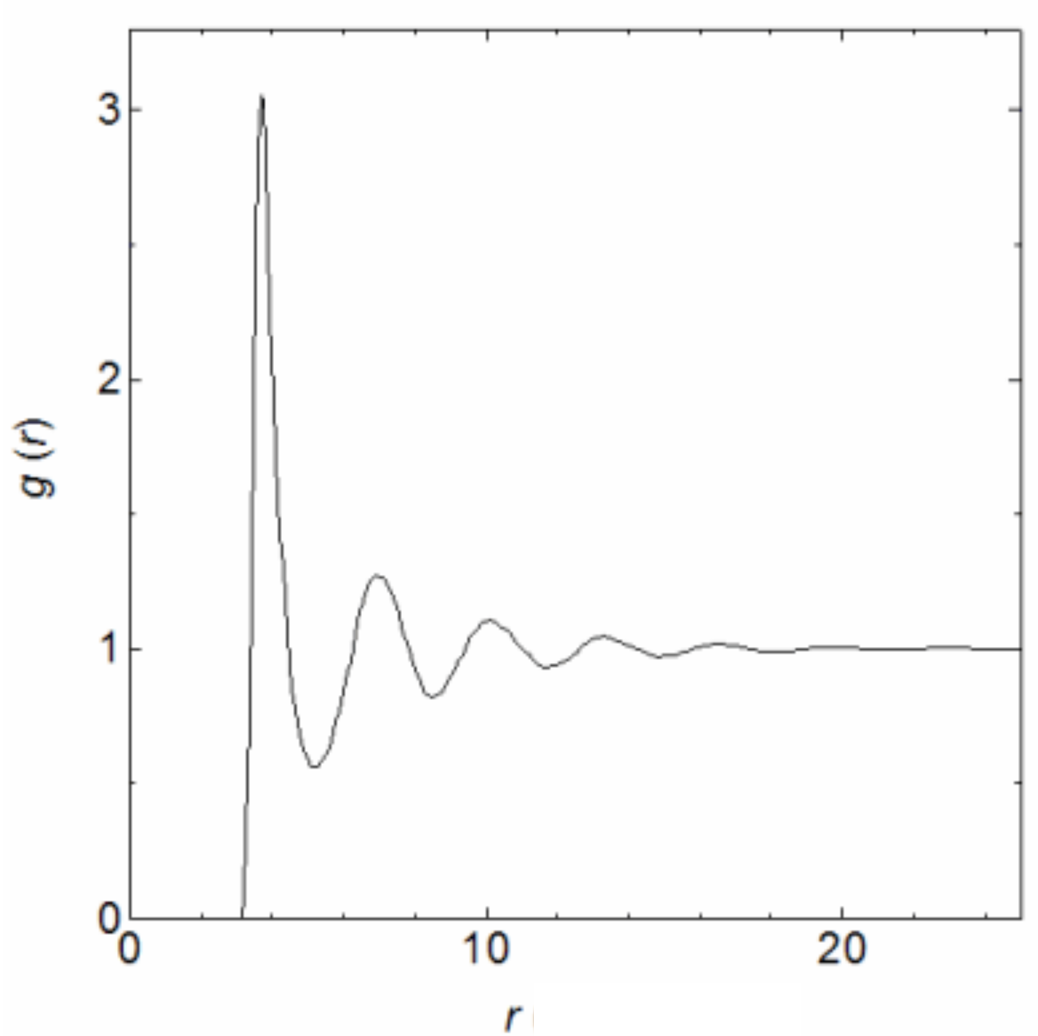
Power-law

Two point correlation function

$$g(r) = \frac{1}{N} \sum_{i \neq j} \delta(r - |\vec{x}_i - \vec{x}_j|)$$

$$\int dr 4\pi r^2 \rho g(r) = N - 1$$

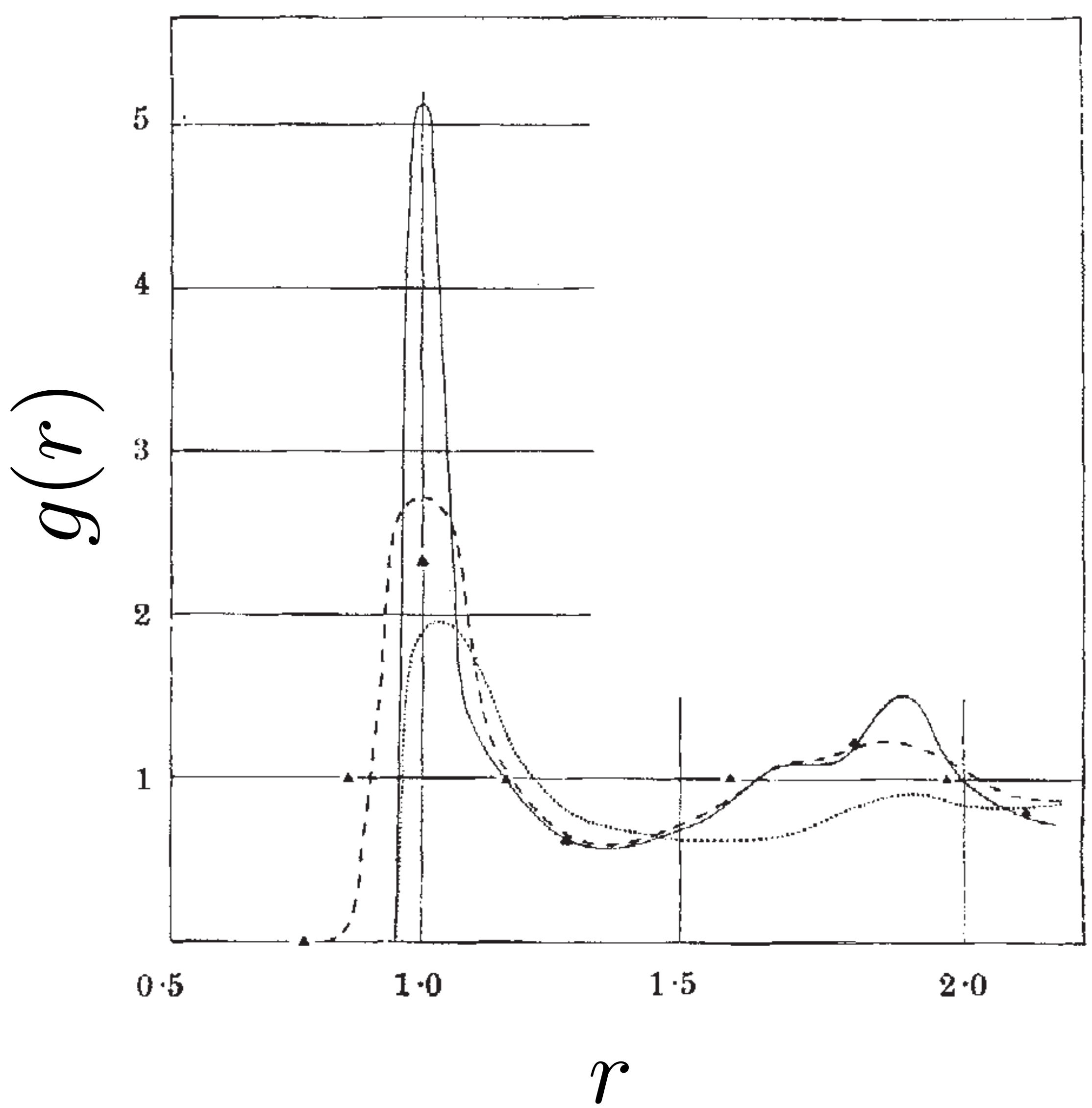




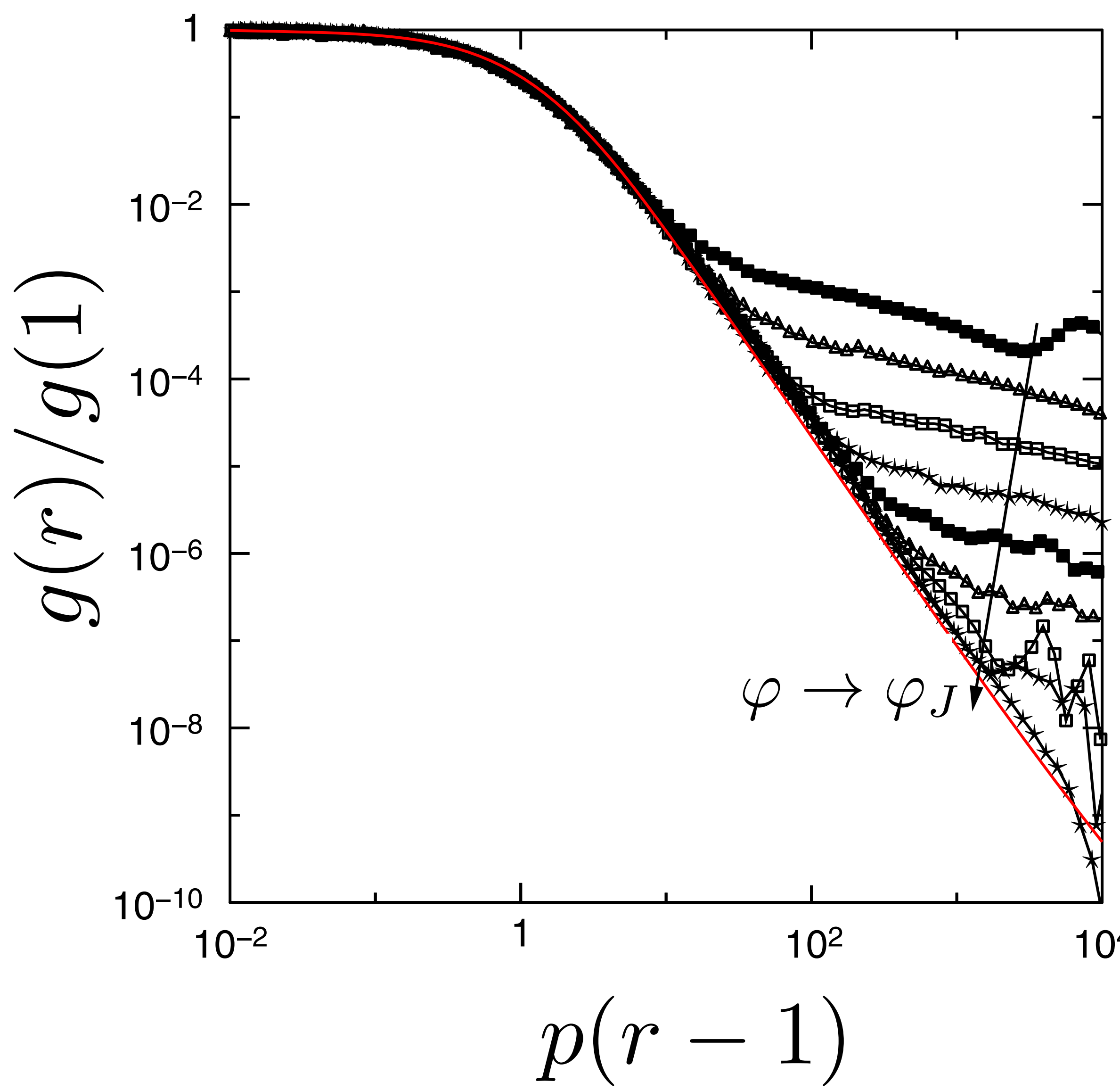
Spherical particles

Power-law

J. D. Bernal (1960)



P. Charbonneau *et al.* (2014)

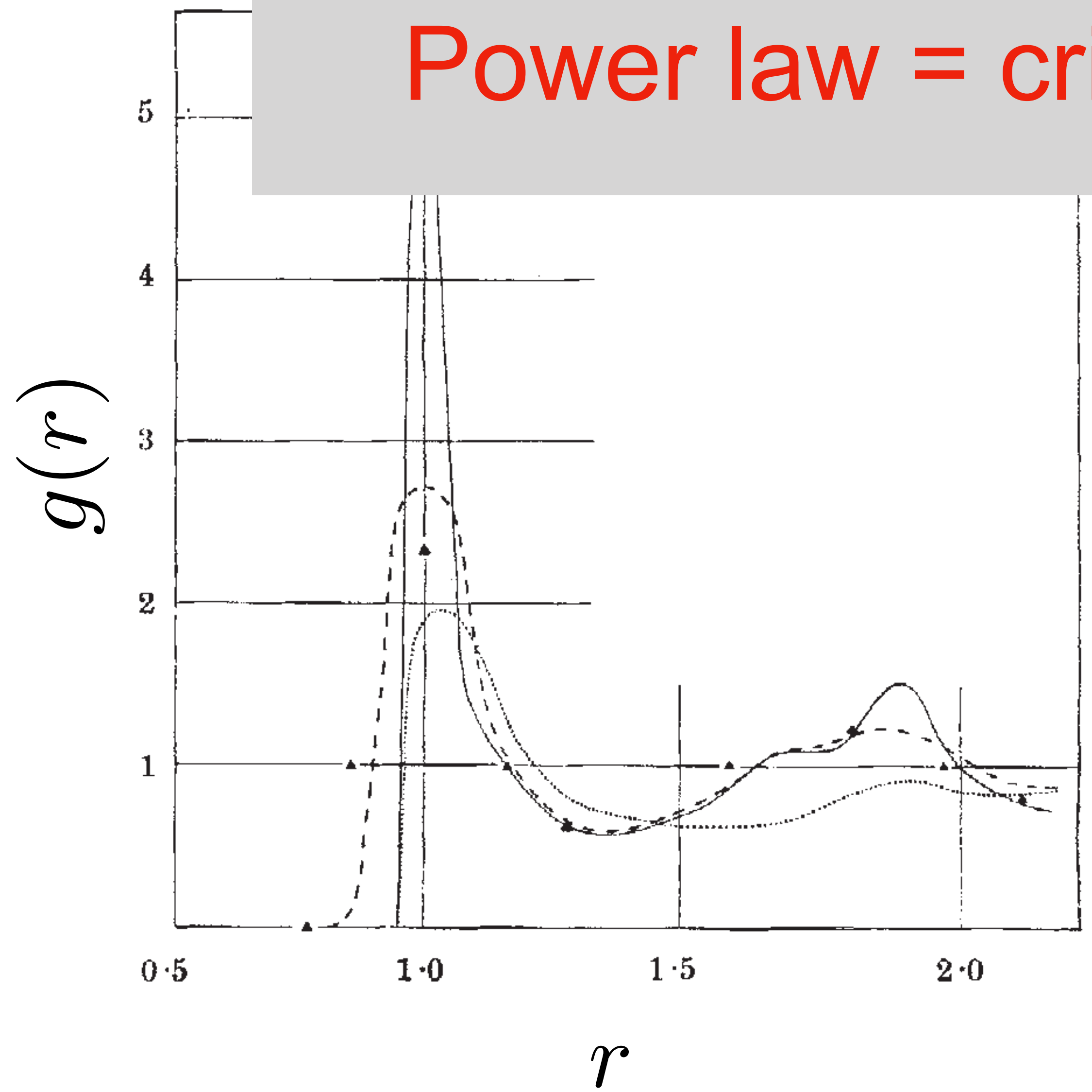


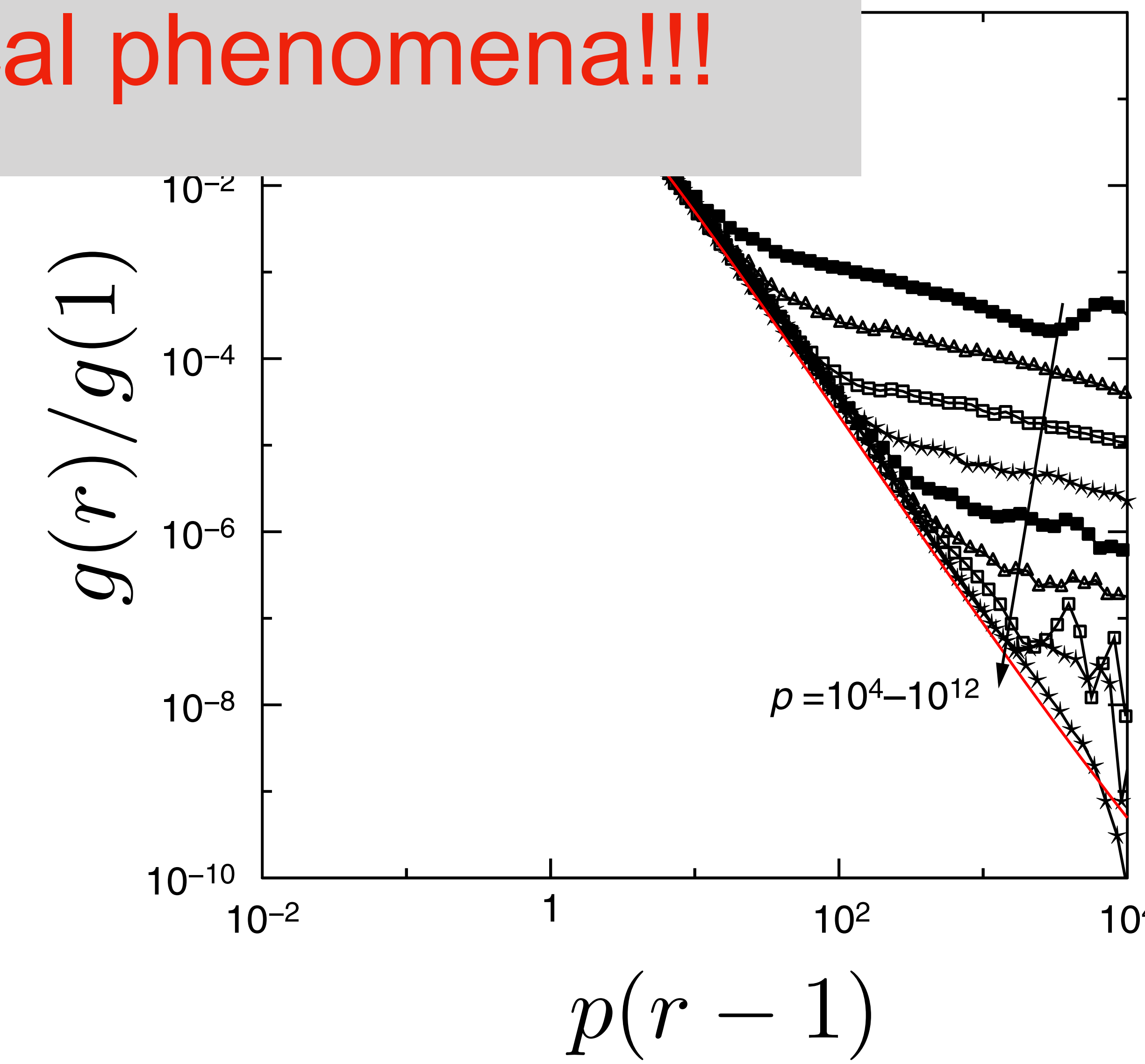
Spherical particles

Power-law

al. (2014)

Power law = critical phenomena!!!

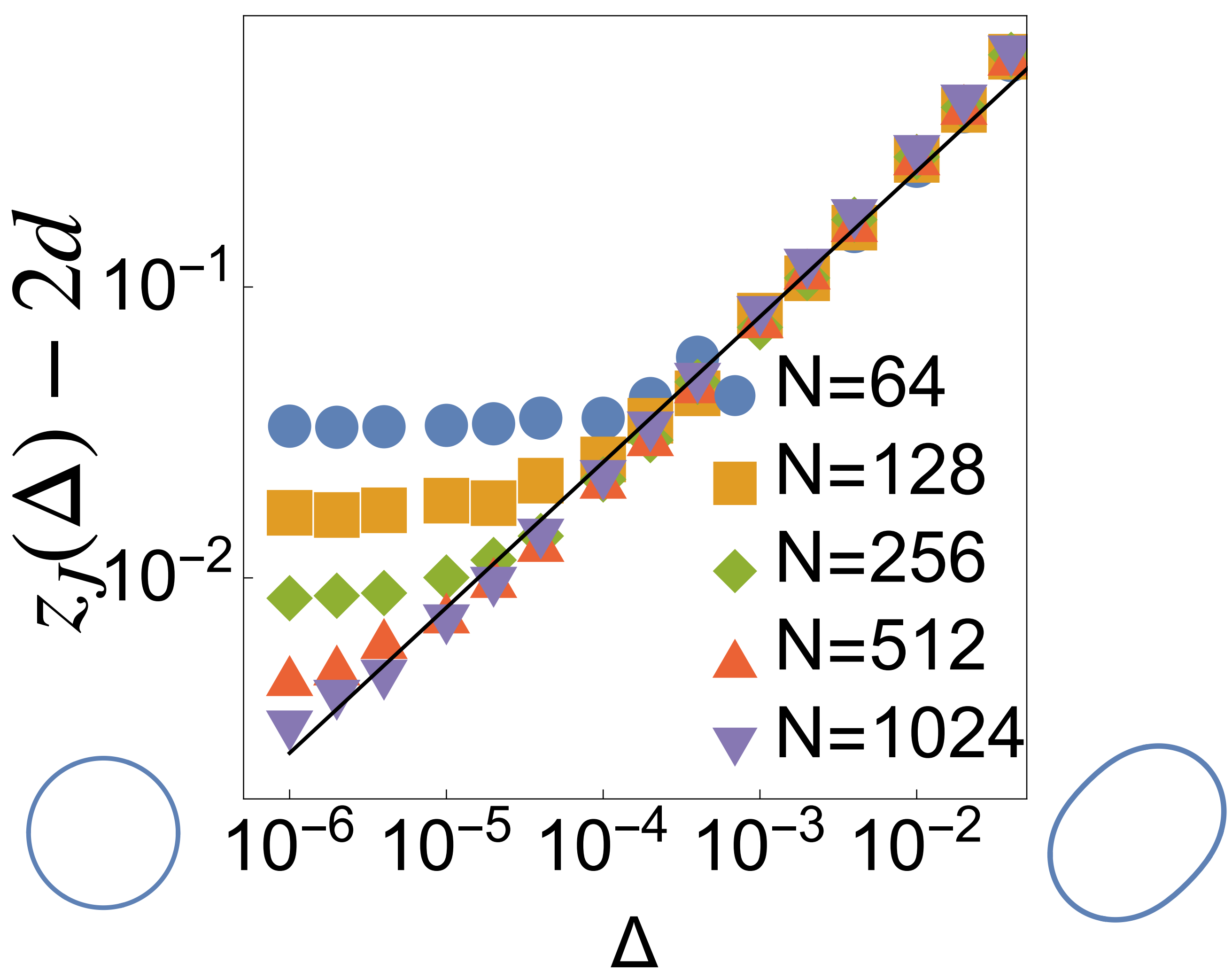




Non-spherical particles

Contact number

Contact number for n=2



The contact number increases with the aspect ratio as

$$z_J(\Delta) - z_J(0) \sim \Delta^{1/2}$$

Spherical particles

Motivation

To simplify the problem, we consider spherical particles

wikipedia.org/wiki/Spherical_cow