Strongly Anharmonic Solids: Vibrational Modes in Jammed Systems

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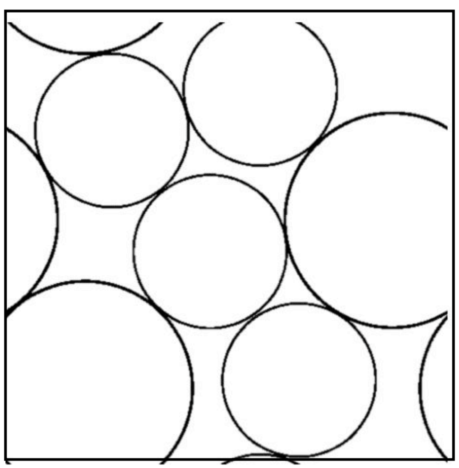
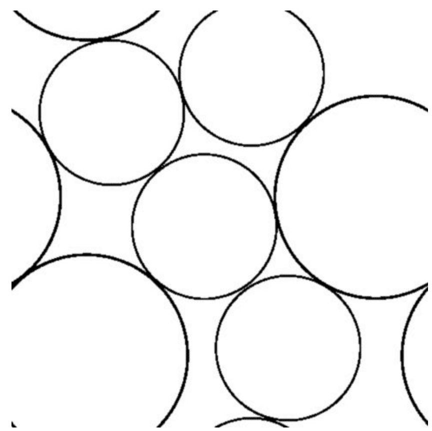
Featured Questions

1. What can we learn about vibrations in amorphous solids from static configurations? Everything vs. Nothing.
2. Are jammed solids harmonic? If not, how anharmonic?
3. Dispersion, nonlinear response, heat transport in particulate media.

N_c=22

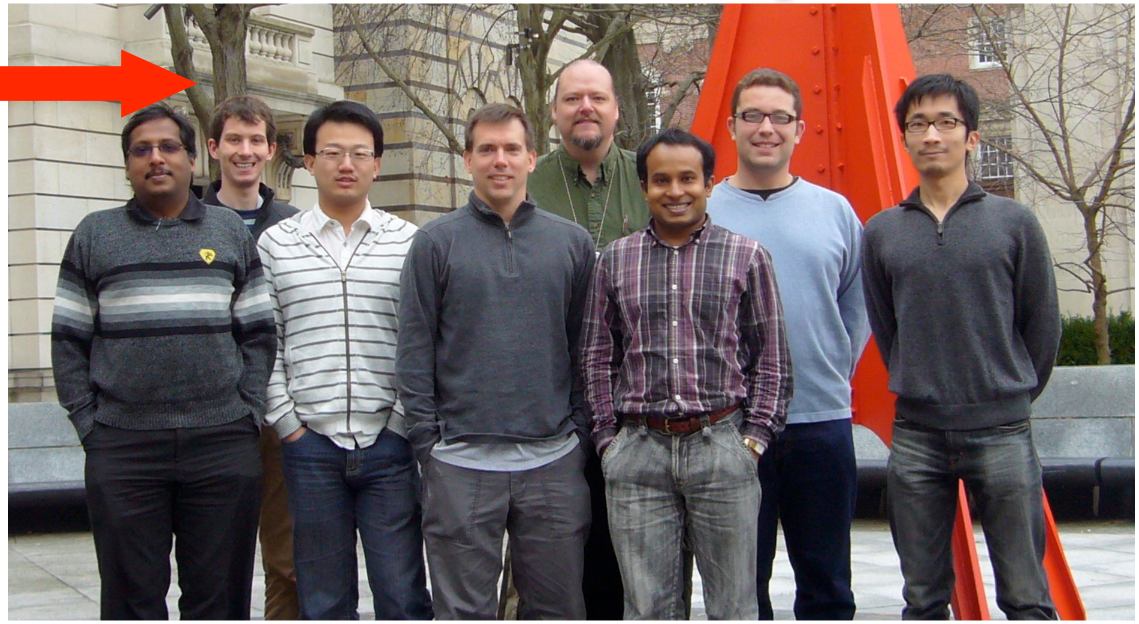


static packing



vibrating

O'Hern Group



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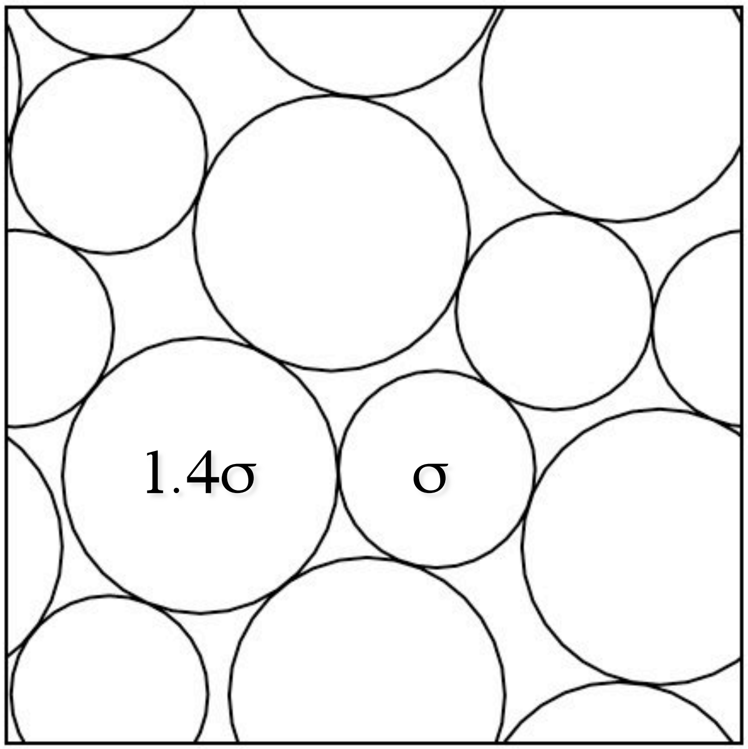
Funding:

NSF DMR-0448838

NSF DMS-0835742

NSF CBET-0967262

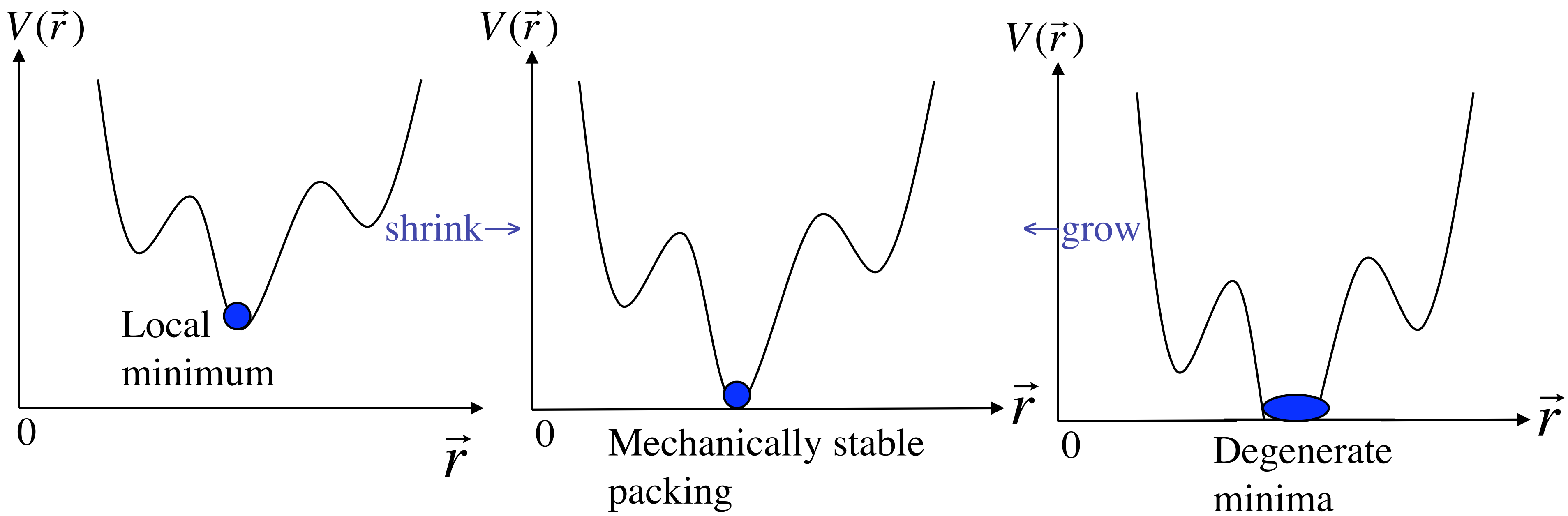
Jammed Solids

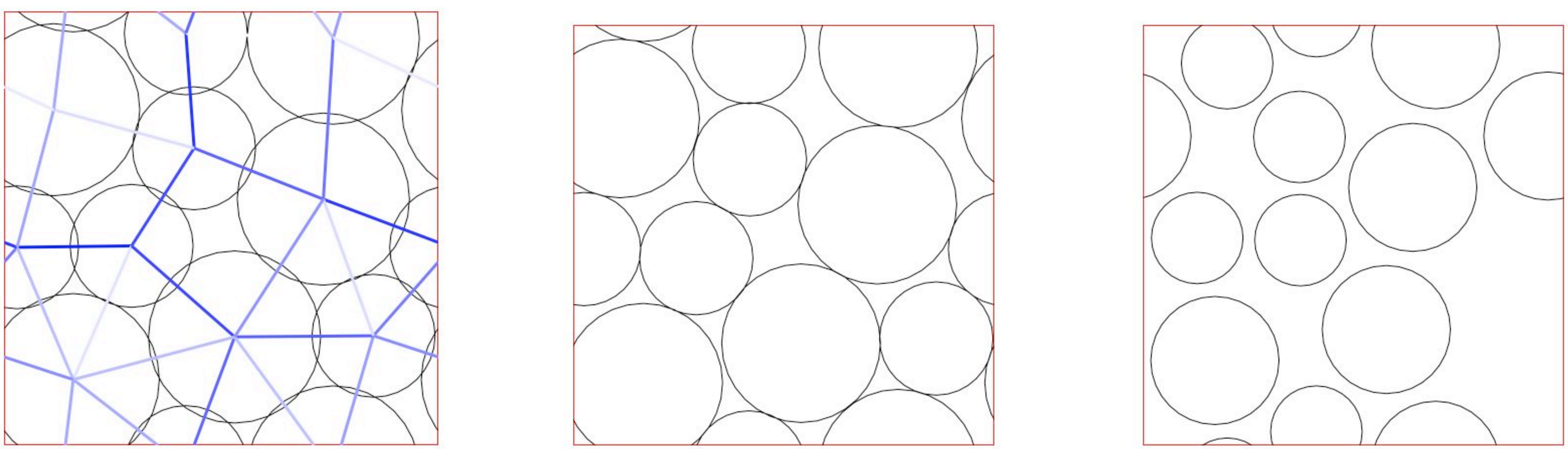


Jammed packing: ϕ_J, z_J, $V \sim P \sim 0$

- Particulate systems
- Contact interactions
- Amorphous
- Frictionless
- Vanishing overlaps
- Isostatic: $N_c = 2(dN - d + 1)$
- Force balance
- Mechanically stable
- collecively jammed hard-sphere inherent structures

Potential Energy Landscape (PEL)





overlapped

Mechanically stable packing

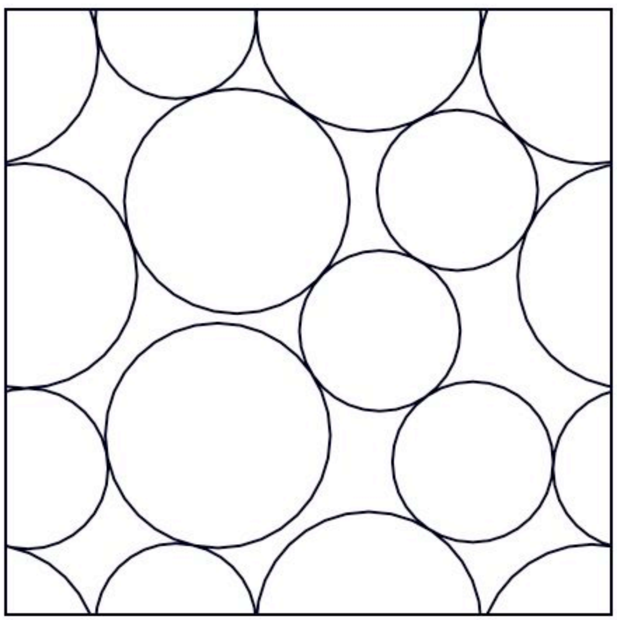
non-overlapped

Interlude: Statistical Descriptions of Jammed Packings

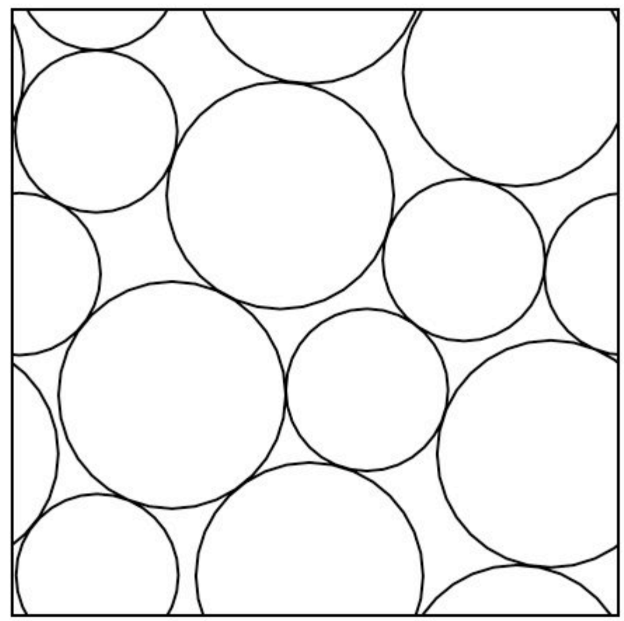
"for a given volume all [jammed] configurations are equally probable"

S. F. Edwards and R. B. S. Oakeshott, "Theory of Powders", Physica A 157 (1989) 1080

…but often jammed packings are not equally likely!

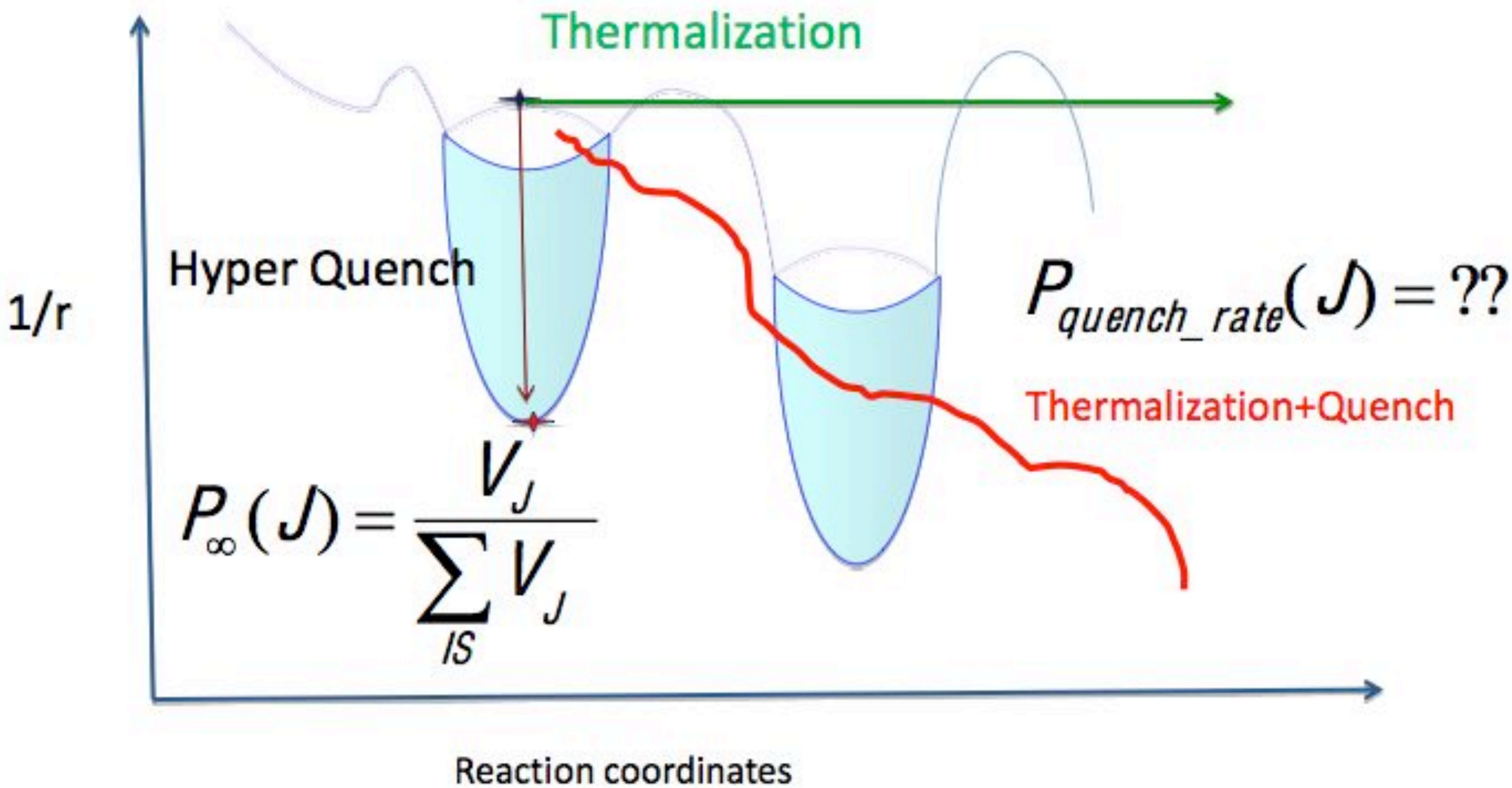


rare

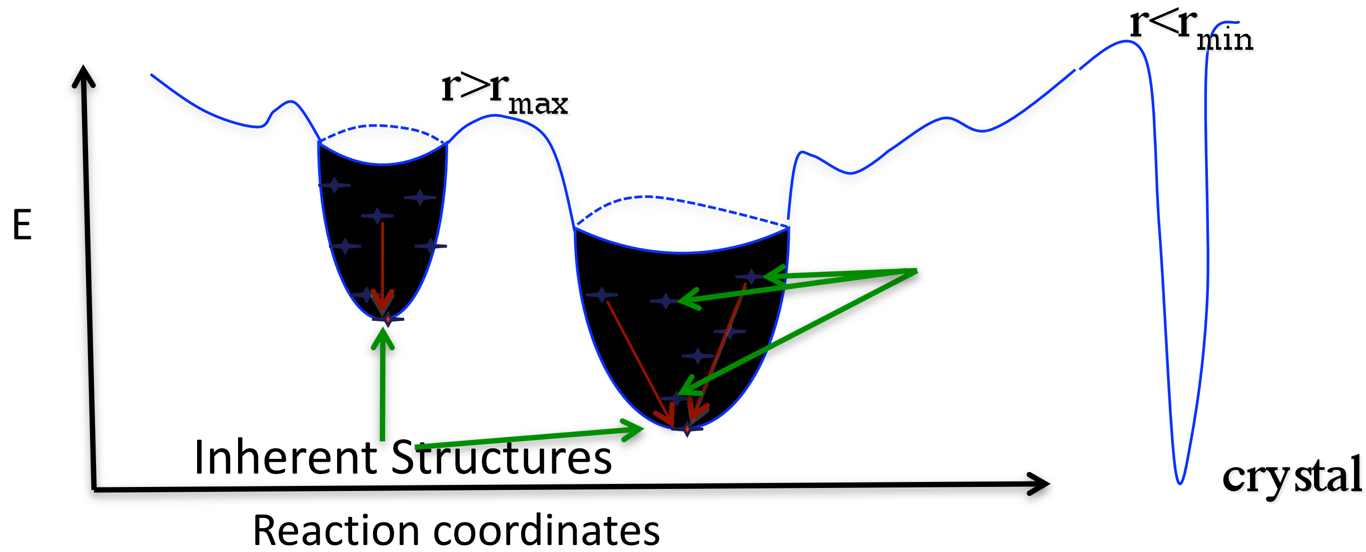


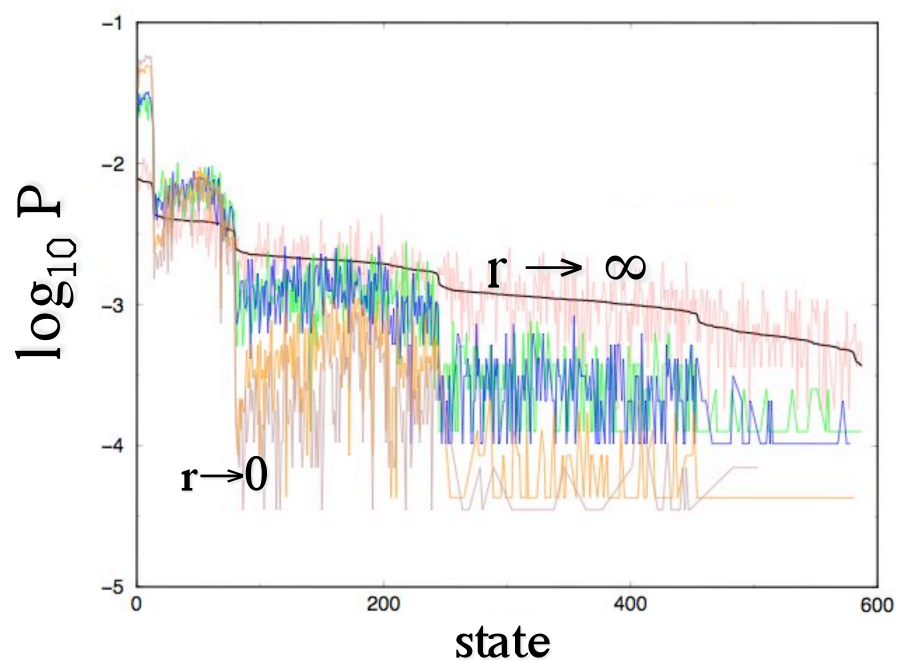
10^6 more frequent

Can we predict probability to obtain jammed packings?



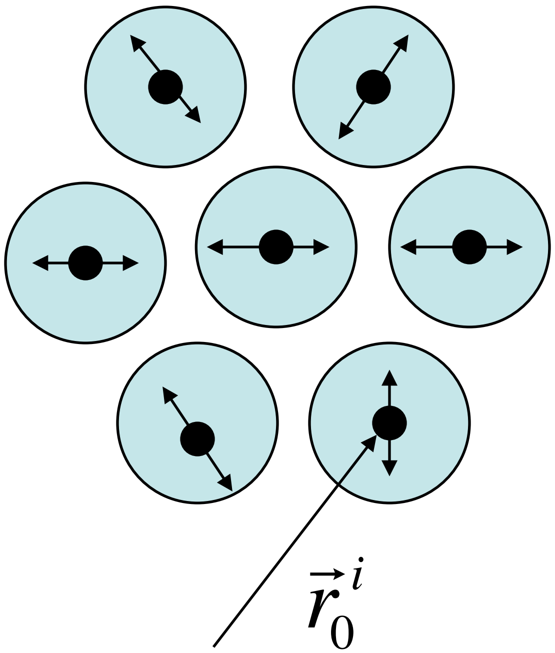
Interlude: Critical Quench Rates

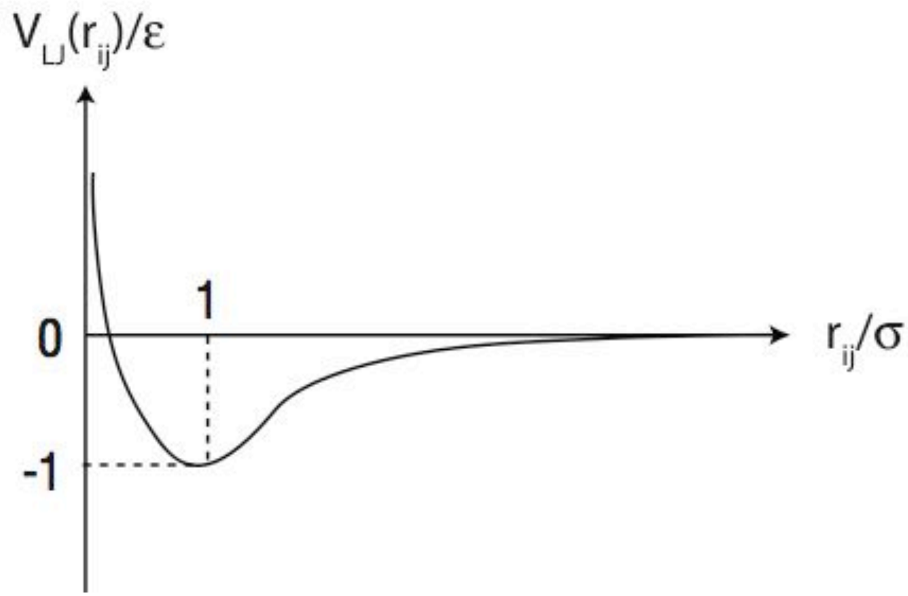




$r_{min} < r < r_{max}$

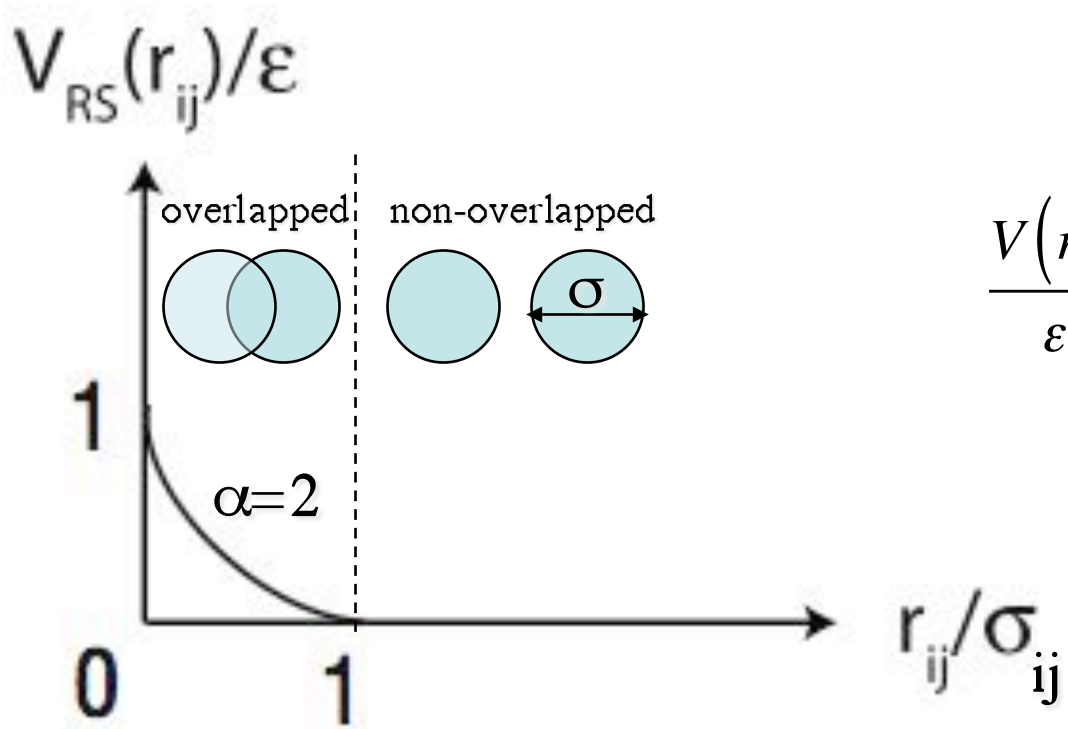
Harmonic Solids





- Pair potential has minimum and are *continuous*; Effective potentials $V_i = \Sigma_j V_{LJ}(r_{ij})$ are harmonic
- Equilibrium positions are well-defined
- Vibrations captured using harmonic approximation

Contact Interactions



$$\frac{V\left(r_{ij}\right)}{\varepsilon}=\begin{cases}\alpha^{-1}\left(1-\dfrac{r_{ij}}{\sigma_{ij}}\right)^{\alpha} & r_{ij}\le\sigma_{ij}\\ 0 & r_{ij}>\sigma_{ij}\end{cases}$$

Total potential energy $V=\sum_{\langle i,j\rangle}V\left(r_{ij}\right)$

Dynamical Matrix: Normal Modes

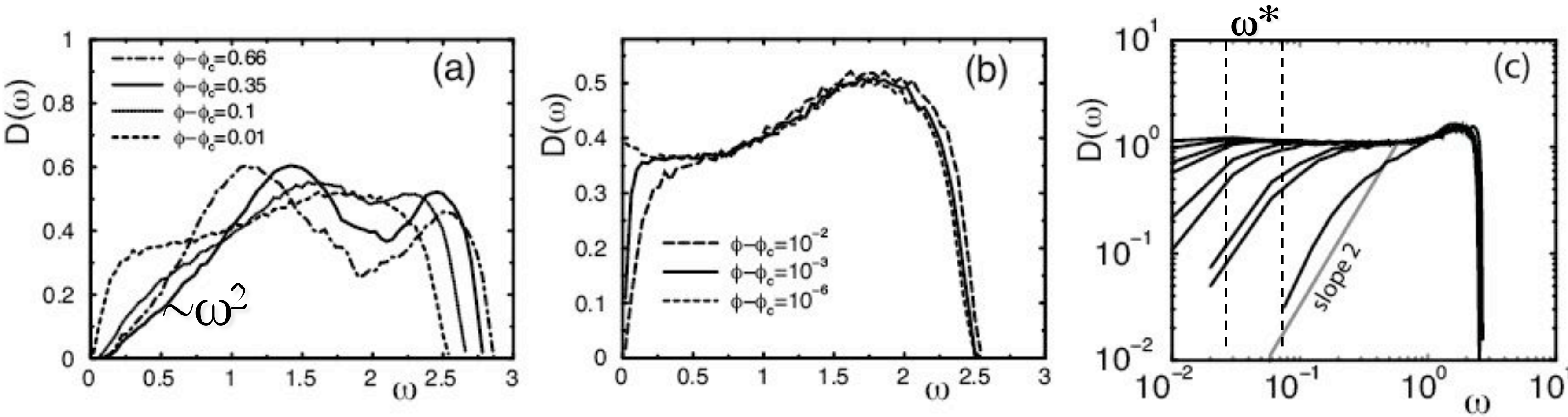
$$M_{\alpha,\beta} = \left.\frac{\partial^2 V(\vec{r})}{\partial r_\alpha \partial r_\beta}\right|_{\vec{r}=\vec{r}_0}$$

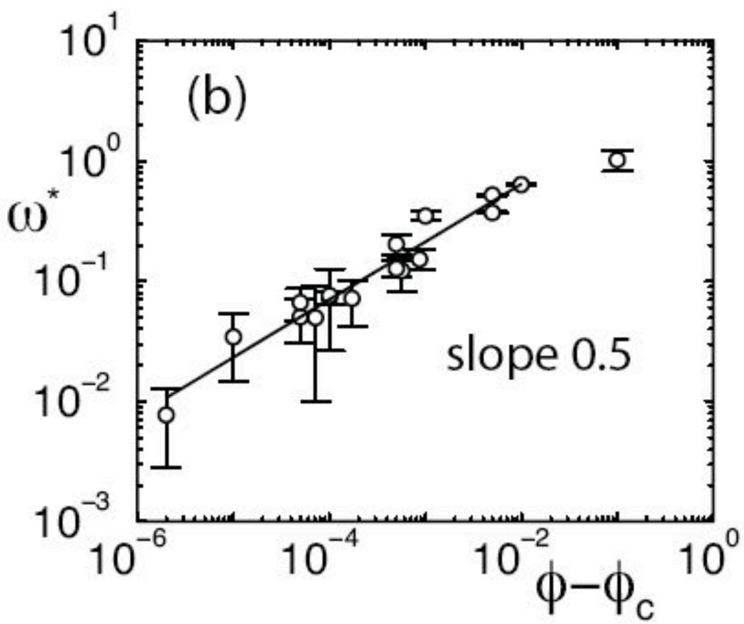
α,β=x, y, z, particle index

$\vec{r}_0$ = positions of MS packing

Calculate d N- d eigenvalues; $m_i = \omega^2_i > 0$.

Density of Vibrational Modes via Dynamical Matrix (DM)





$$D(\omega)d\omega = N(\omega + d\omega) - N(\omega)$$

- Formation of plateau in D(ω) (excess of low-frequency modes) as $\Delta\phi \rightarrow 0$
- $\omega^* \sim \Delta z \sim \Delta\phi^{0.5}$ responsible for anomalous static structural/mechanical properties

A. J. Liu, S. R. Nagel, W. van Saarloos, and M. Wyart, "The jamming scenario--an introdcution and outlook," Soft Matter (2010).

Causes of anharmonicity

- Nonlinear interaction potential
- Breaking existing contacts and forming new contacts

- Explicit dissipation from normal contacts
- Sliding and rolling friction

1. Energy Expansion of Stressed Springs

$$V(\vec{r})-V(\vec{r}_0)=\epsilon\sum_{<i,j>}((1-\frac{r_{ij,0}}{\sigma_{ij}})\frac{\hat{r}_{ij,0}\cdot\Delta\vec{r}_{ij}}{\sigma_{ij}}+\frac{1}{2}\frac{\Delta r_{ij}^2}{\sigma_{ij}^2}-\frac{1}{2}\frac{(\hat{r}_{ij,0}\times\Delta\vec{r}_{ij})^2}{r_{ij,0}\sigma_{ij}}+\frac{\hat{r}_{ij,0}\cdot\Delta\vec{r}_{ij}}{r_{ij,0}}\frac{(\hat{r}_{ij,0}\times\Delta\vec{r}_{ij})^2}{r_{ij,0}\sigma_{ij}})$$

3rd order

$$\vec{r}=\{x_1,y_1,...,x_N,y_N\}$$

$$\Delta\vec{r}_{ij}=\vec{r}_{ij}-\vec{r}_{ij,0}$$

$$\vec{r}_{ij}=\{x_j-x_i,y_j-y_i\}$$

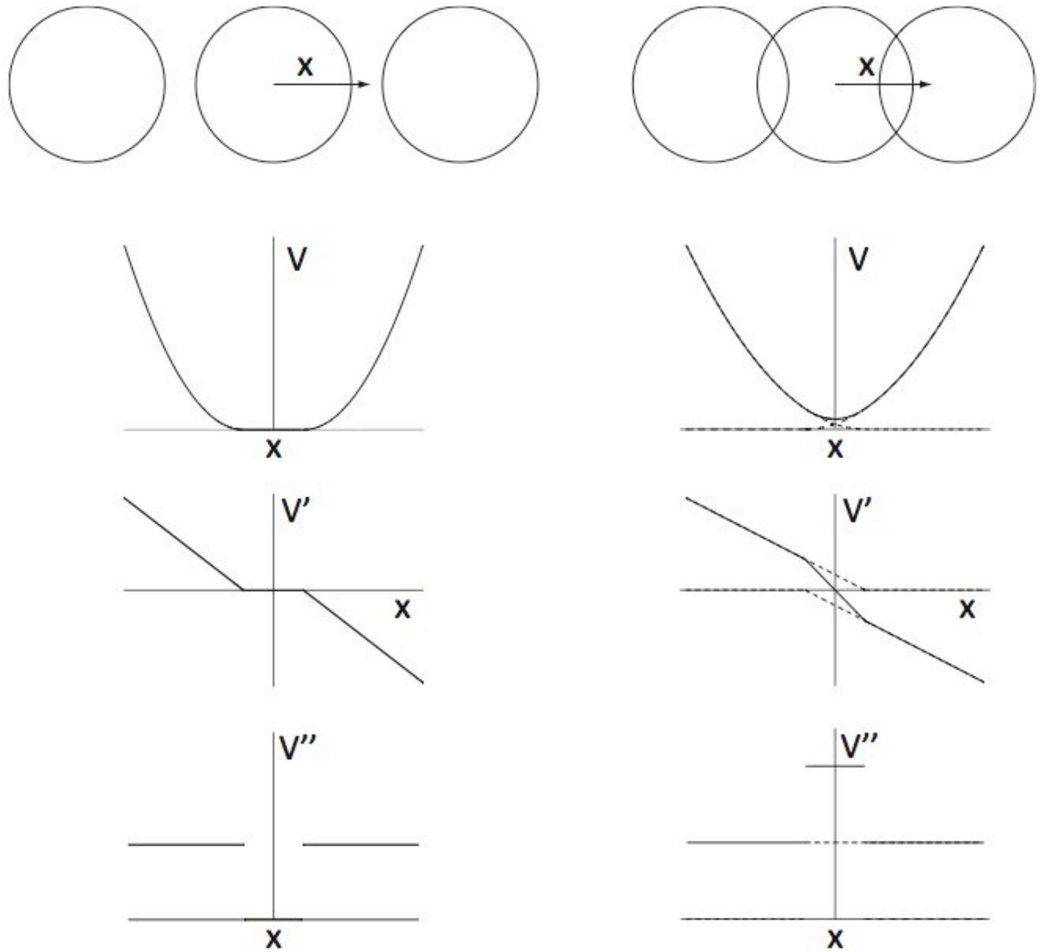
$$\hat{r}_{ij}=\frac{\vec{r}_{ij}}{|\vec{r}_{ij}|}$$

$$\vec{r}_{ij,0}=\{x_{j,0}-x_{i,0},y_{j,0}-y_{i,0}\}$$

$$\hat{r}_{ij,0}=\frac{\vec{r}_{ij,0}}{|\vec{r}_{ij,0}|}$$

$$\sigma_{ij}=\frac{\sigma_i+\sigma_j}{2}$$

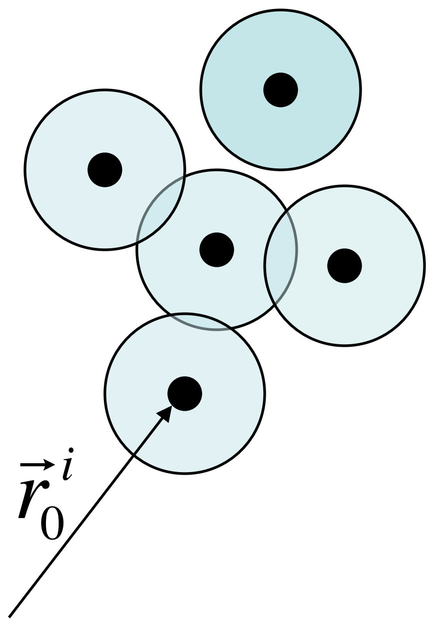
2. What happens during overlap and underlap?



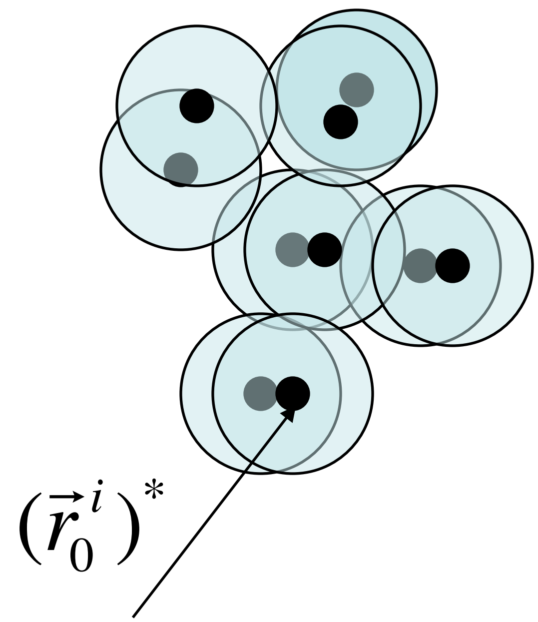
underlap

overlap

3. Do jammed solids have equilibrium positions?



Static, force-balanced configuration

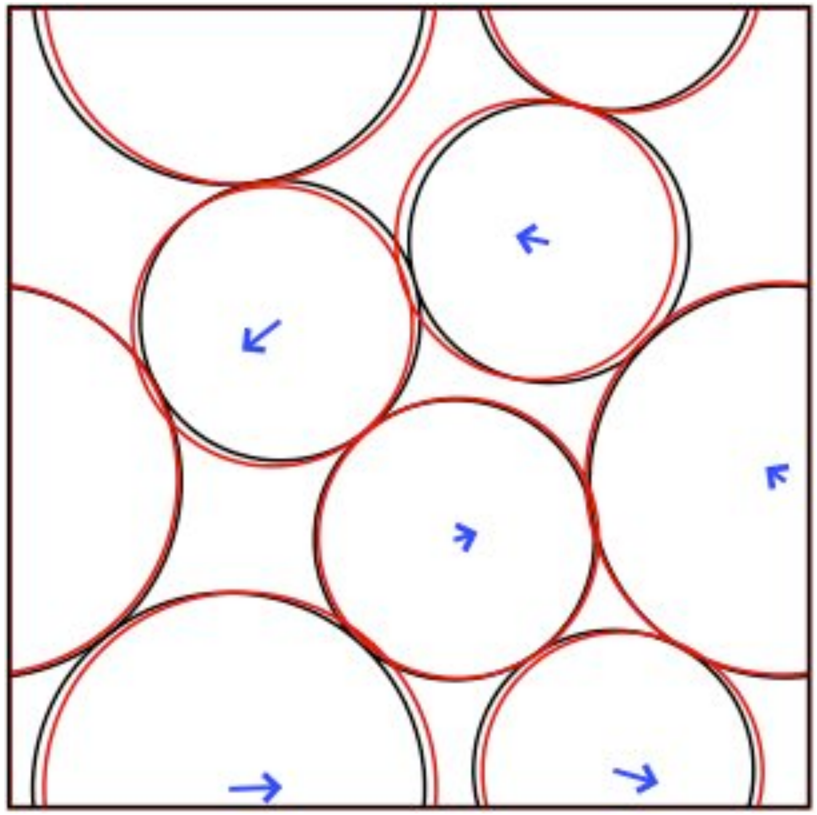


Weakly vibrating configuration

…Answer depends on breaking and forming of contacts…

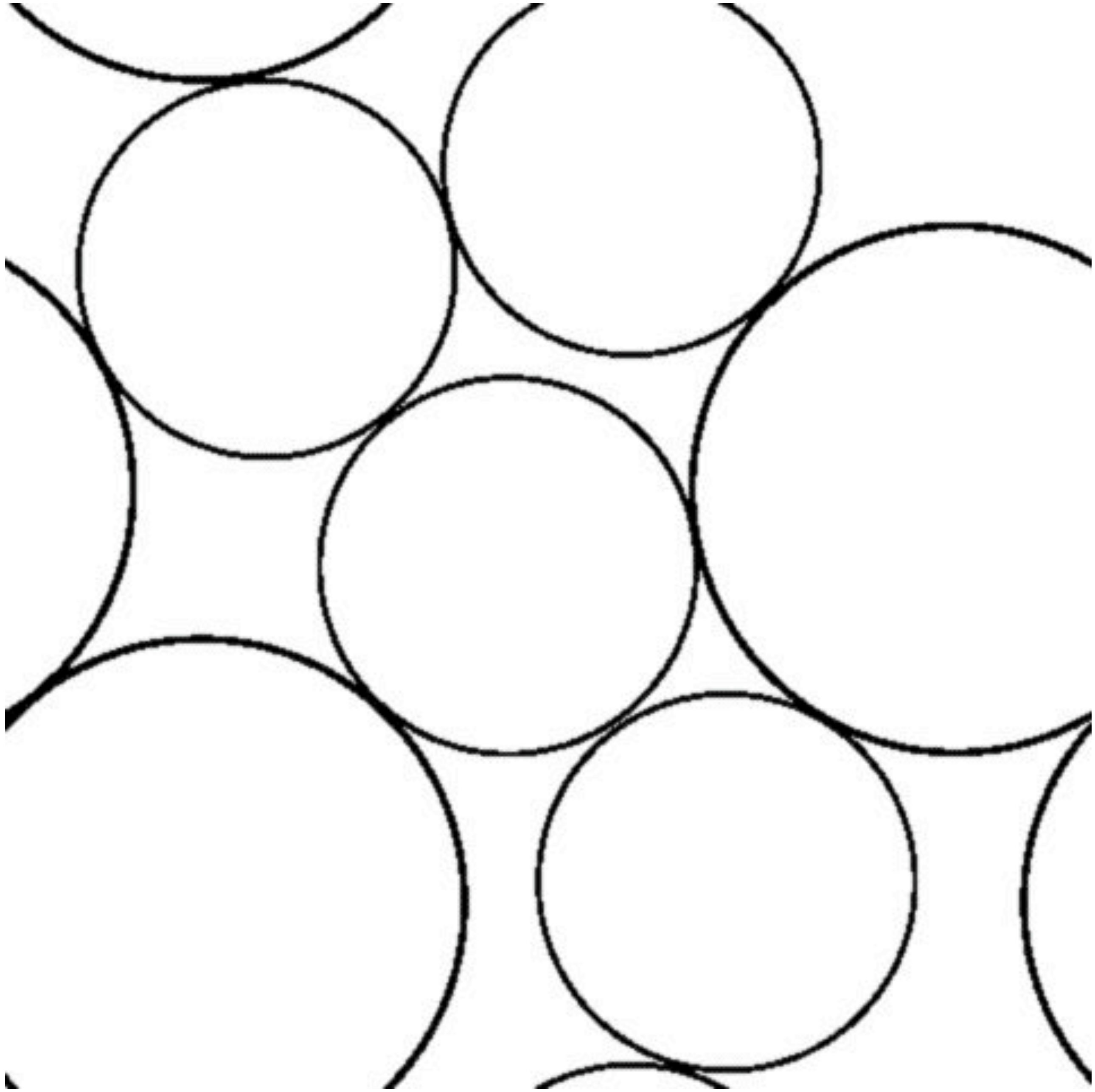
Deform along each 'Eigenmode'

$$\vec{r}_i^{\,'} = \vec{r}_i + \delta \hat{e}_4$$

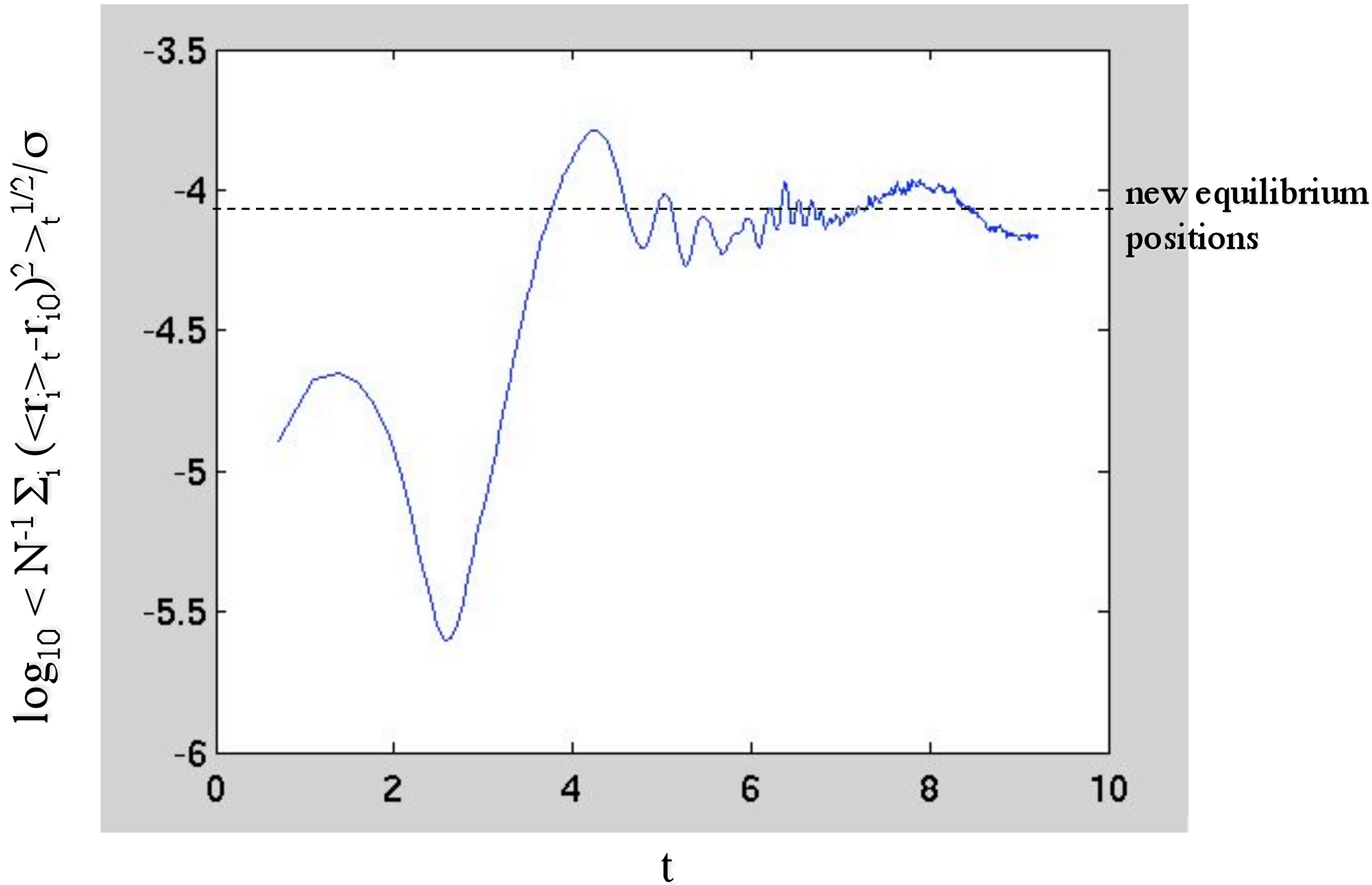


- Does system oscillate at frequency ω_4 from DM?
- Apply deformation, run at NVE

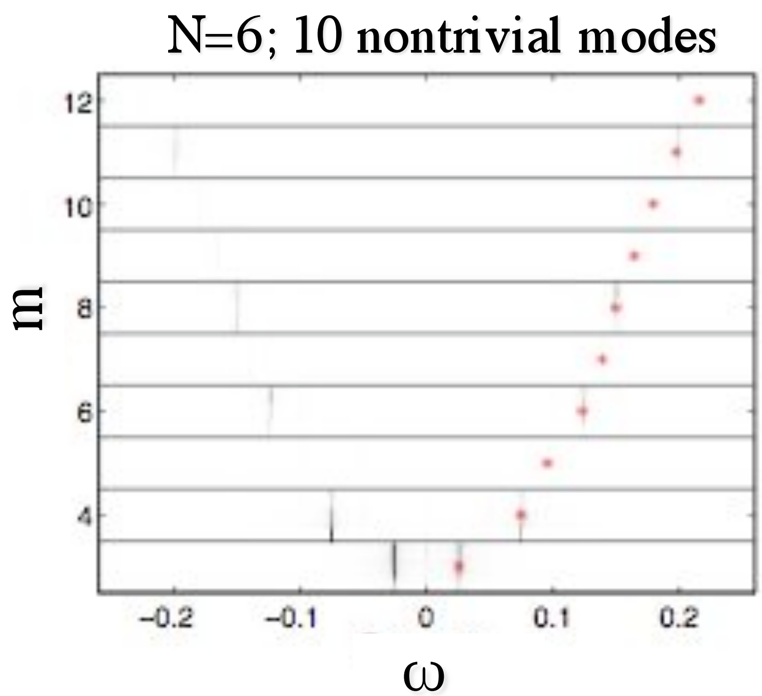
$\delta=10^{-2}$

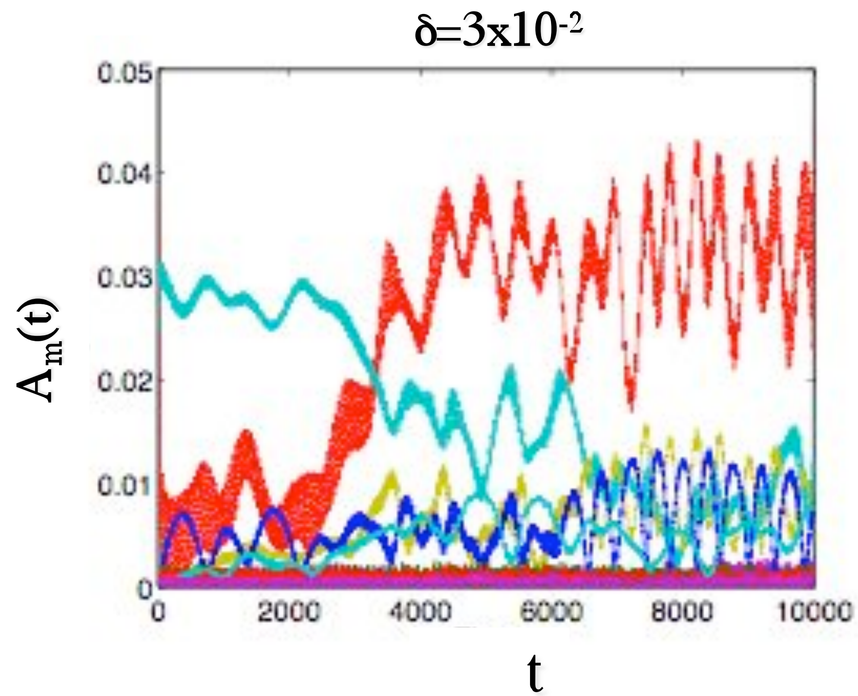


Break to New Vibrational Equilibrium, Not New Packing



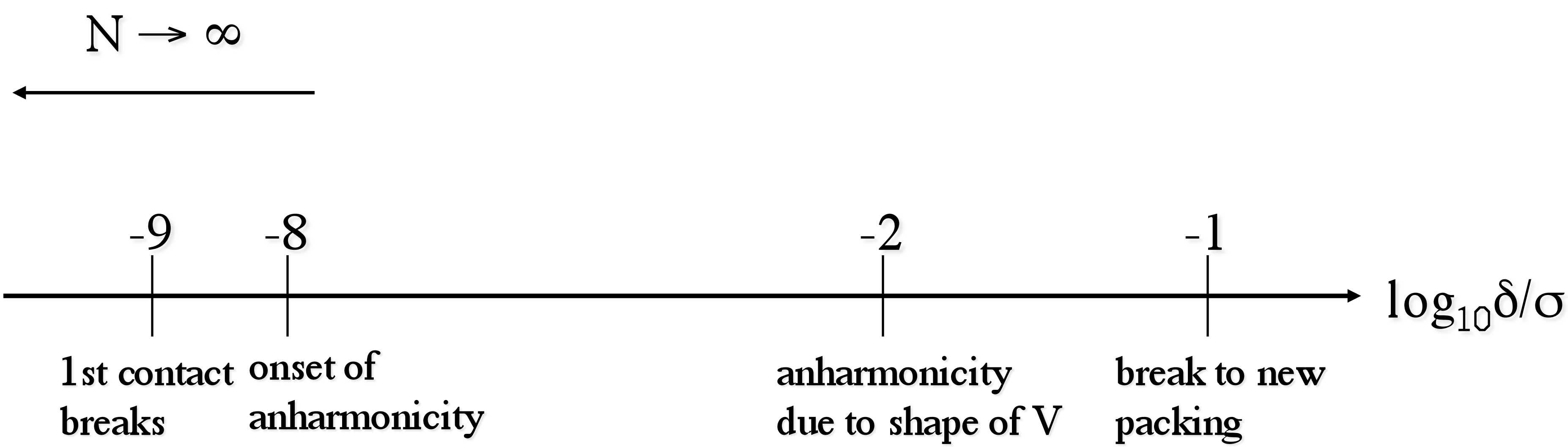
Dispersion from double-sided potentials



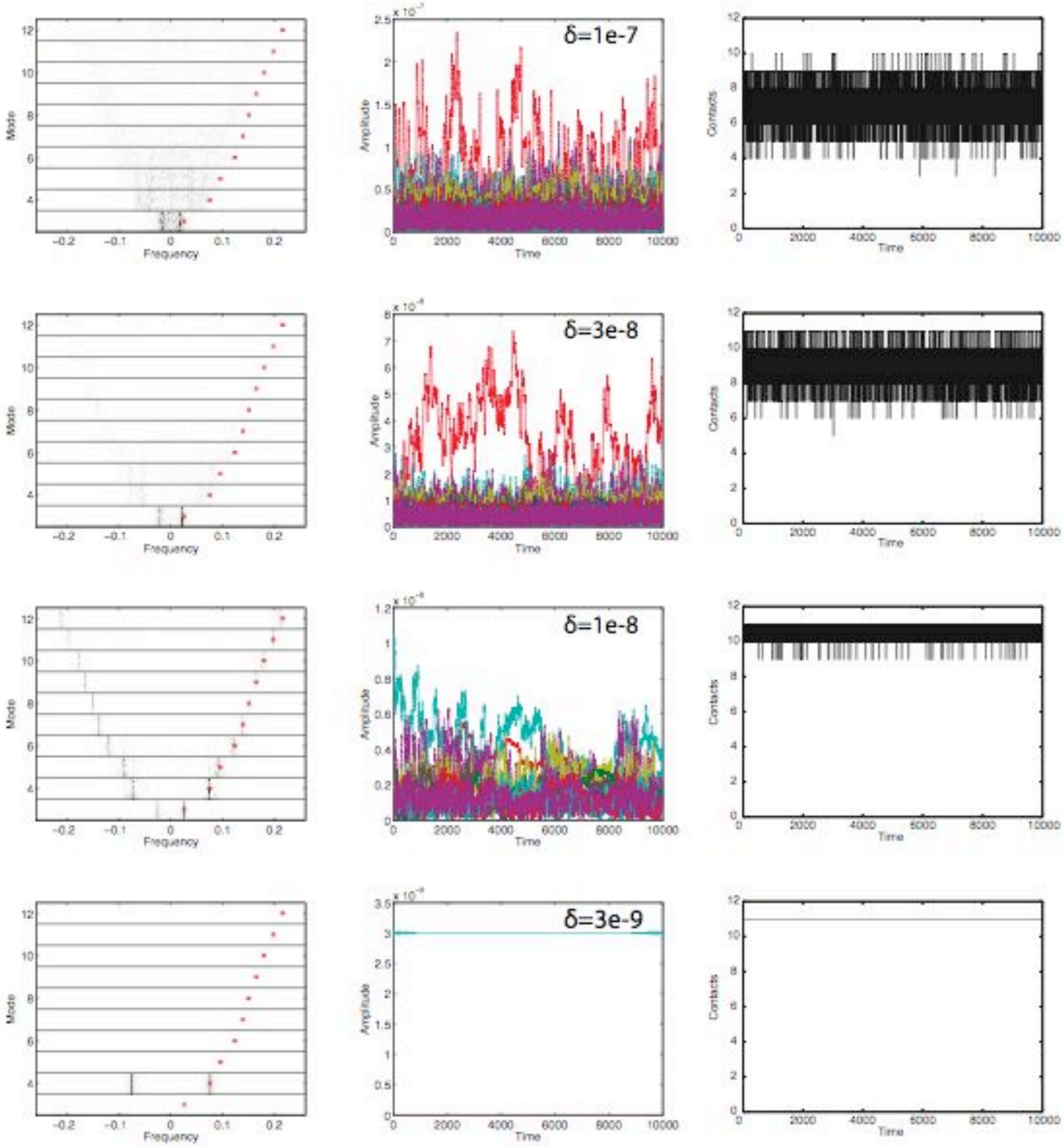


$$A_m(t) = \int d\omega e^{-i\omega t} H(\omega)\left(\int dt \Delta\vec{r}(t)\bullet\hat{e}_m e^{i\omega t}\right)$$

`Phase Diagram'



Dispersion due to Contact Breaking

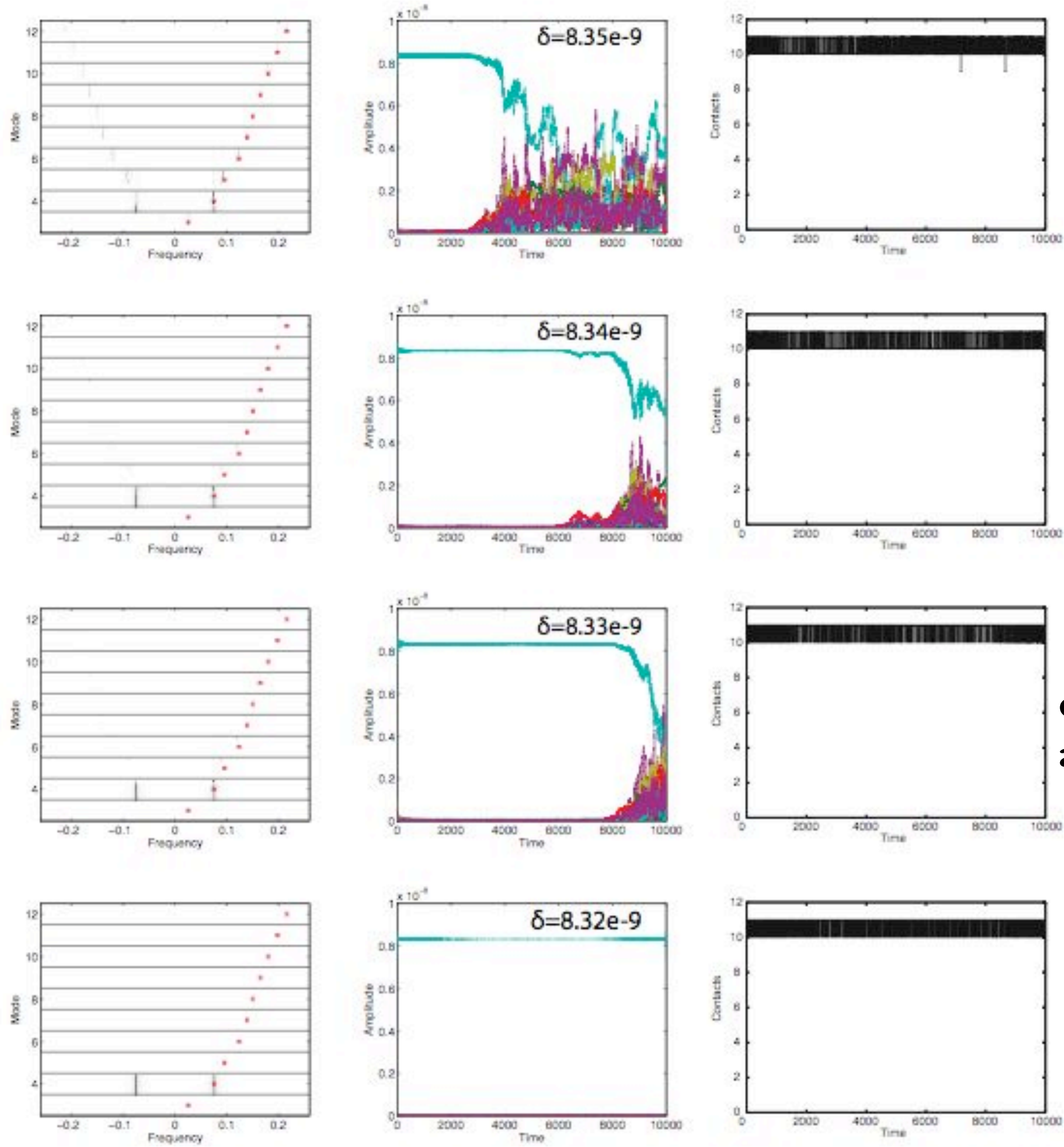


continuous spectrum

contacts break/reform

no contacts break

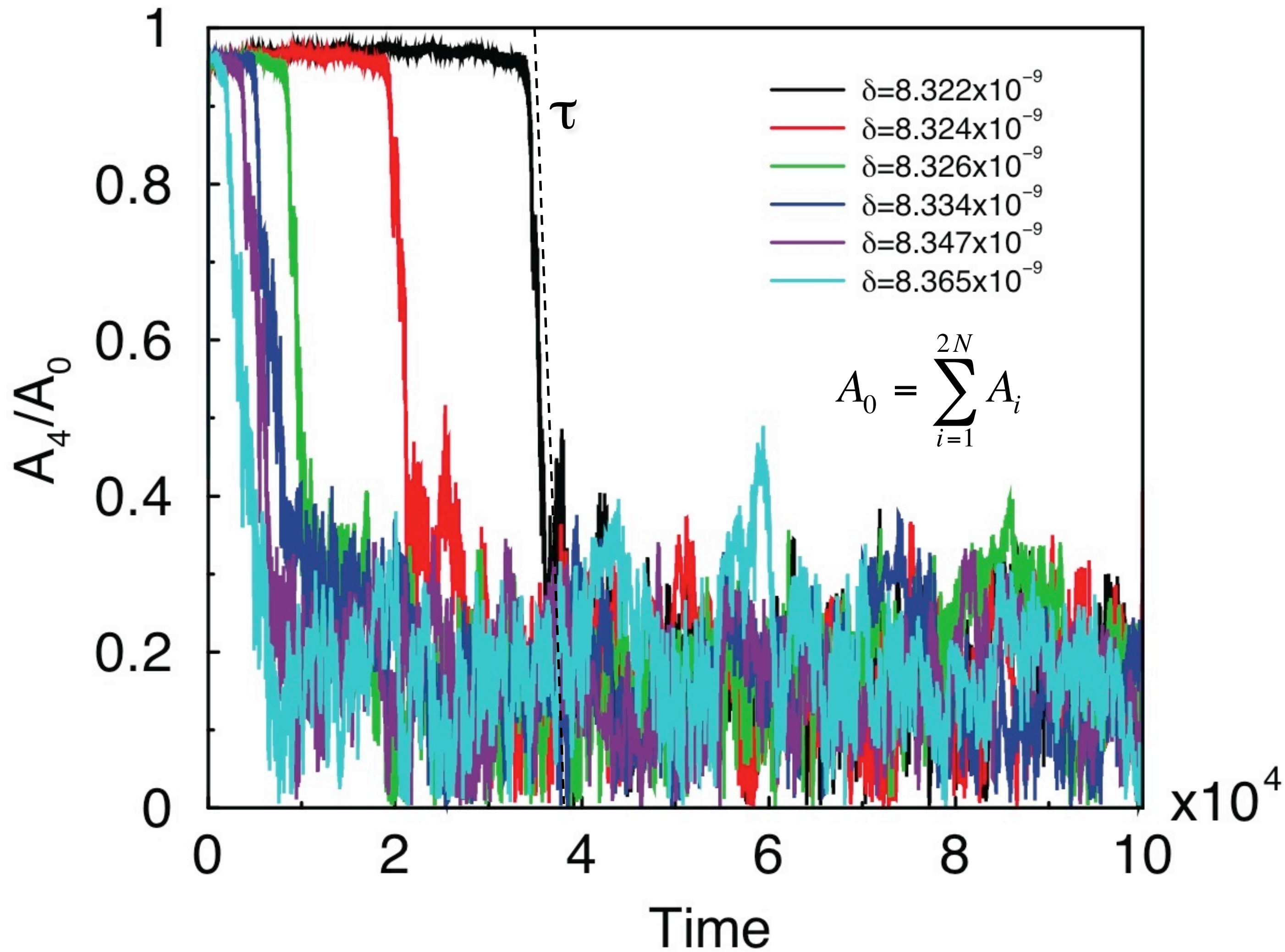
close-up



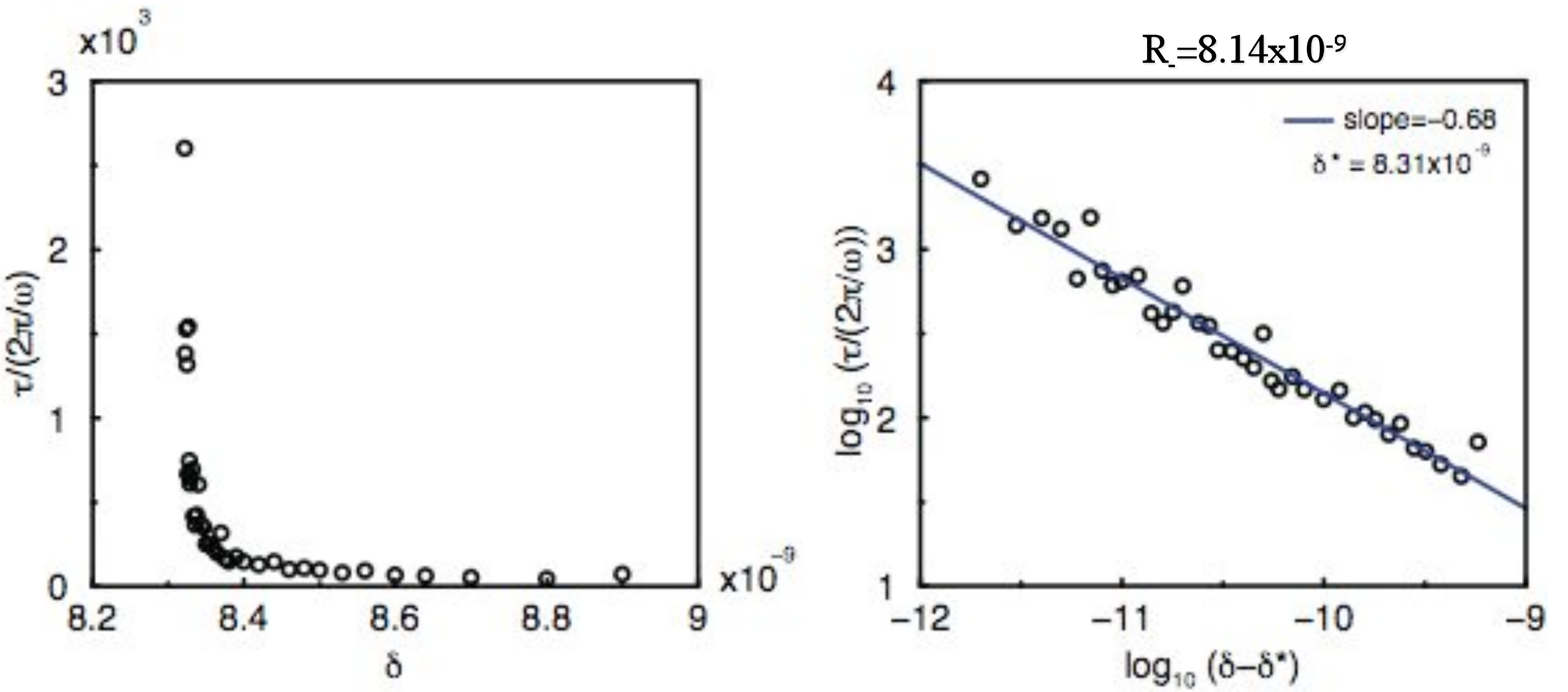
onset of anharmonicity

contacts break/reform

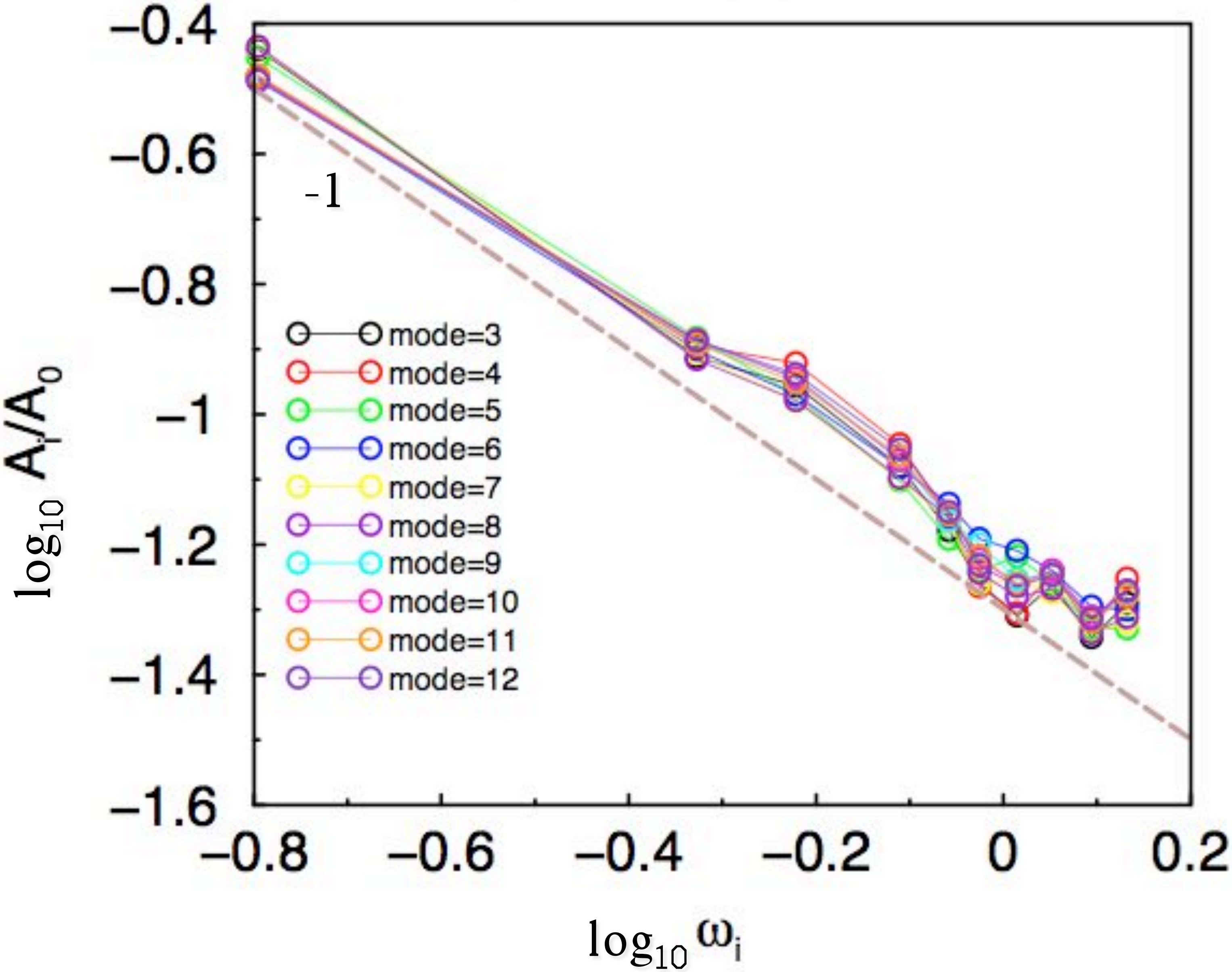
Time Dependence of Anharmonicity



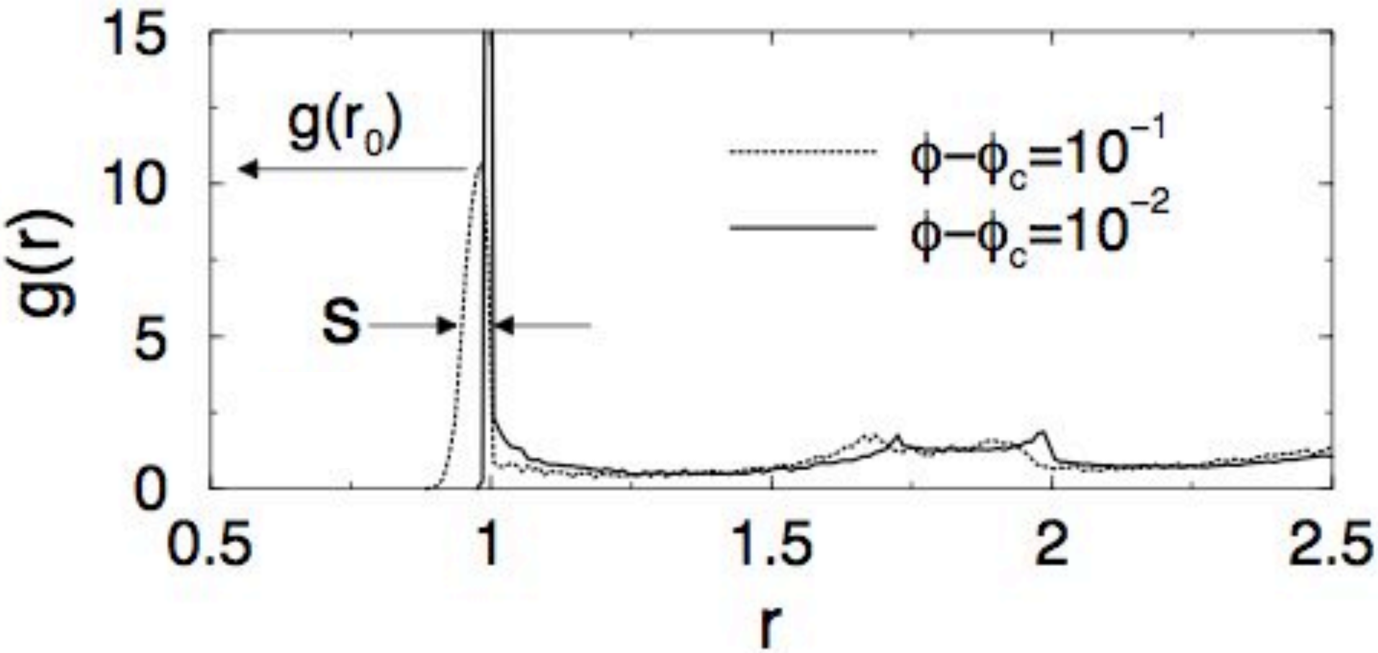
Can we extract timescale τ to become anharmonic?



Steady State: Equipartition



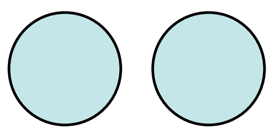
Can we predict onset of anharmonicity from g(r)?



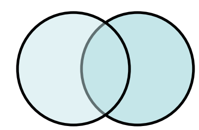
Focus on first peak of g(r)

$$R = \frac{r_{ij} - \sigma_{ij}}{\sigma_{ij}}$$

R > 0: underlap

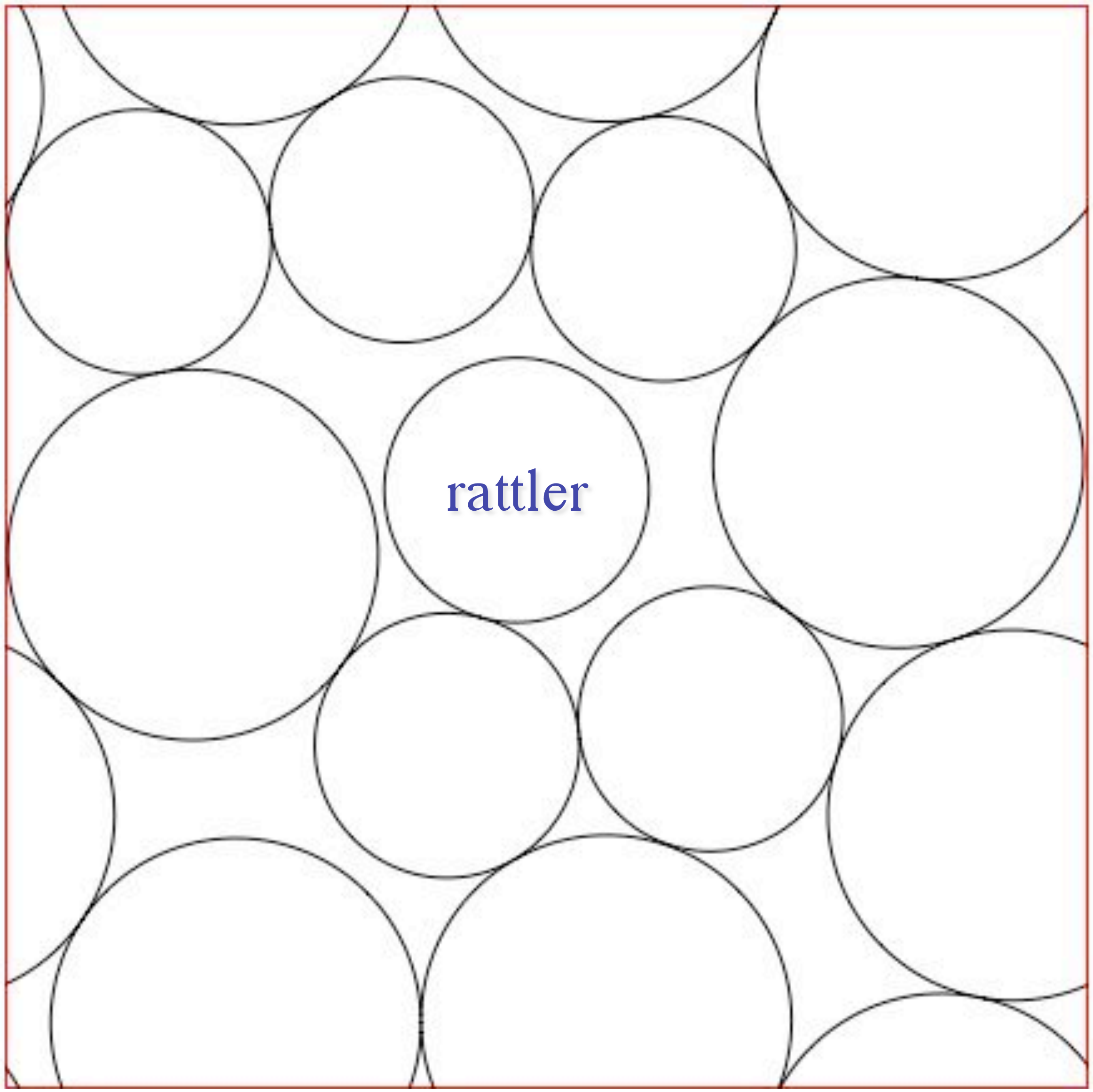


R < 0: overlap



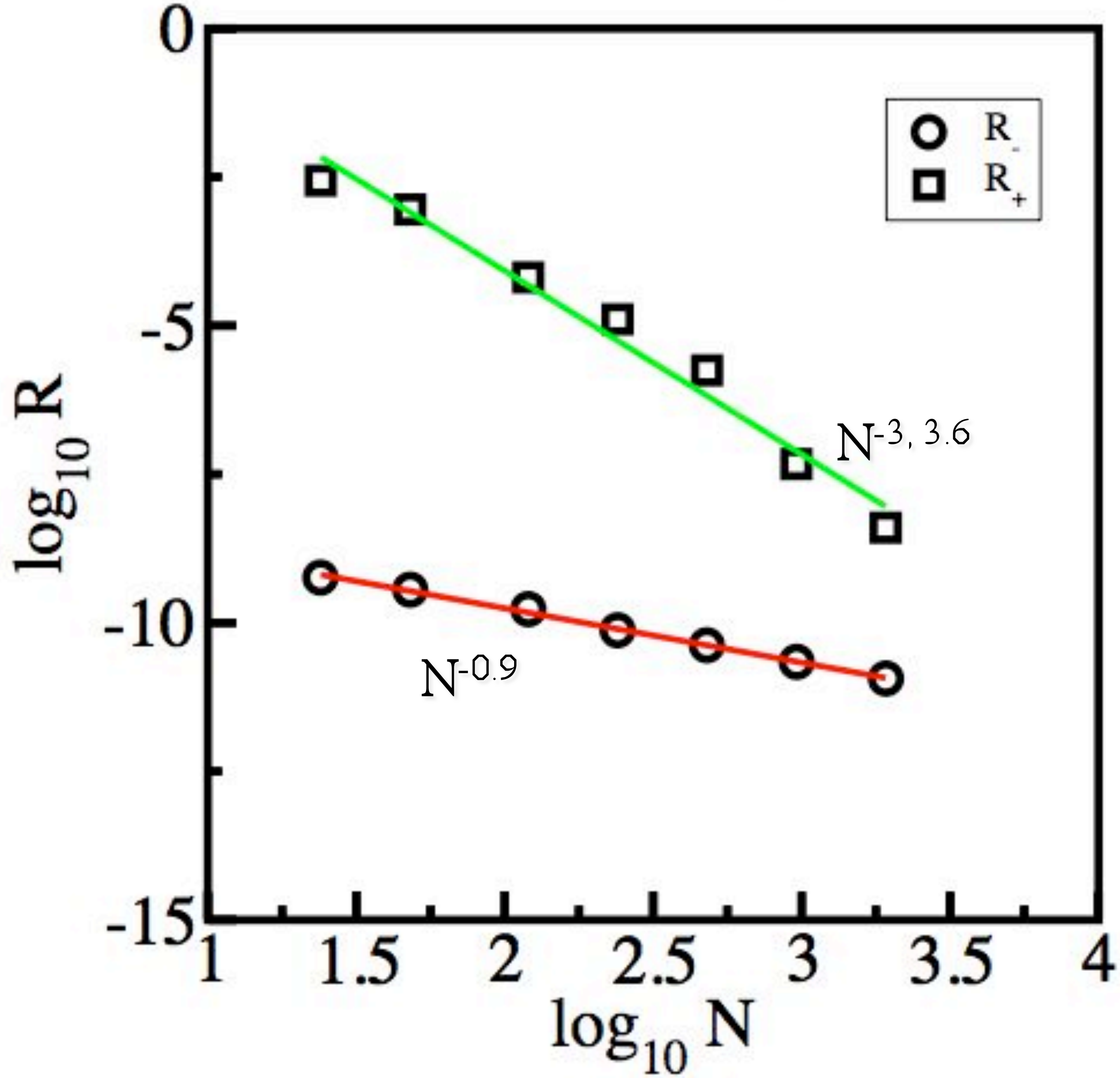
R+: smallest R>0; first contact to form

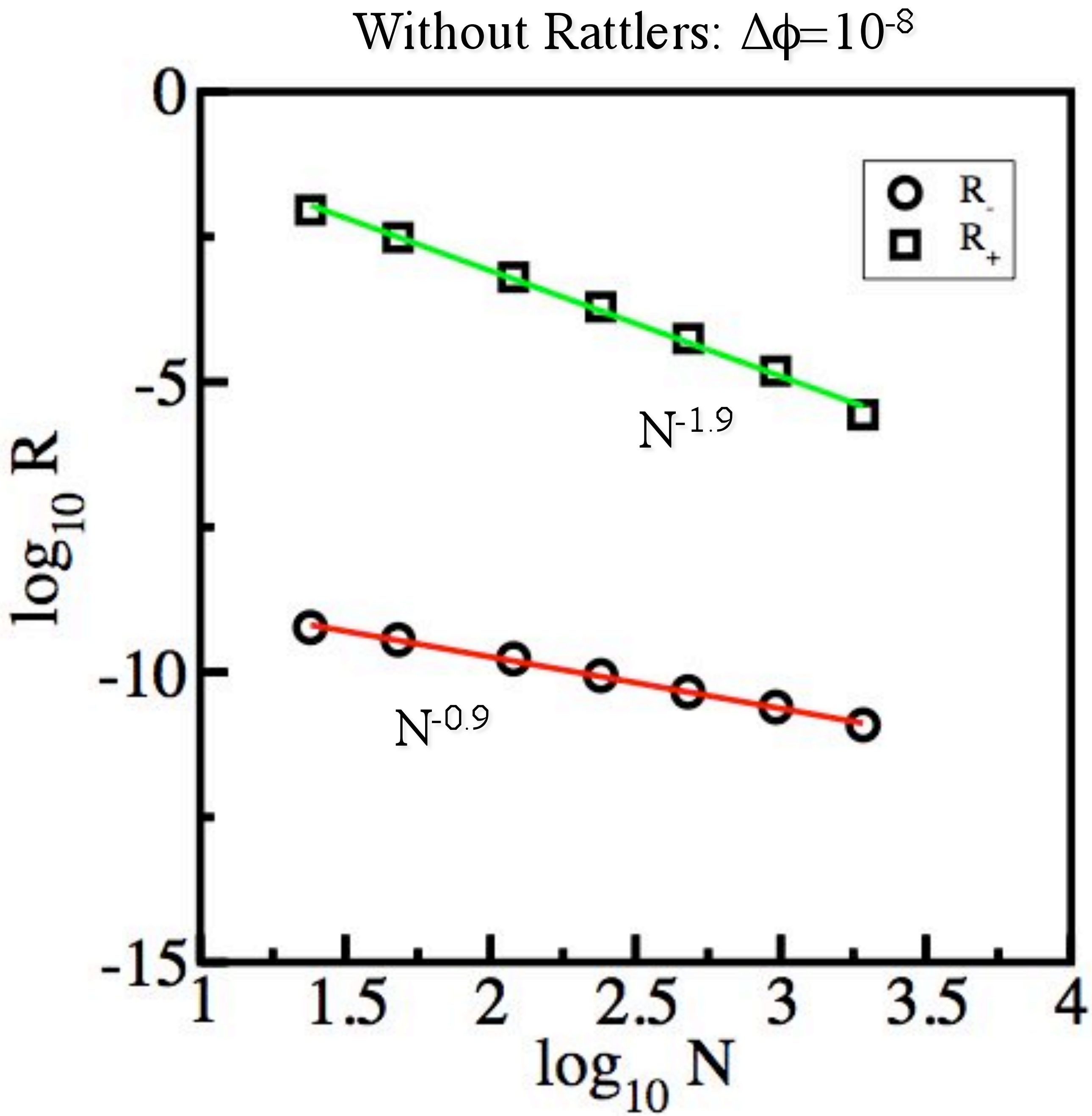
R-: smallest R<0; first contact to break



Rattler: < 3 contacts*

With Rattlers: $\Delta\phi=10^{-8}$





Without Rattlers: Δϕ=10-8
0
-5
-10
-15
1
1.5
2
2.5
3
3.5
4
log10 R
log10 N
R-
R+
N-1.9
N-0.9

Predictions from g(r)

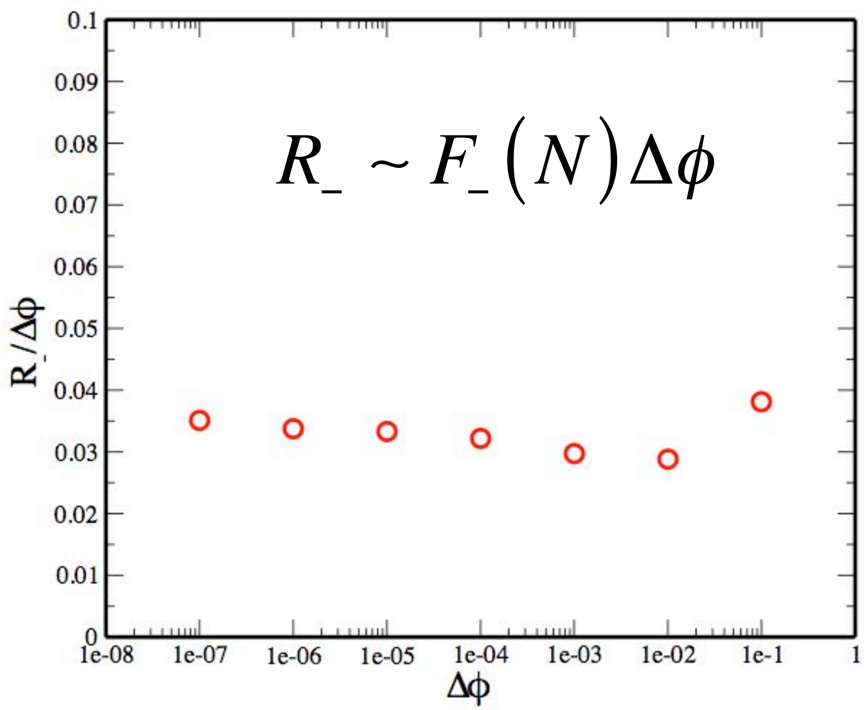
$$x = 1 - \frac{r}{\sigma} > 0 \qquad g(x) = g_0 \exp\left[-\left(\frac{\alpha_1}{x} + \frac{\alpha_2}{x^2}\right)^{-1}\right] \qquad R_- \sim N^{-1}$$

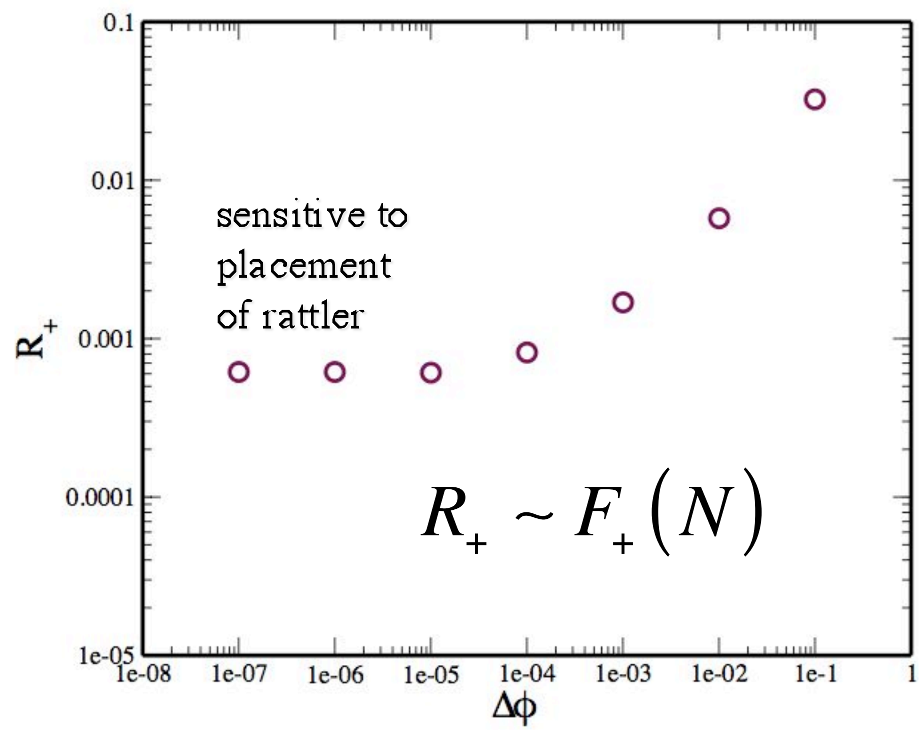
$$x = 1 - \frac{r}{\sigma} < 0 \qquad g(x) \sim x^{-\eta} \qquad R_+ \sim N^{\frac{1}{\eta-1}}$$

η~0.4-0.5

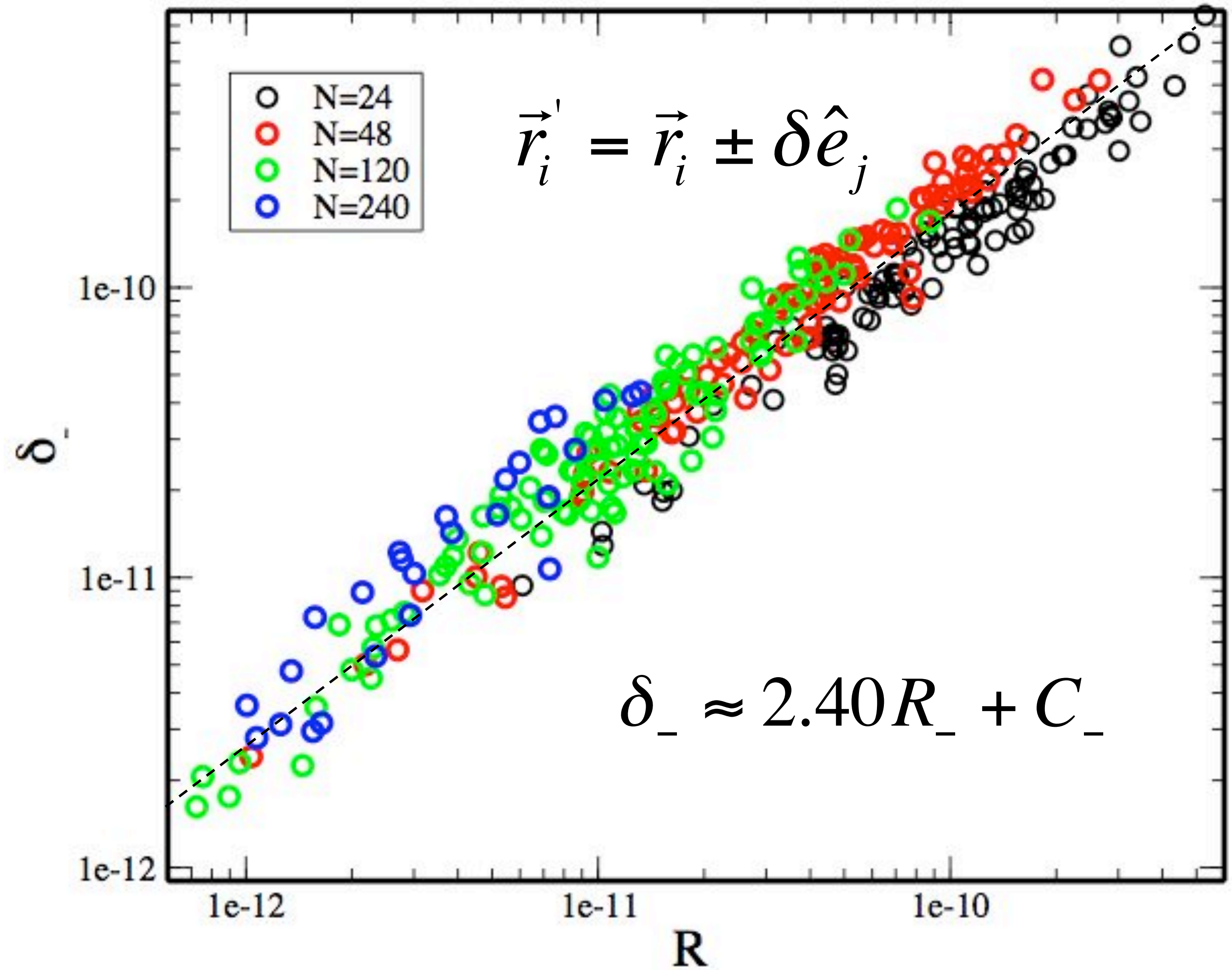
L. E. Silbert, A. J. Liu, and S. R. Nagel, "Structural signatures of the unjamming transition at zero temperature," Phys. Rev. E 73 (2006) 041304.
A. Donev, S. Torquato, and F. H. Stillinger, "Pair correlation function characteristics of nearly jammed disordered and ordered hard-sphere packings," Phys. Rev. E 71 (2005) 011105.

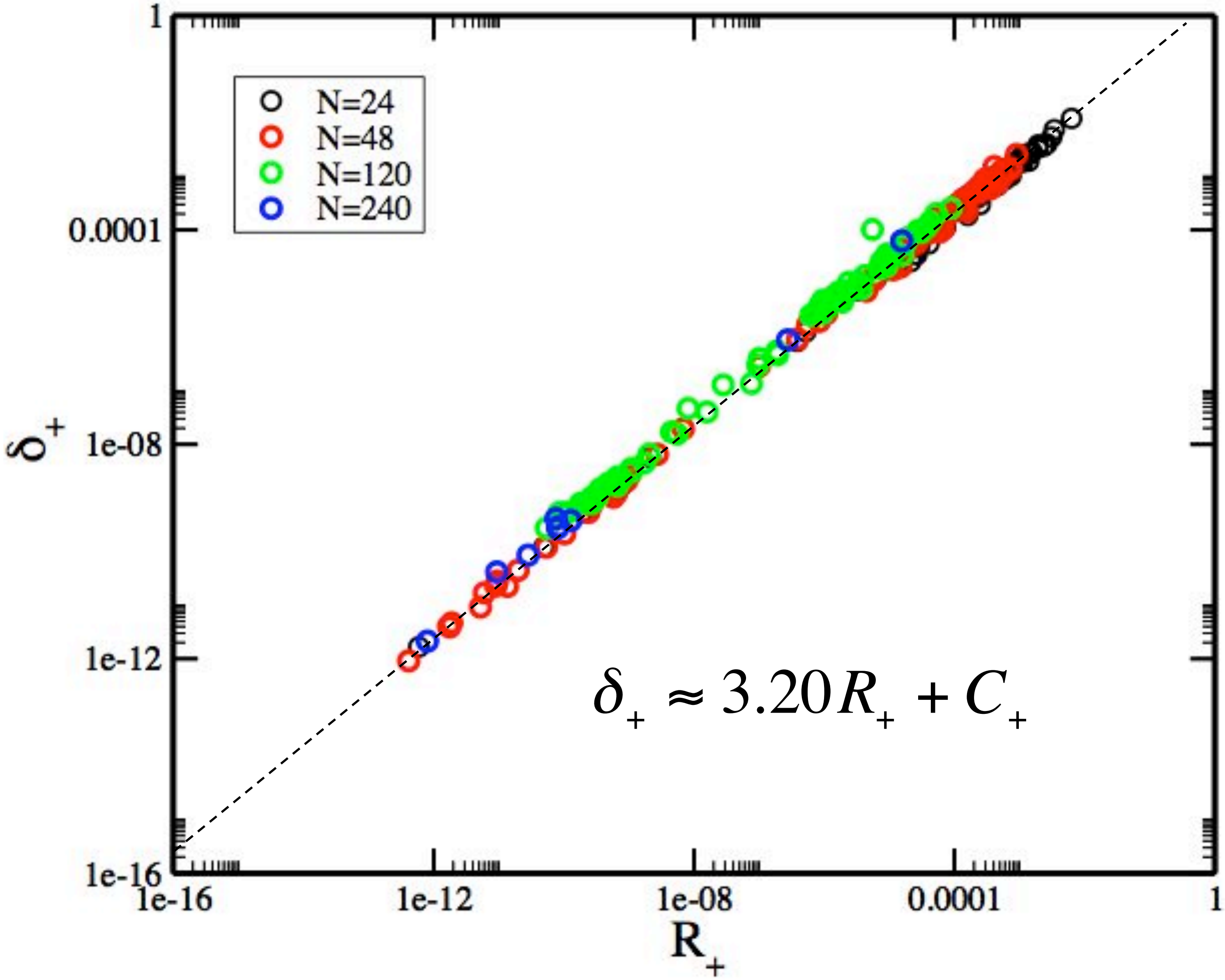
Dependence on Compression Δϕ





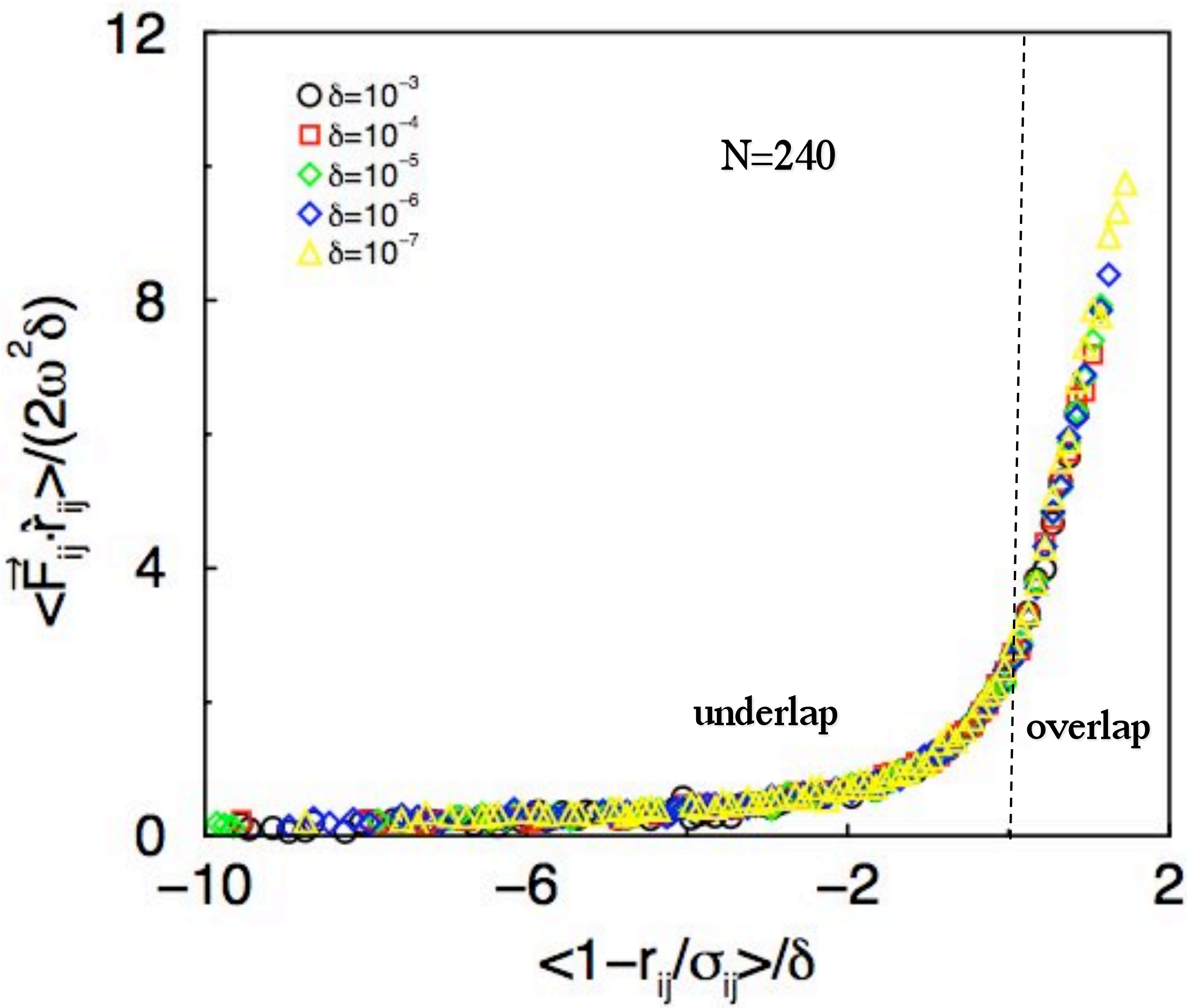
Are R_+ and R_- relevant?



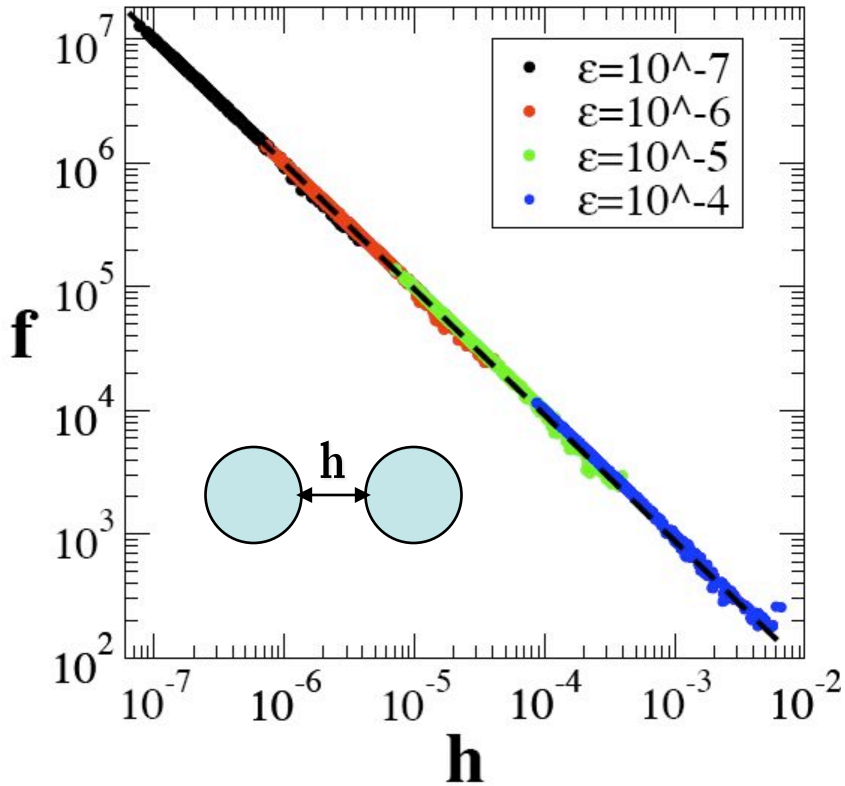


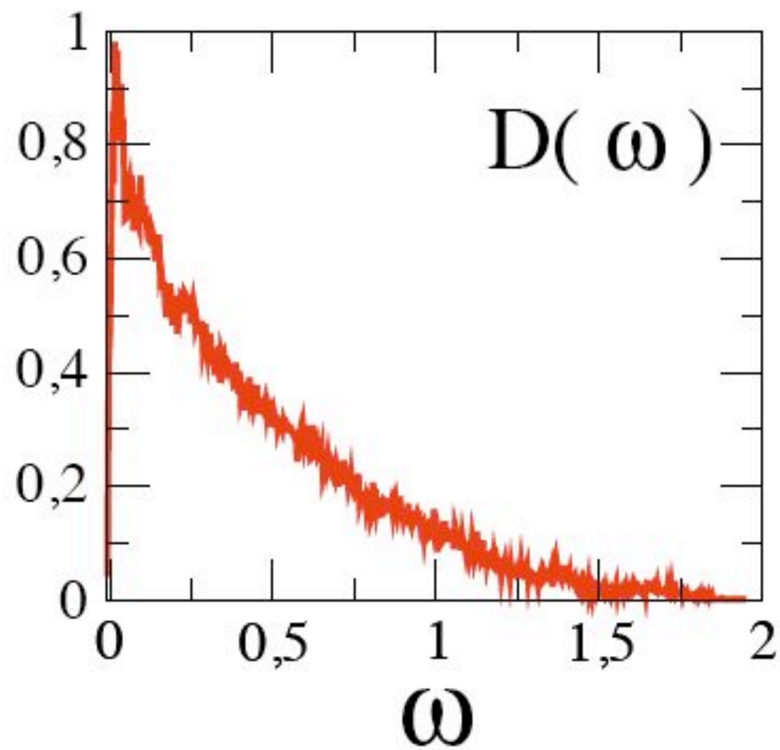
N=24
N=48
N=120
N=240
1
0.0001
1e-08
1e-12
1e-16
1e-16
1e-12
1e-08
0.0001
1
δ+
R+
δ+ ≈ 3.20 R+ + C+

Effective Pair Force

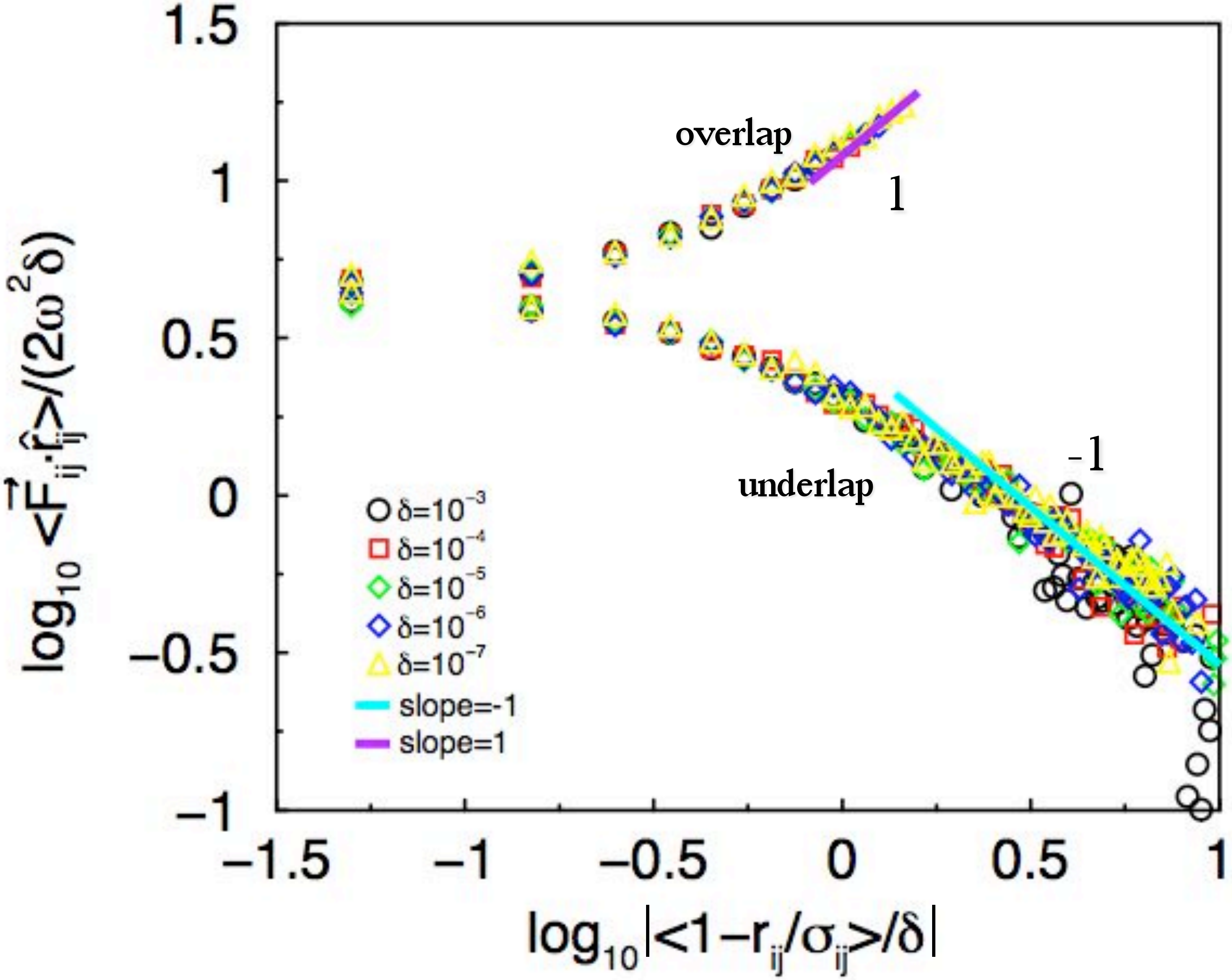


Effective hard-sphere interactions





C. Brito and M. Wyart, " On the rigidity of a hard-sphere glass near random close packing," Europhys. Lett. 76 (2006) 149.



overlap
1
underlap
-1
δ=10^-3
δ=10^-4
δ=10^-5
δ=10^-6
δ=10^-7
slope=-1
slope=1
1.5
1
0.5
0
−0.5
−1
−1.5
log10 <F_ij·r̂_ij>/(2ω^2δ)
log10|<1−r_ij/σ_ij>/δ|

To-do List

- Determine fraction of contacts near breaking or forming as a function of $\Delta\phi$ and N
- Determine fraction of contacts that must break/form to cause anharmonicity?
- Measure effective potential in steady-state; Calculate dynamical matrix and determine to what extent there is harmonic regime
- Add explicit dissipation