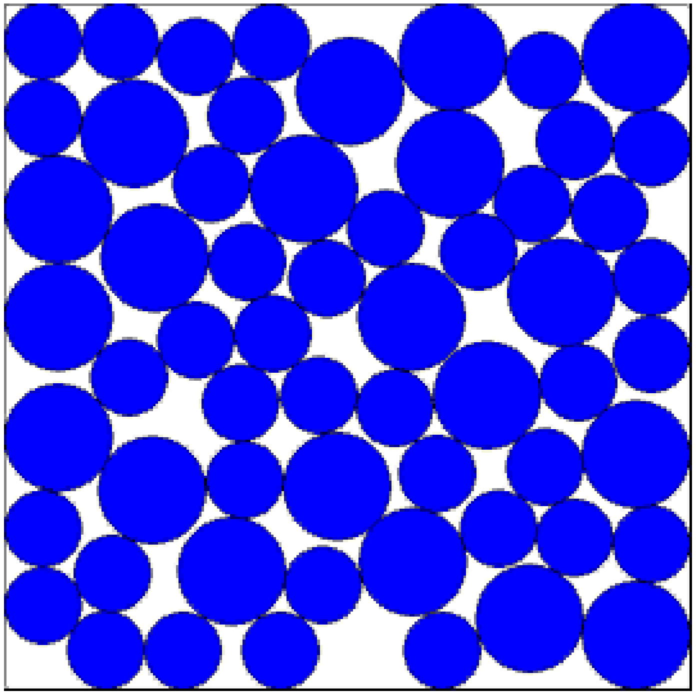
Granular Materials Laboratory



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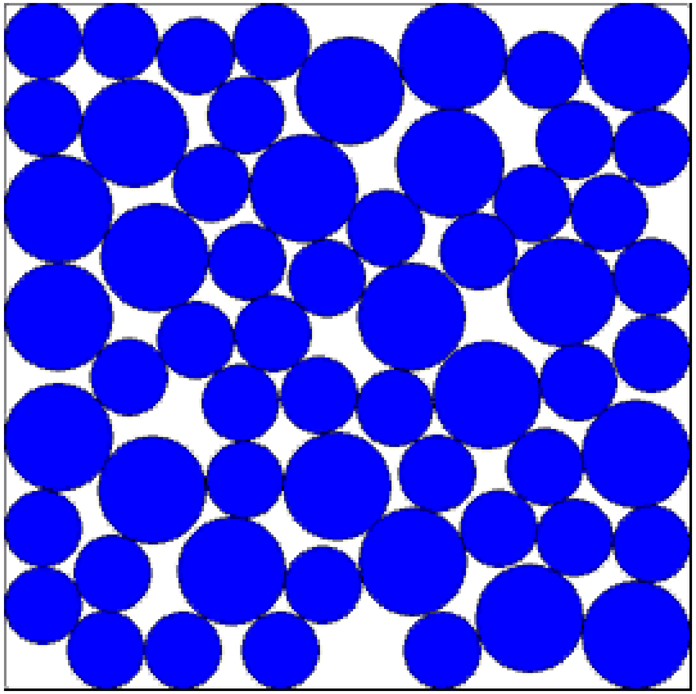
the City College of New York

OF THE CITY UNIVERSITY OF NEW YORK

Novel plasticity of purely repulsive solids near jamming



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NSF-DMR-PREM-0934206
NSF-CBET-0968013

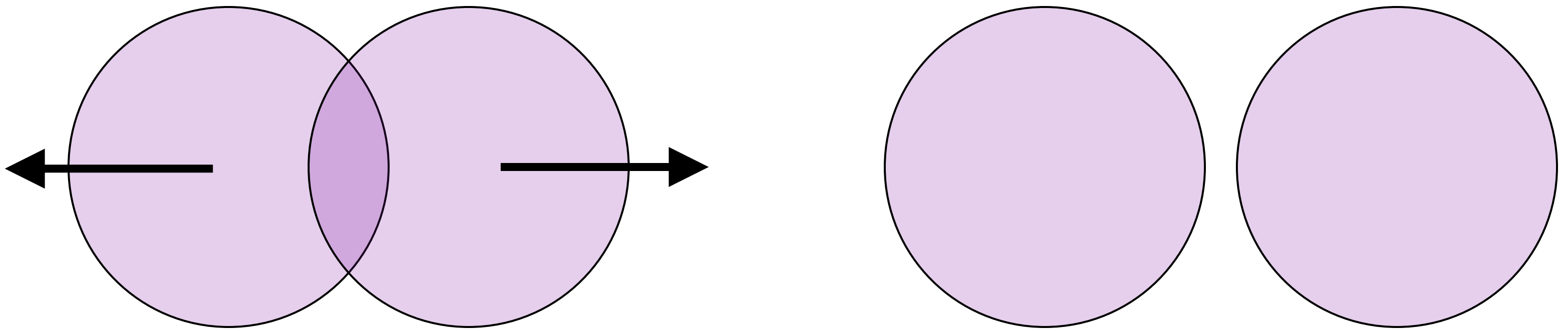
KITP 2014

Purely Repulsive Jammed Solids

2D Molecular Dynamics

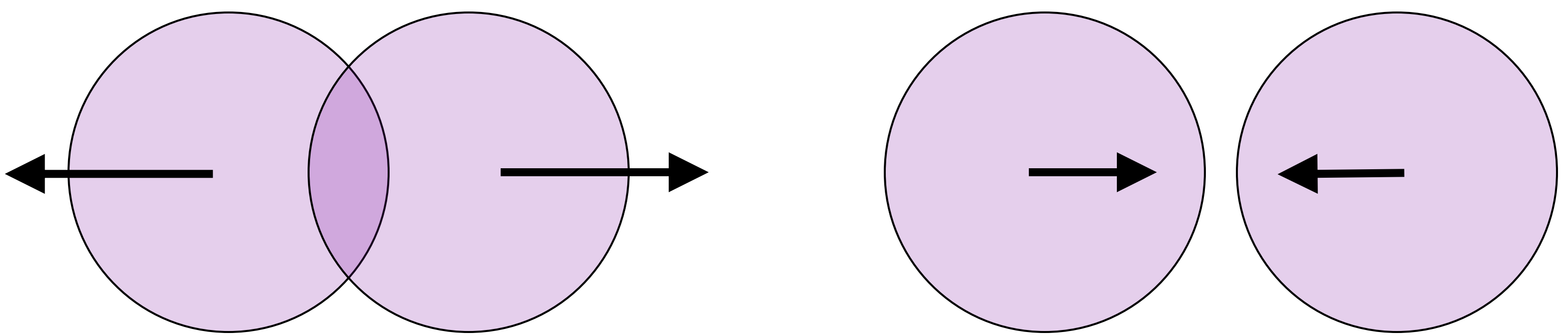
- 2D frictionless bidisperse mechanically stable disk packings.
  - 50:50 mixture, $D_L / D_S = 1.4$
  - Jammed (ϕ_J), many $\Delta\phi = \phi - \phi_J$
  - Vary Temperature
  - Measure Density of Vibrational States
  - Measure Response to Shear
    - Compare repulsive interaction to two-sided springs

Purely Repulsive



F=-Kδ F=0

Double Sided Springs



F=-Kδ F=Kδ

Normal Modes in Disorder System

Displacements:

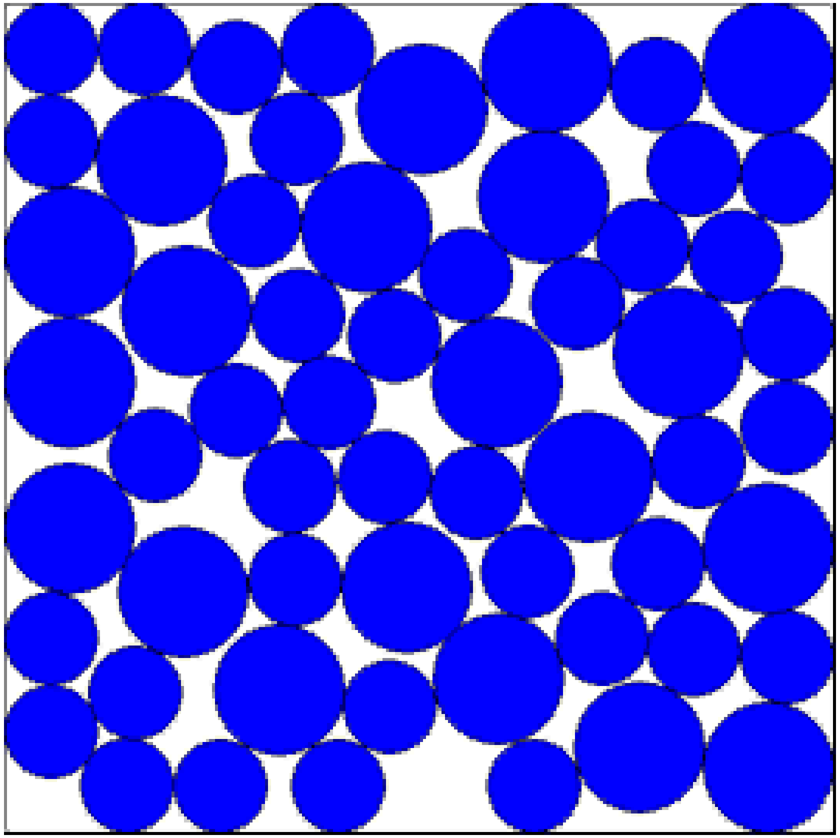
$$\mathbf{U}_n = \mathbf{X}_n - \mathbf{X}_n^{\mathbf{0}}$$

Dynamical Matrix:

$$\kappa_{nk} = \nabla_n \nabla_k V(\mathbf{X}_n^0)$$

Newton's Law:

$$m\ddot{\mathbf{U}}_n \cong \sum_{k=1}^{2N} \kappa_{nk} \mathbf{U}_k$$



Solution:

$$\mathbf{U}_n = \sum_{k=1}^{2N} A_k \hat{\varepsilon}_{kn} \cos(\omega_k t + \varphi_k)$$

Vibrational Density of States

Vibrational Density of States

Dynamical Matrix:

$$\kappa_{nk} = \nabla_n \nabla_k V(\mathbf{X}_n^0)$$

Covariance Matrix:

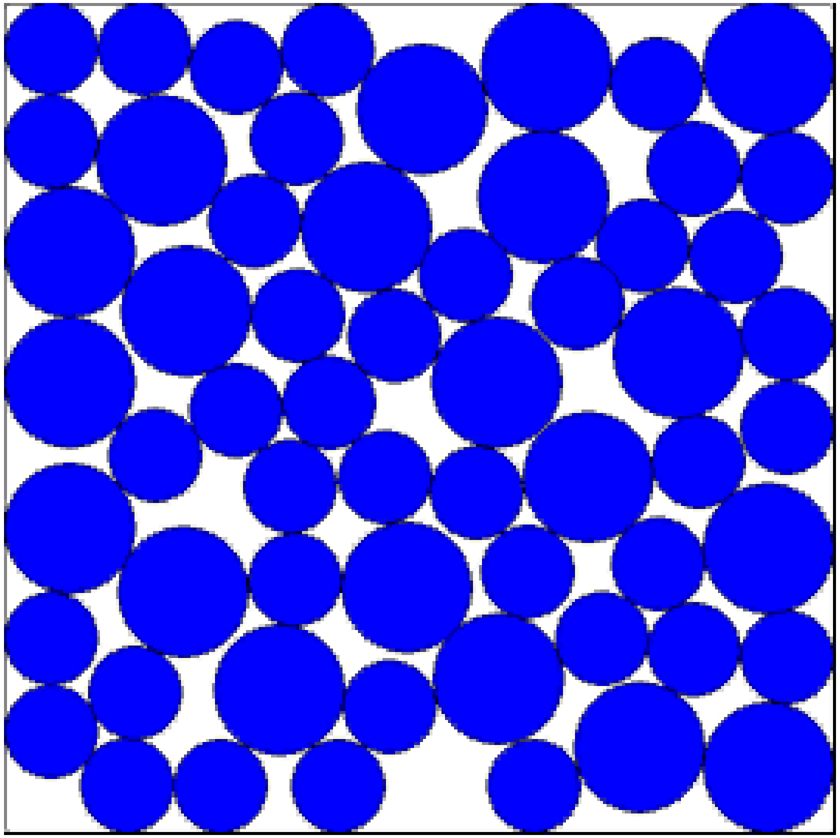
$$\tilde{\kappa}_{nk} = C_{nm}^{-1} V_{mk}$$

$$C_{nm} = \langle \mathbf{U}_n \mathbf{U}_m \rangle$$

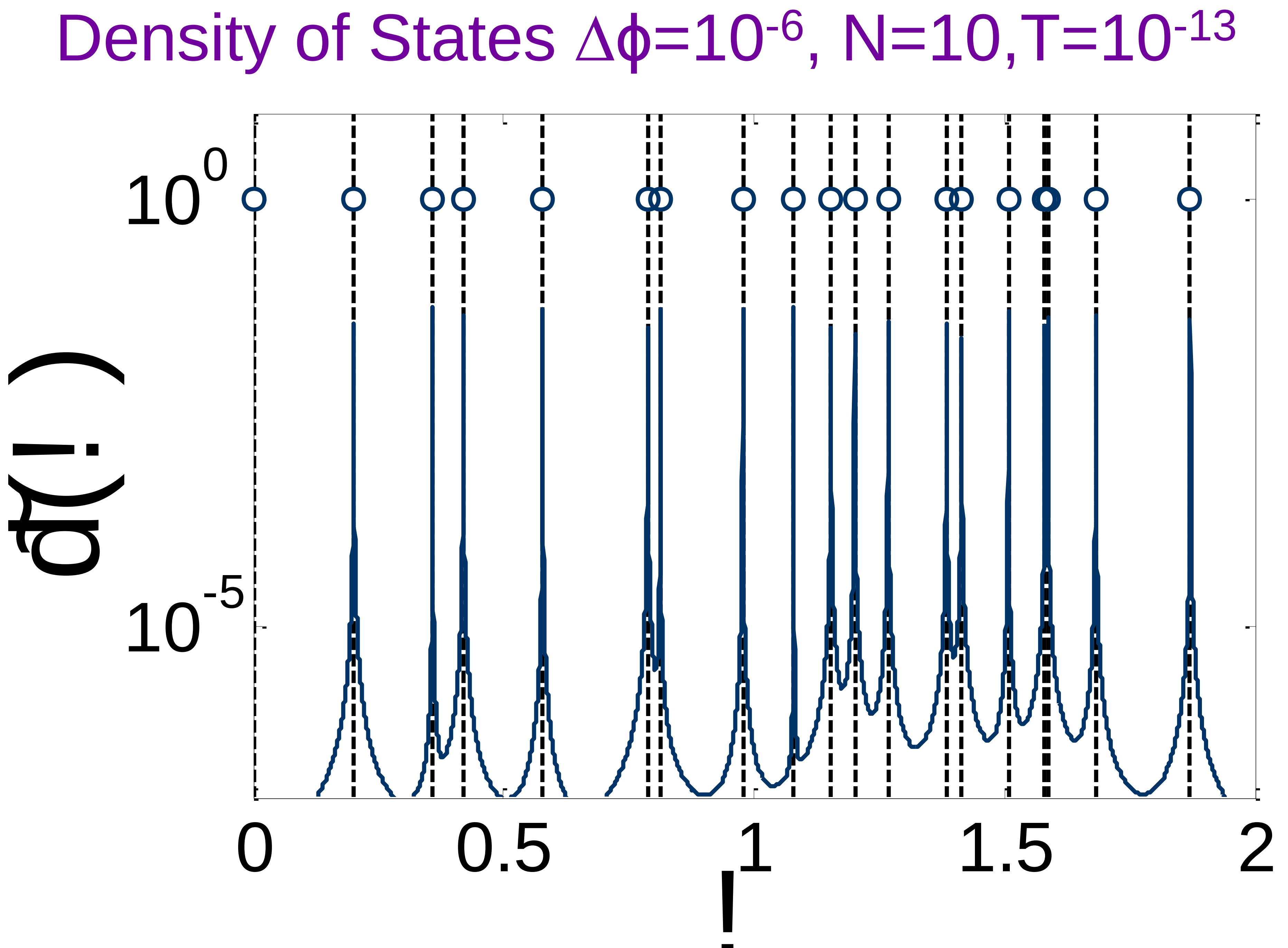
$$V_{nm} = \langle \mathbf{V}_n \mathbf{V}_m \rangle$$

Eigenvalues:

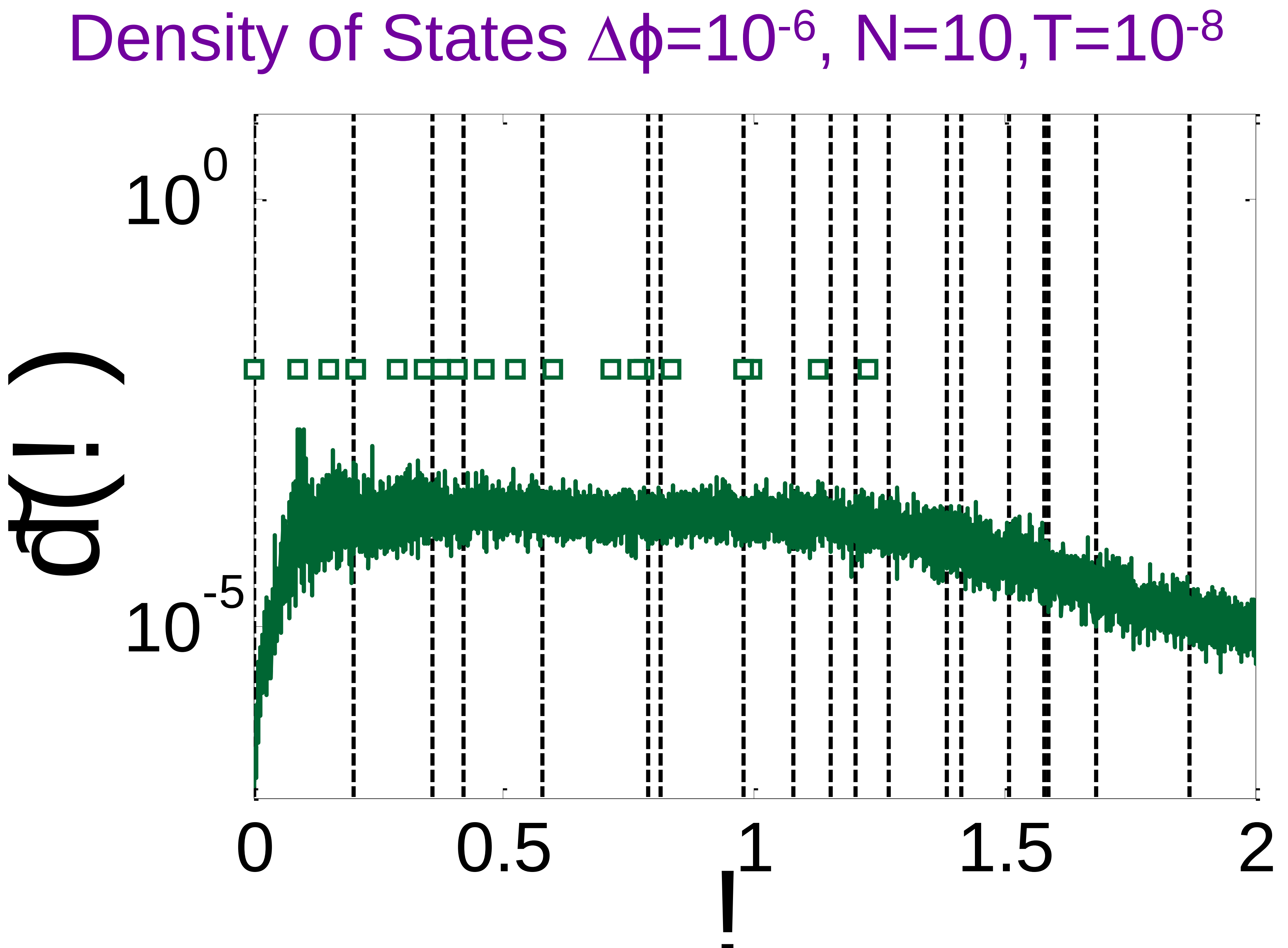
$$\omega_n = \sqrt{\lambda_n / m} = \tilde{\omega}_n = \sqrt{\tilde{\lambda}_n / m}$$



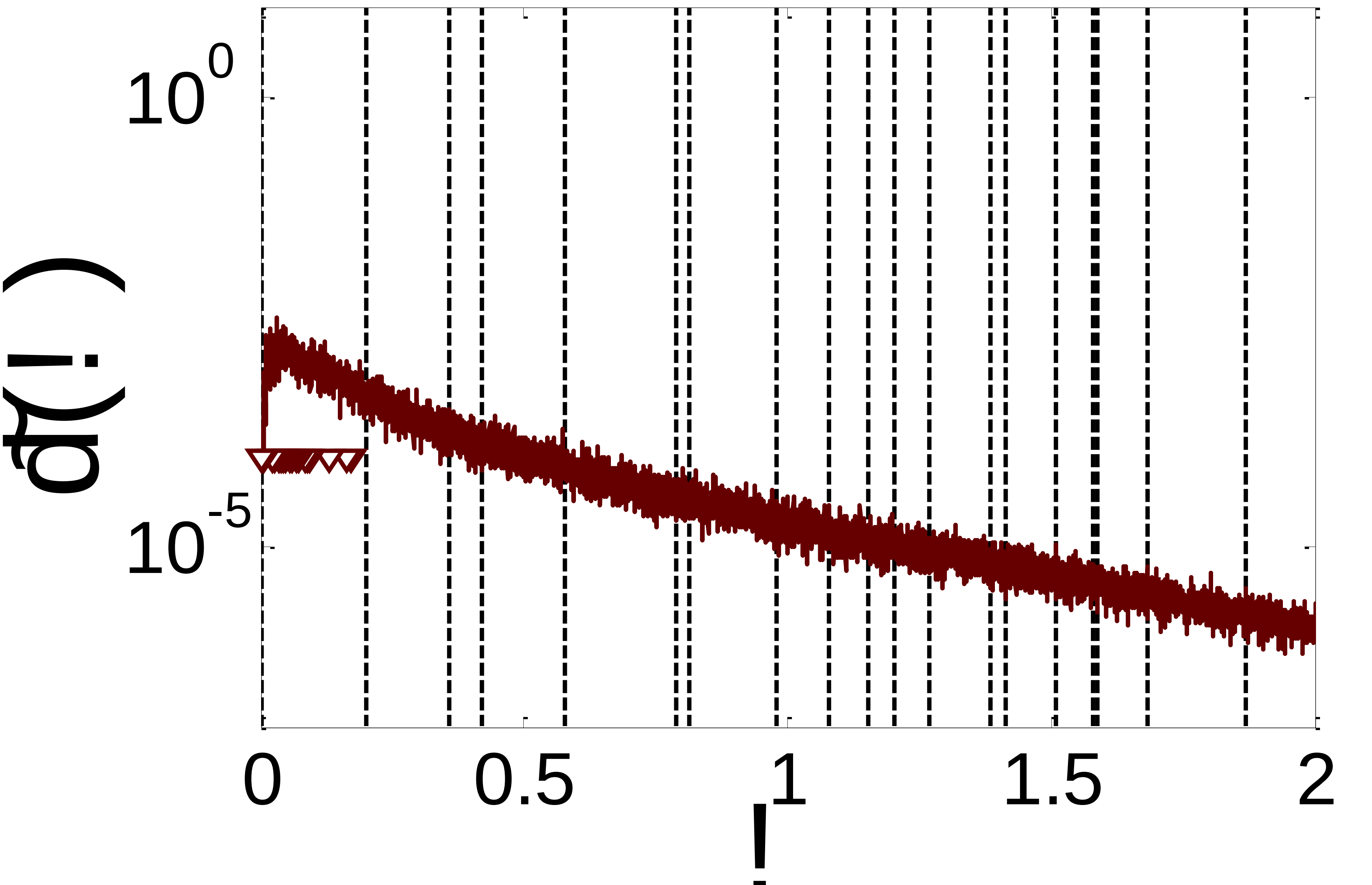
$$D(\omega) = \sum_n \delta(\omega - \omega_n) = \sum_n \delta(\omega - \tilde{\omega}_n) = \sum_k \int \frac{\vec{V}_k(t) \cdot \vec{V}_k(0)}{\sum_m \vec{V}_m(0) \cdot \vec{V}_m(0)} e^{i\omega t} dt$$

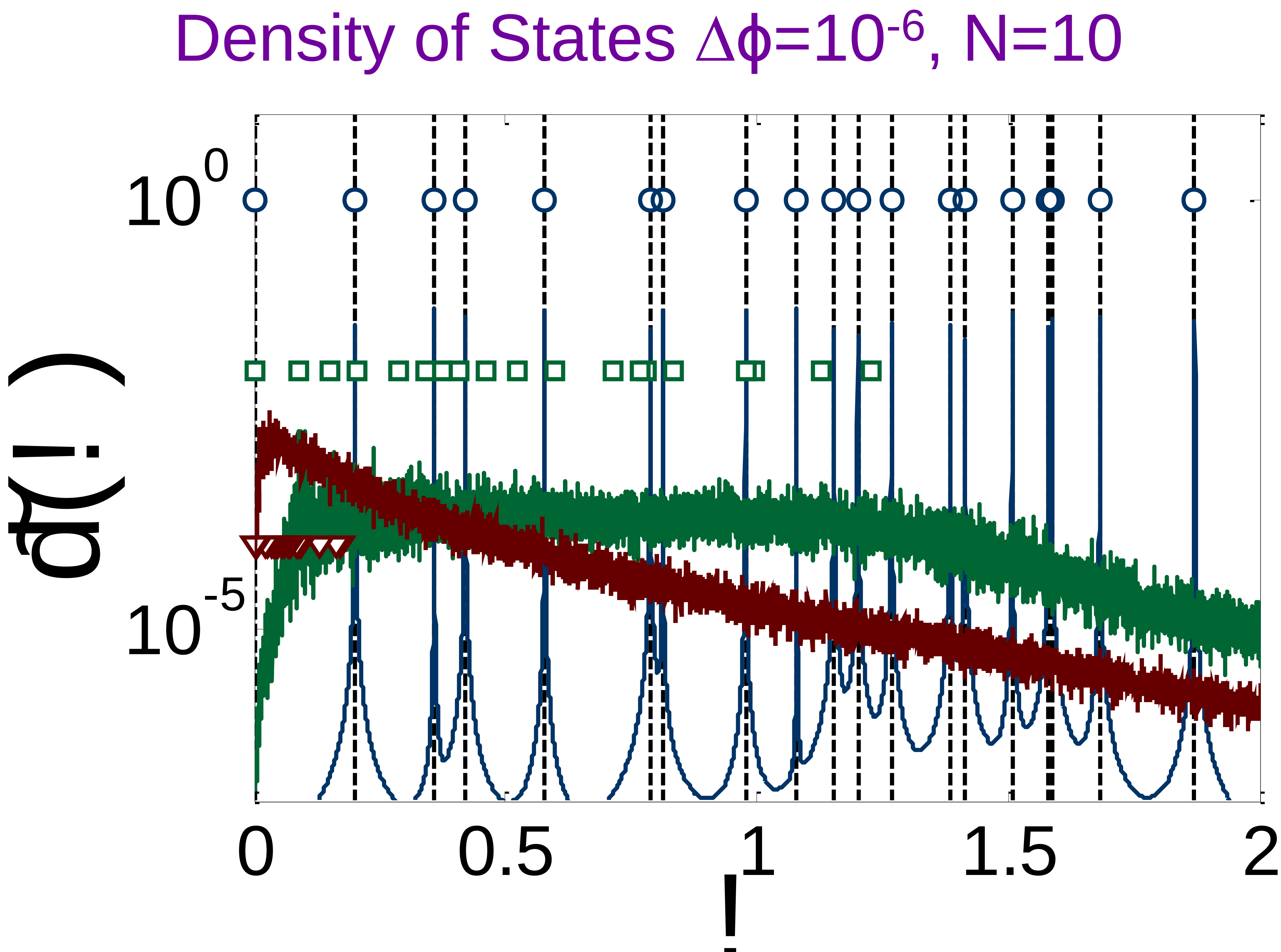


Density of States Δϕ=10-6, N=10,T=10-13
10^0
10^-5
0
0.5
1
1.5
2


Density of States Δφ=10-6, N=10,T=10-8
10^0
10^-5
0
0.5
1
1.5
2

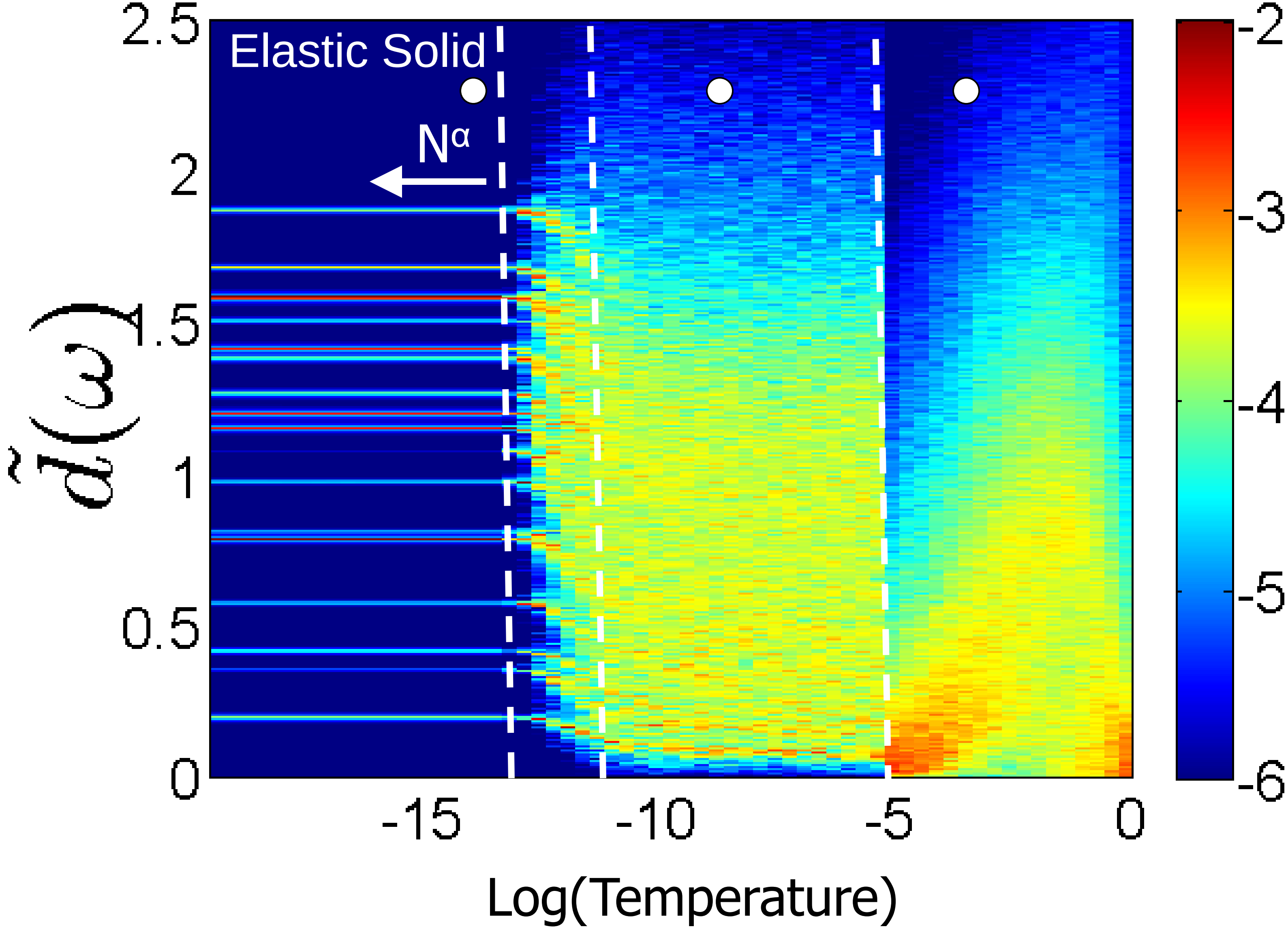
Density of States $\Delta\phi=10^{-6}$, N=10,T=10^{-3}



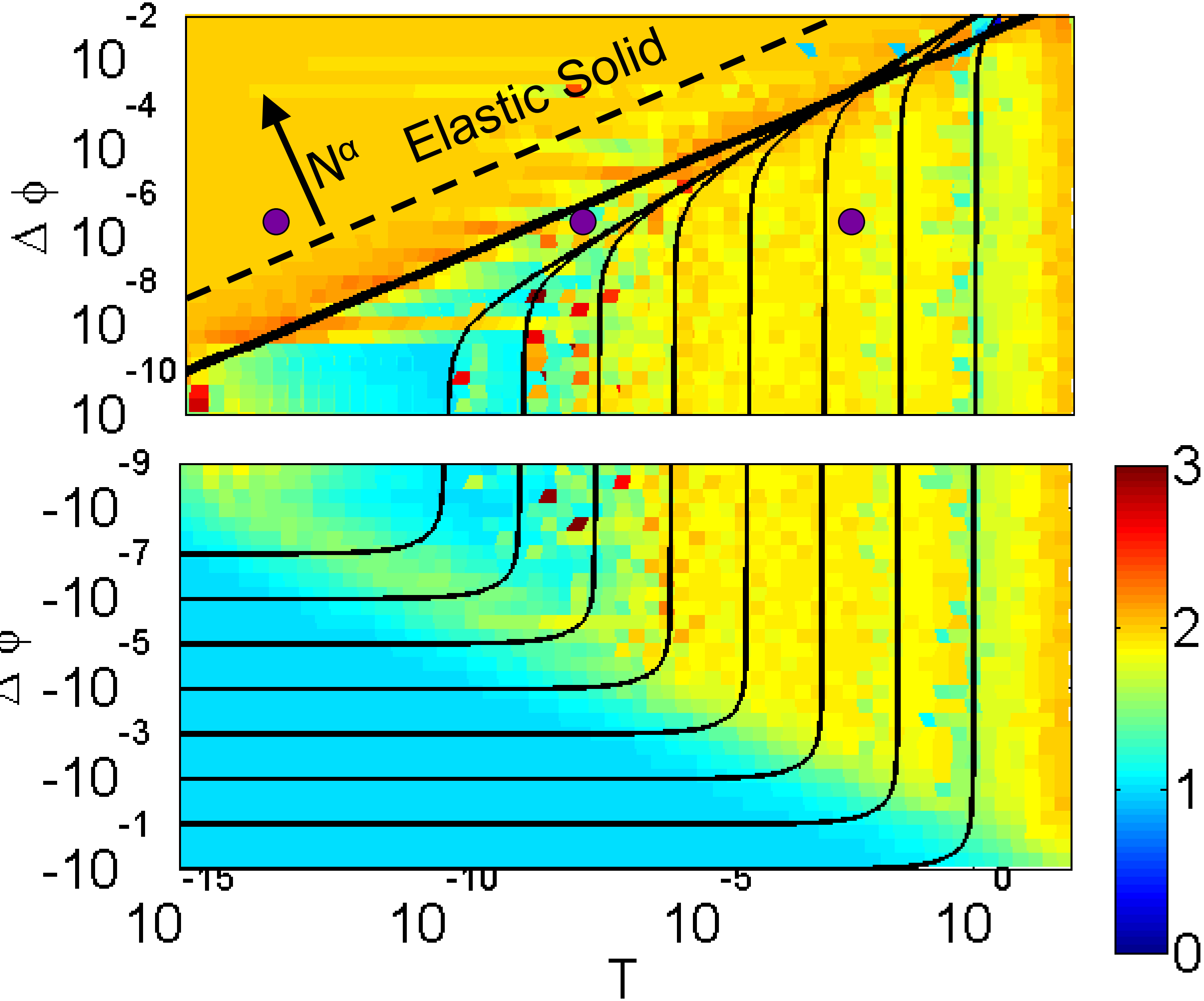


Density of States Δφ=10^-6, N=10
10^0
10^-5
0
0.5
1
1.5
2

Density of States N=10



Heat Capacity



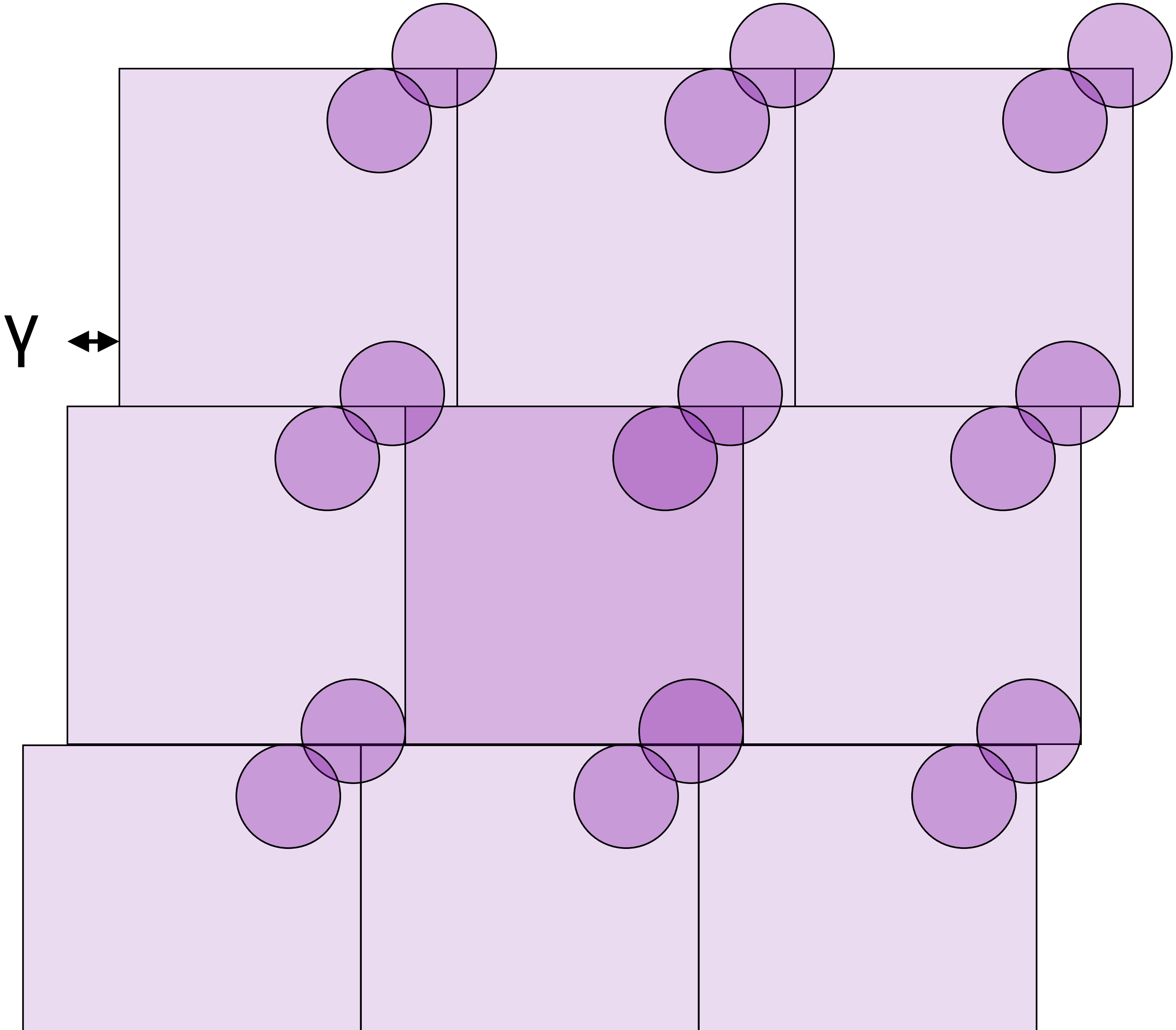
Stress vs. Strain

Purely Repulsive

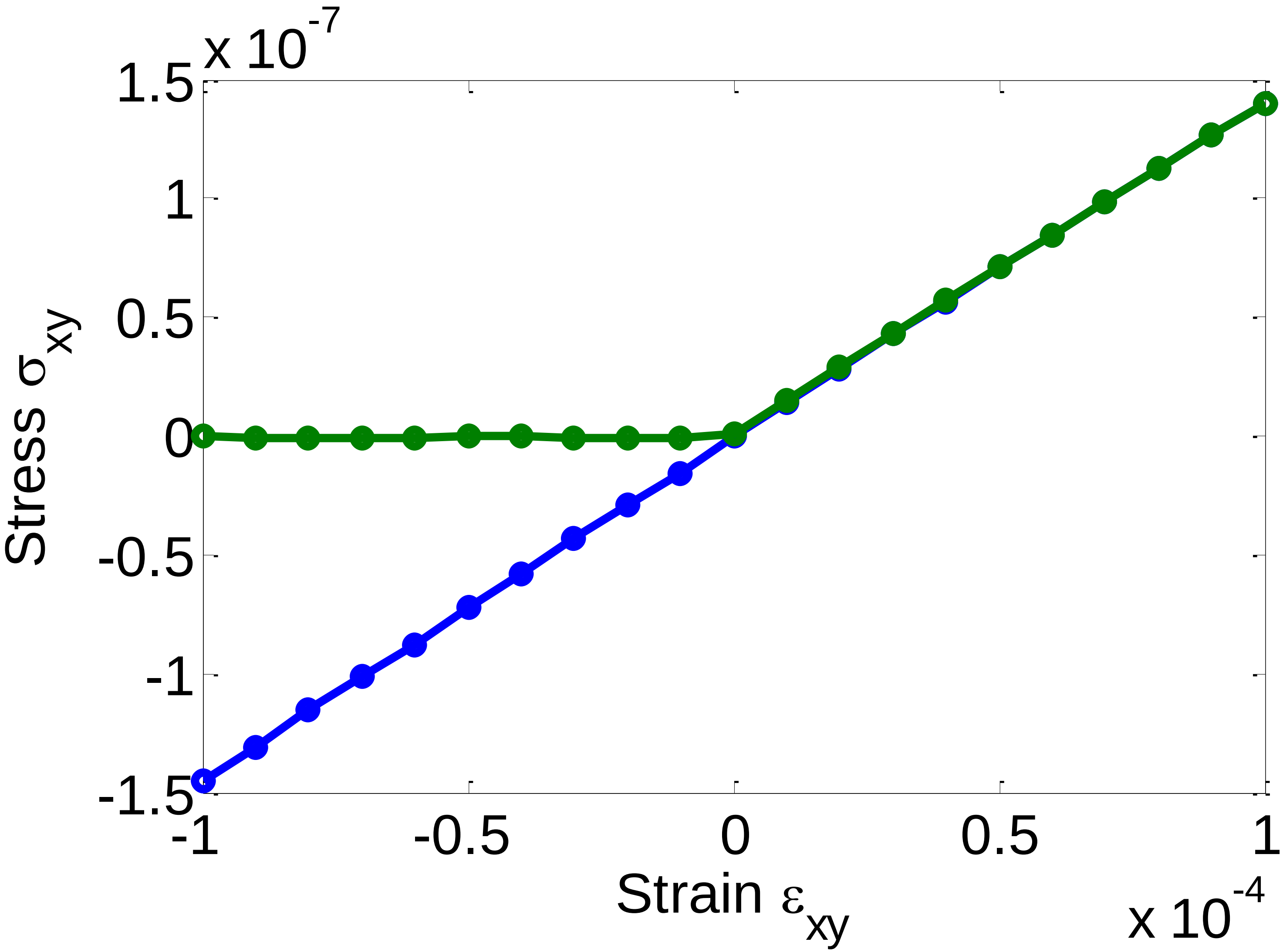
vs.

Double-Sided

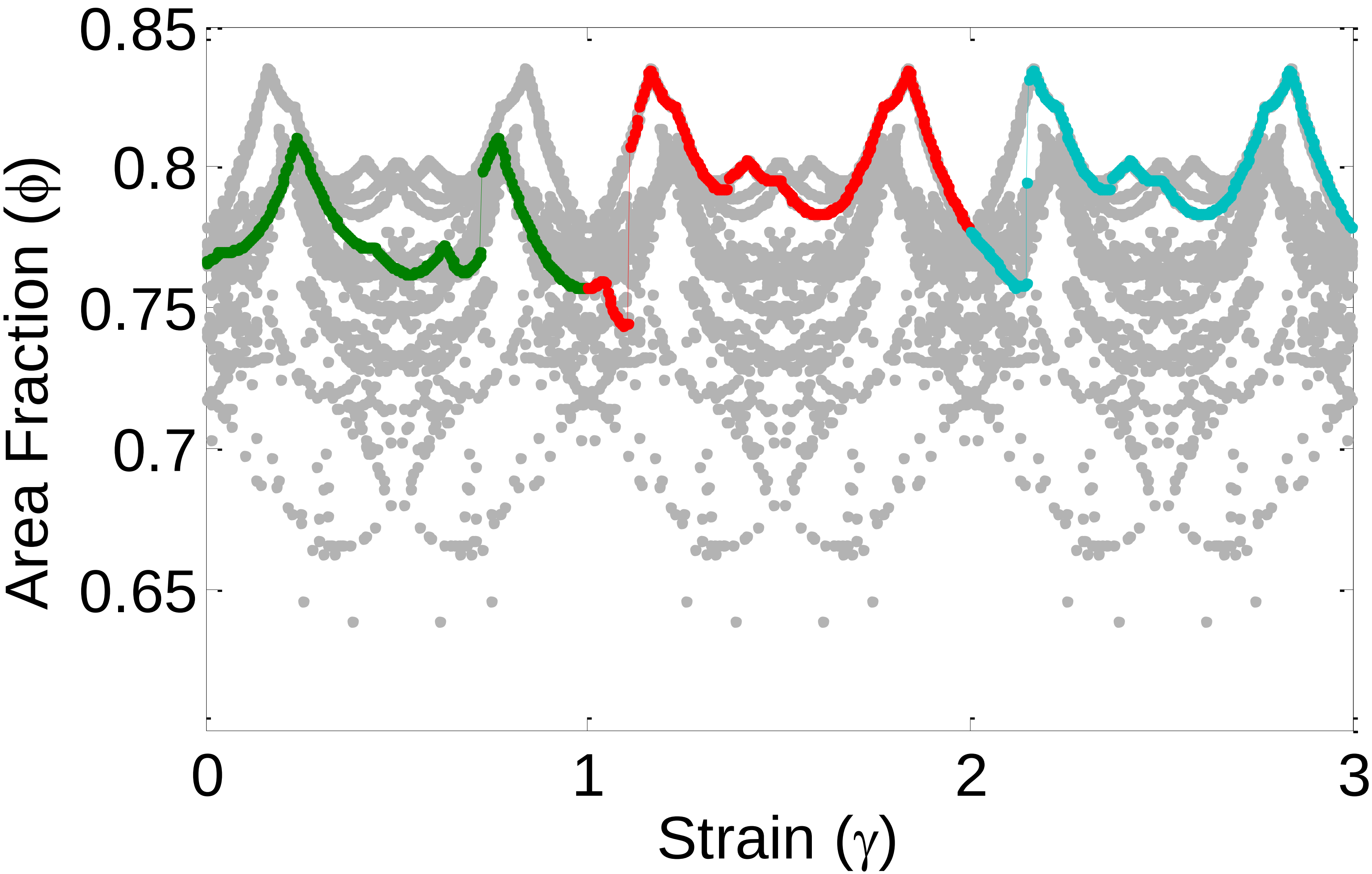
Stress vs Strain



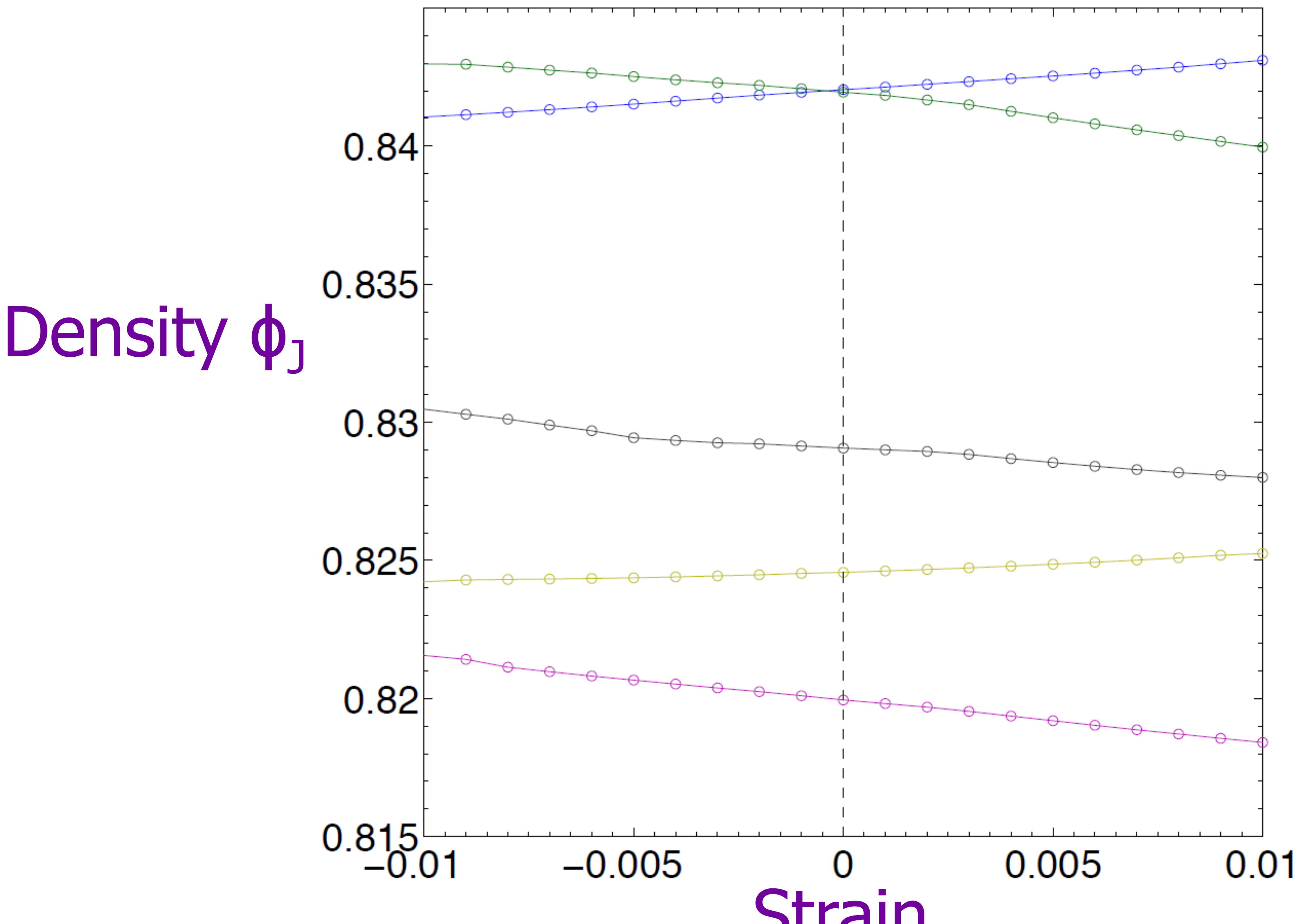
Stress vs Strain T=0



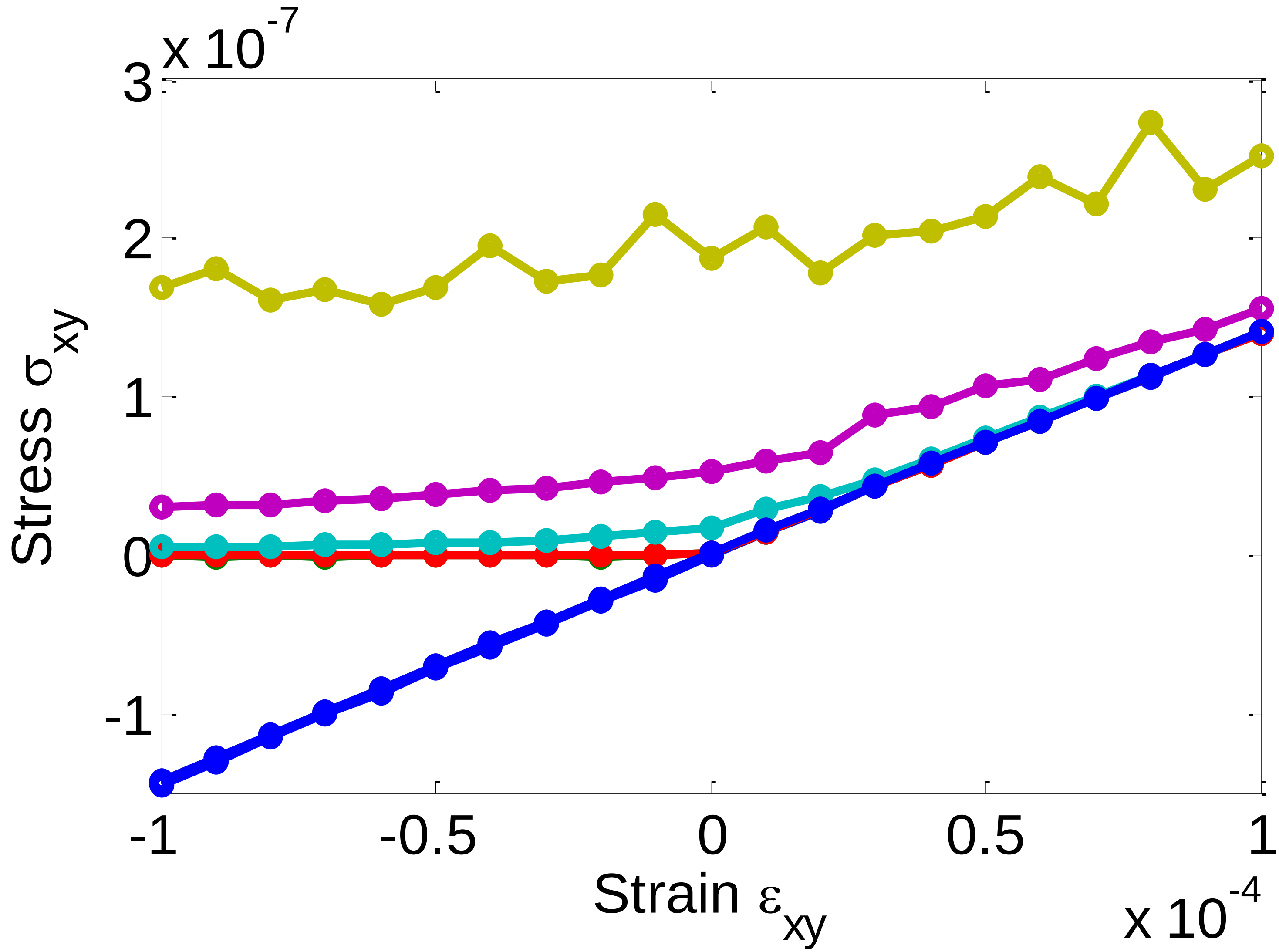
Jamming Density (ϕ_J) vs Strain



Jamming Density (ϕ_J) vs Strain



Stress vs Strain T>0

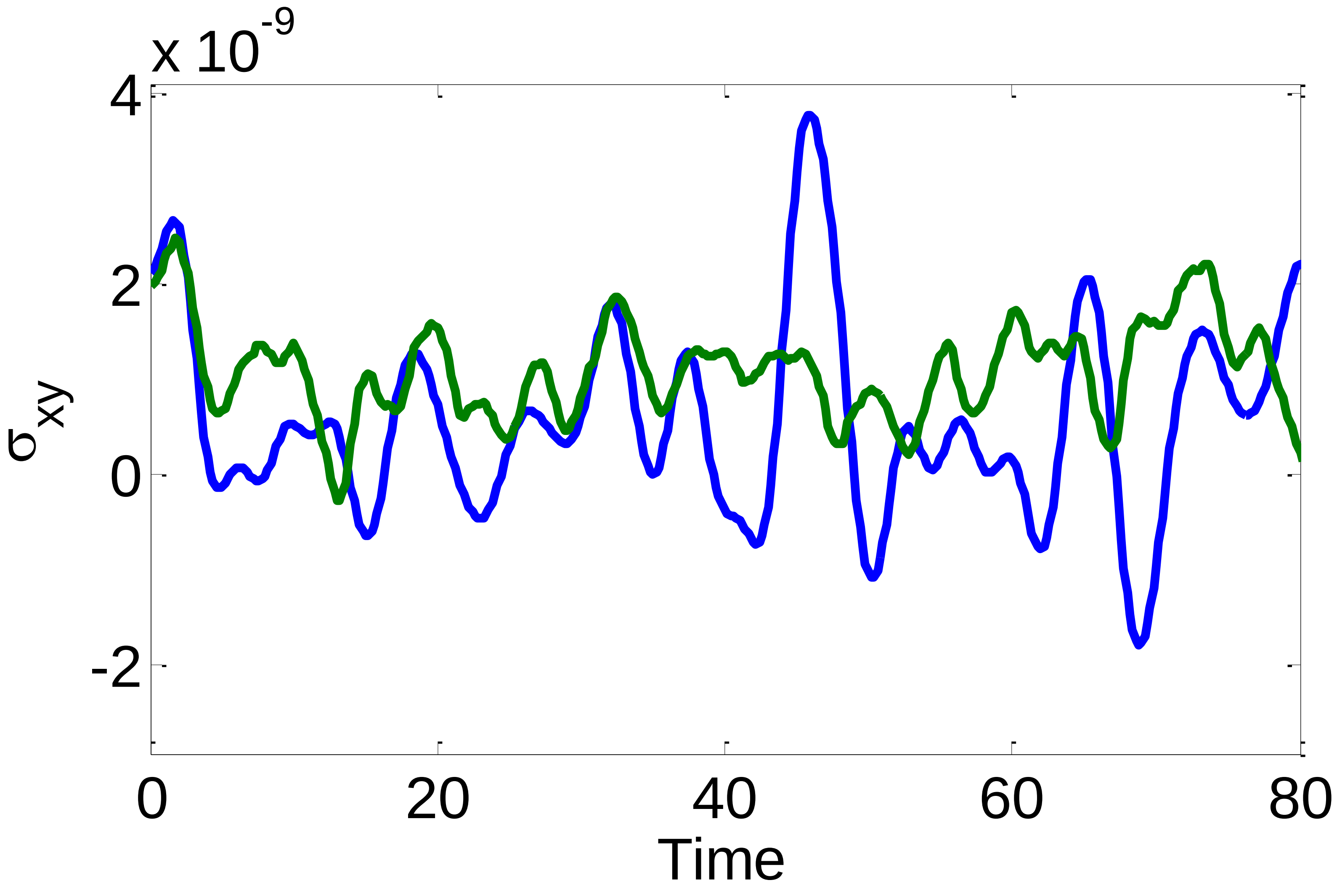


Stress vs. Time
(shear step displacement)

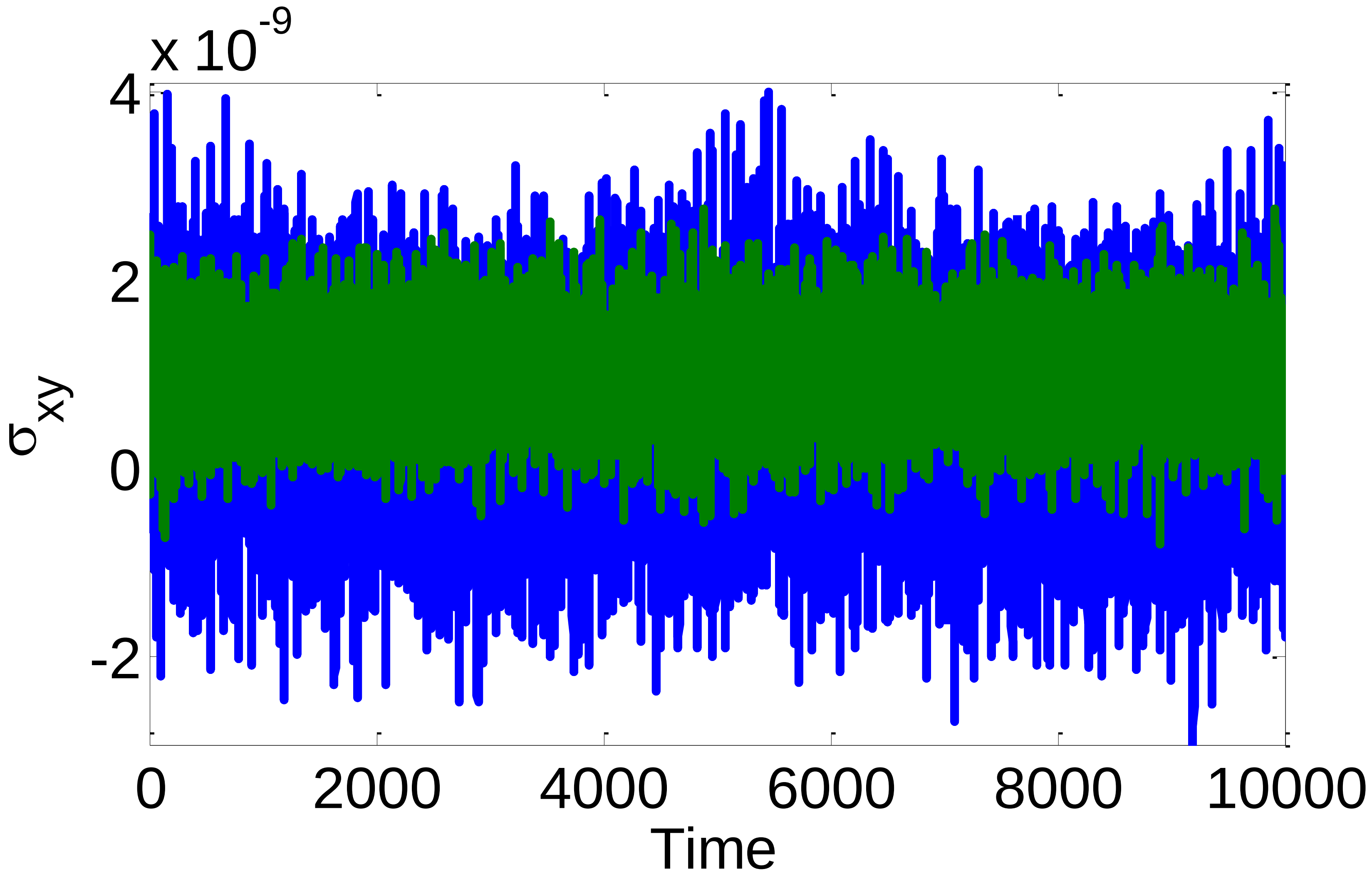
2D Molecular Dynamics

- Apply a shear displacement to all particles at time t=0.
- Let system evolve under constant NVE for both double and single sided springs.

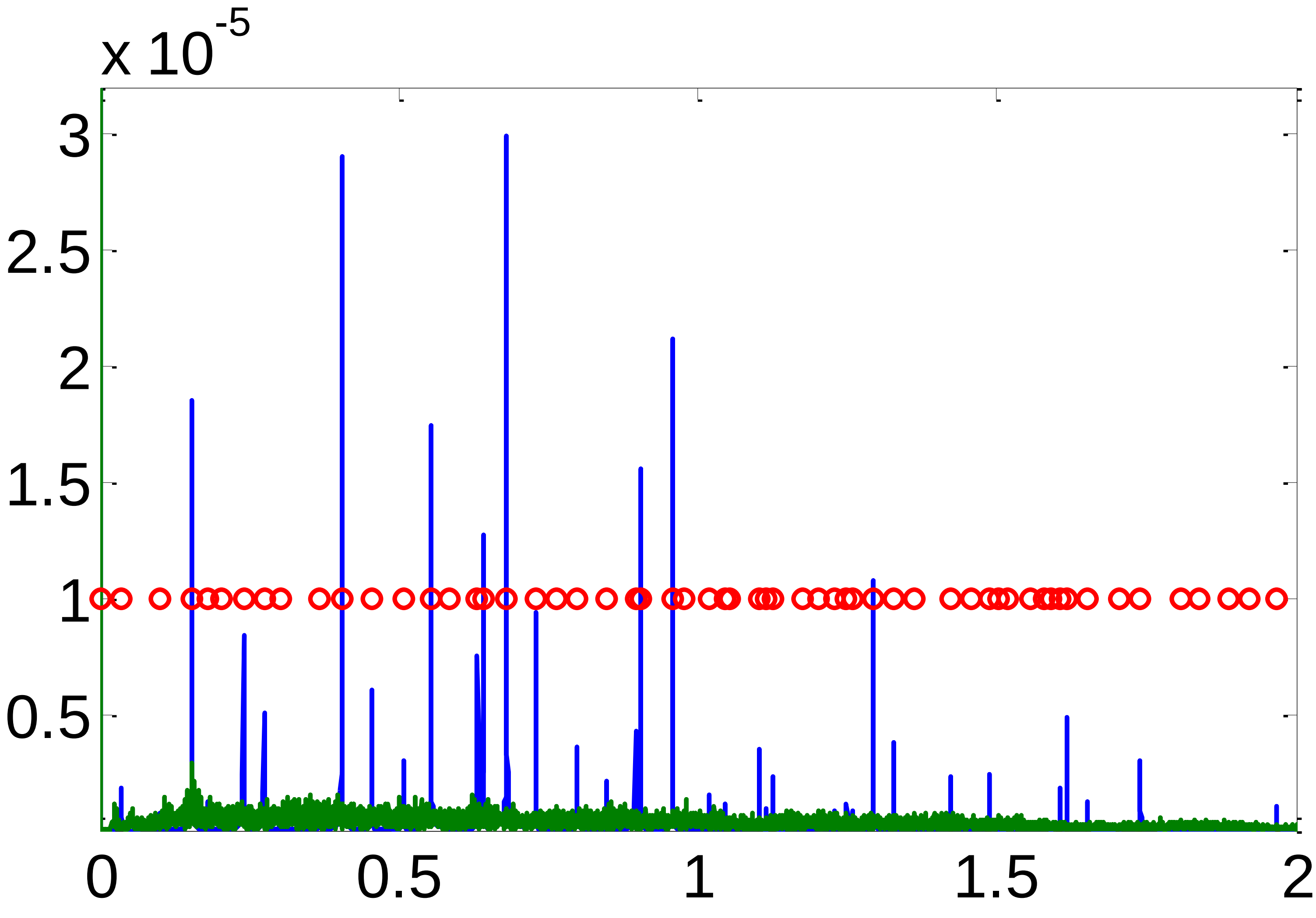
Stress vs. Time
(shear step displacement)



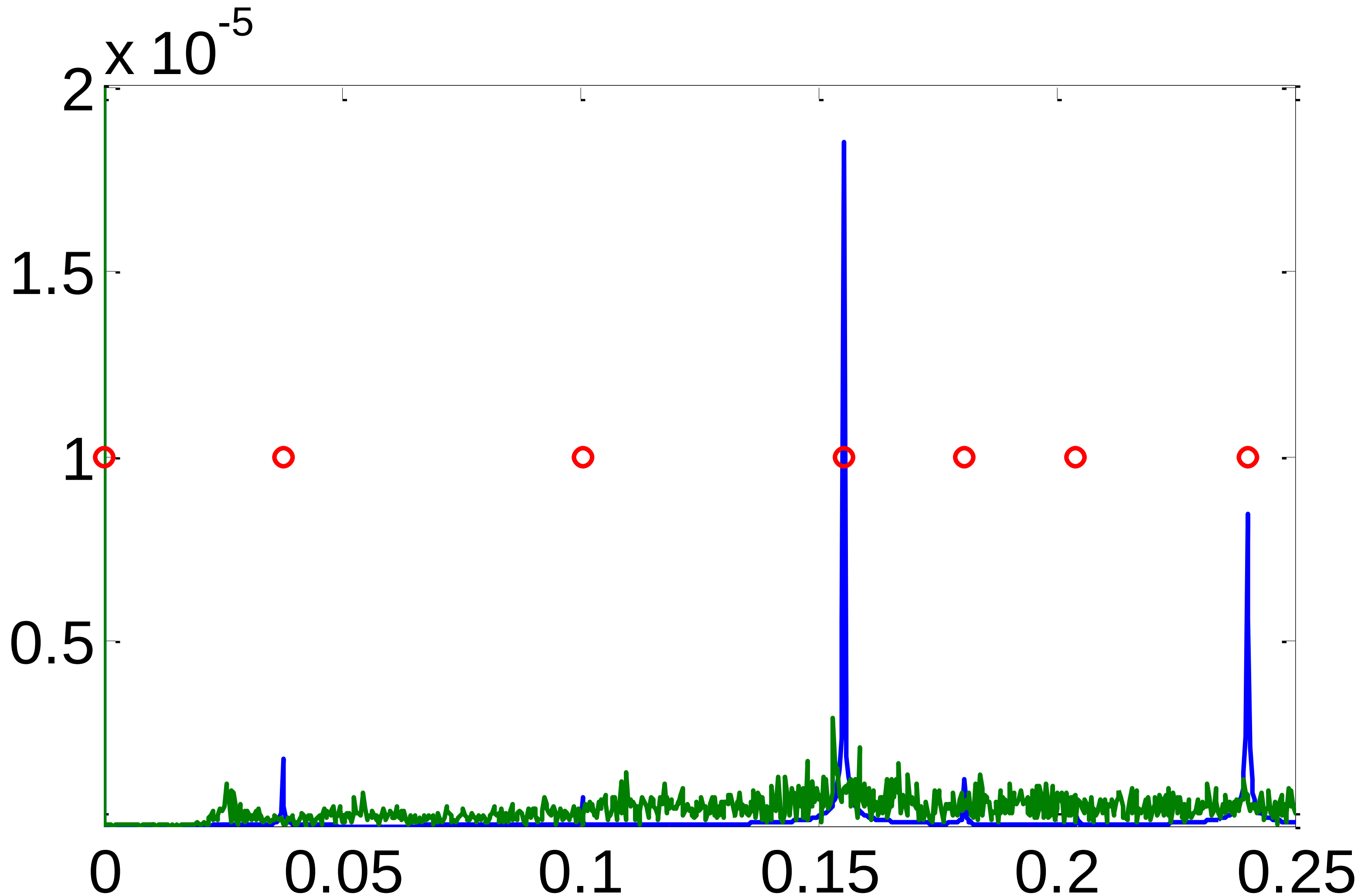
Stress vs. Time
(shear step displacement)



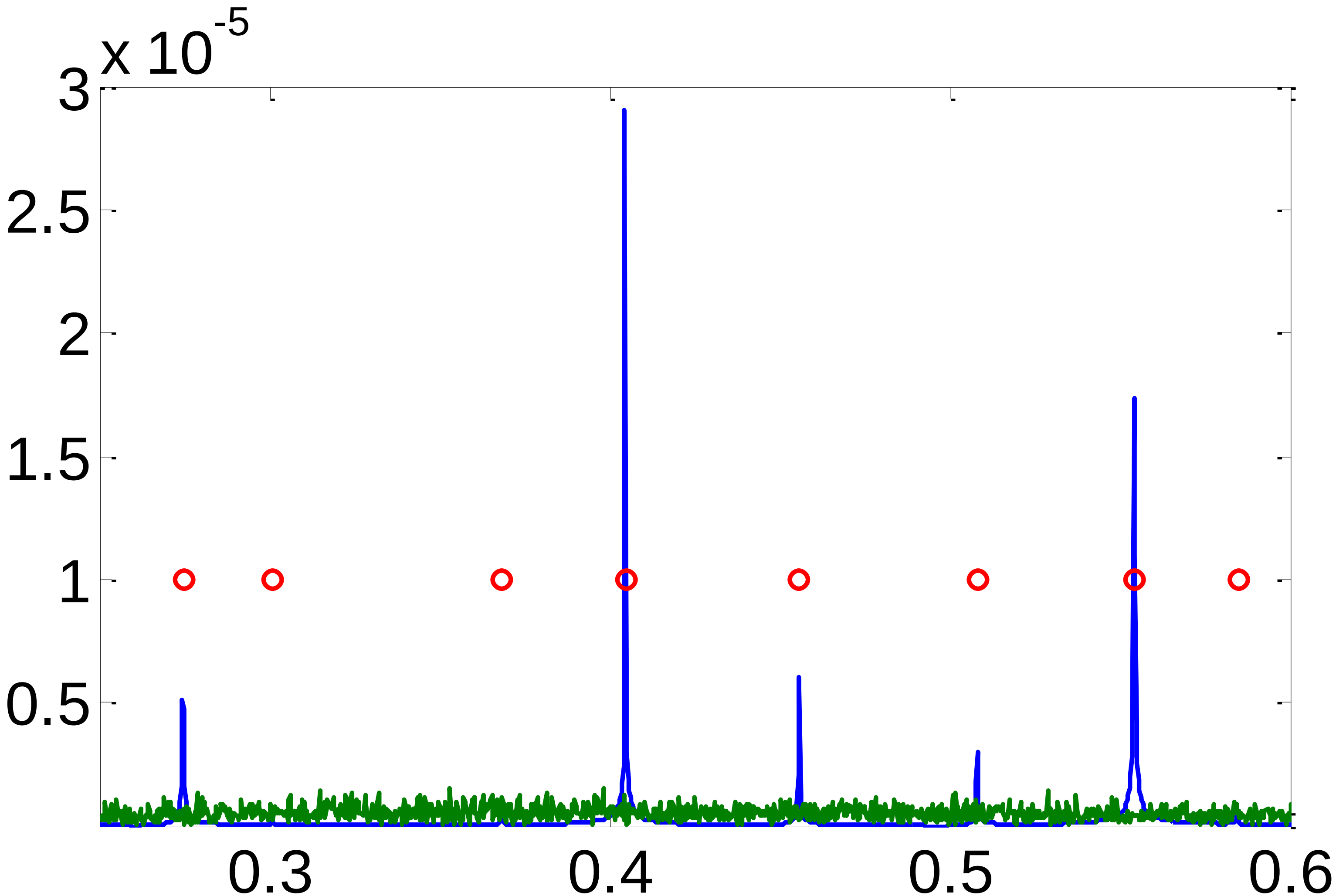
FFT of Stress
(shear step displacement)



FFT of Stress
(shear step displacement)

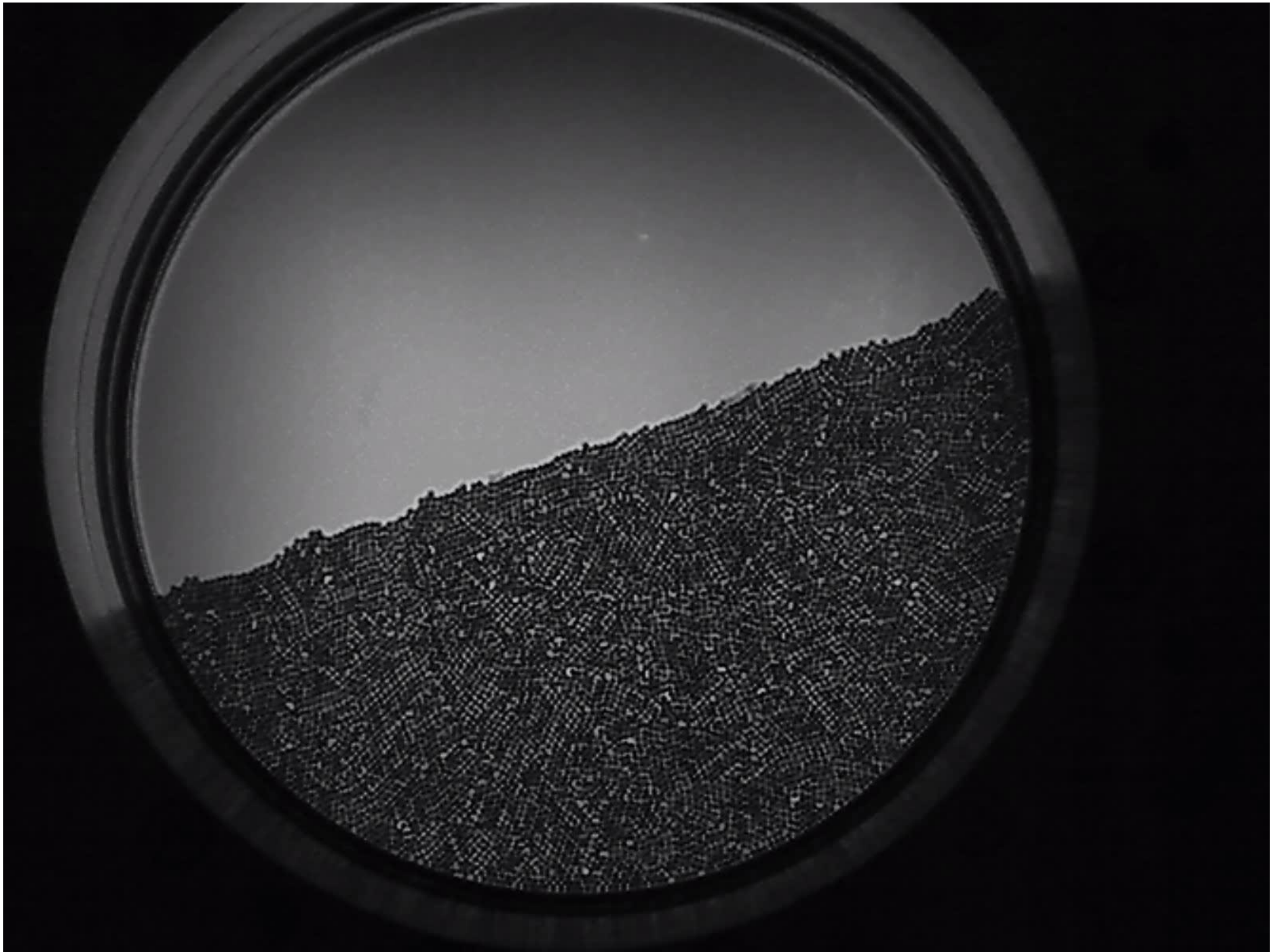


FFT of Stress
(shear step displacement)



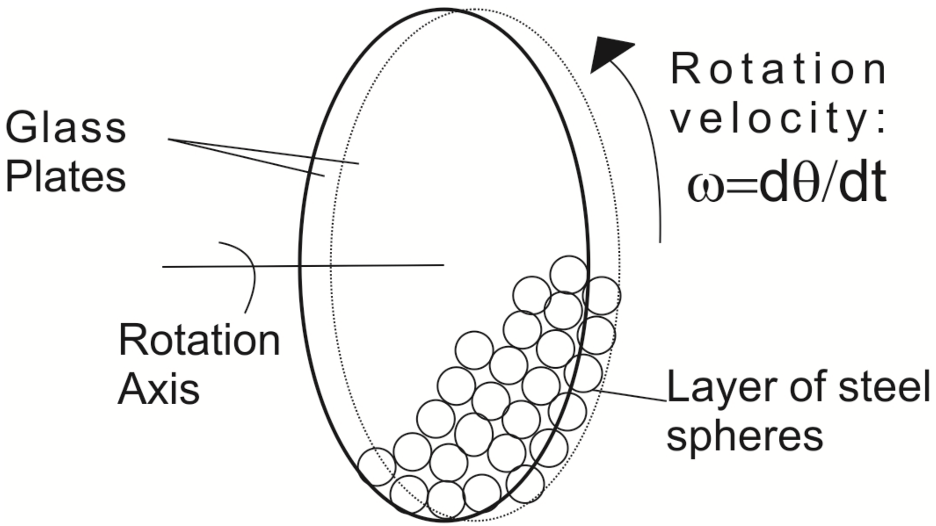
Avalanches in a Rotating Drum.

Aline Hubard Escalera



Our Rotating Drum

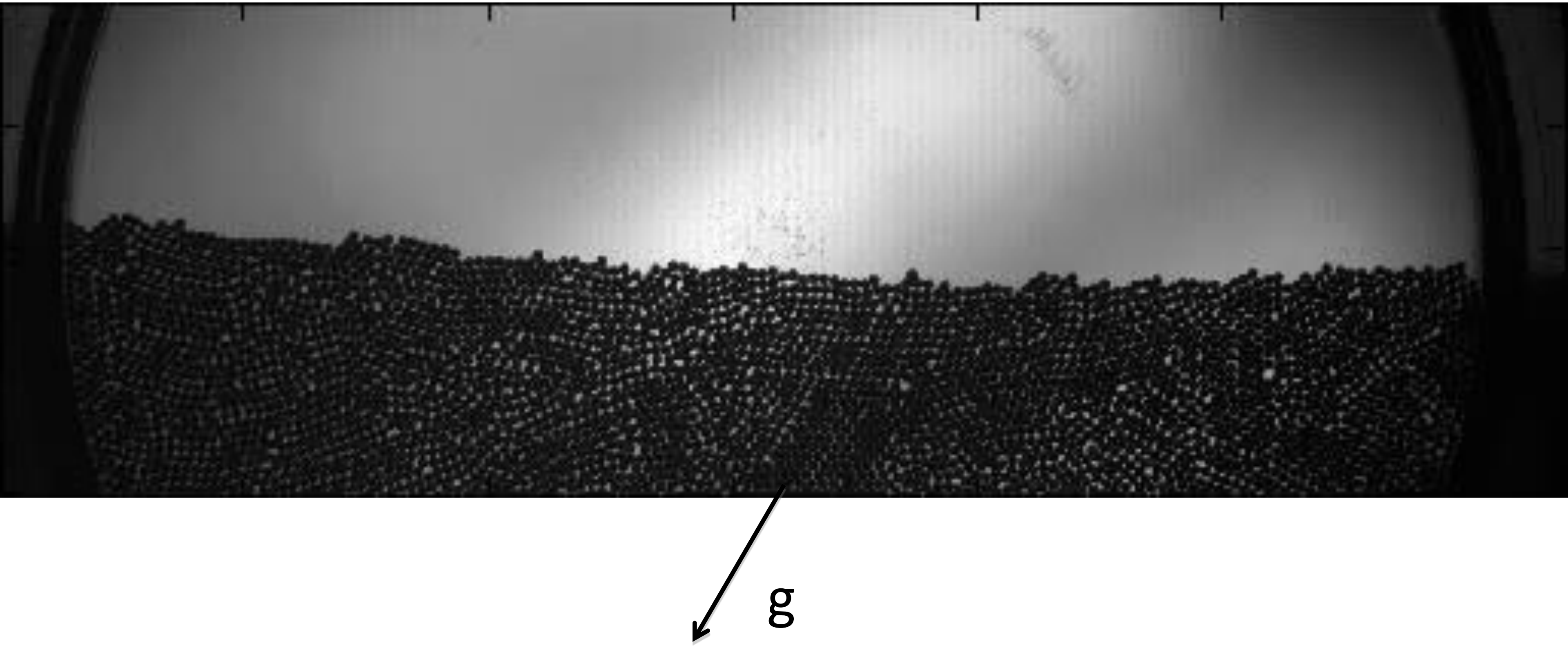
ω=0.01degrees/s



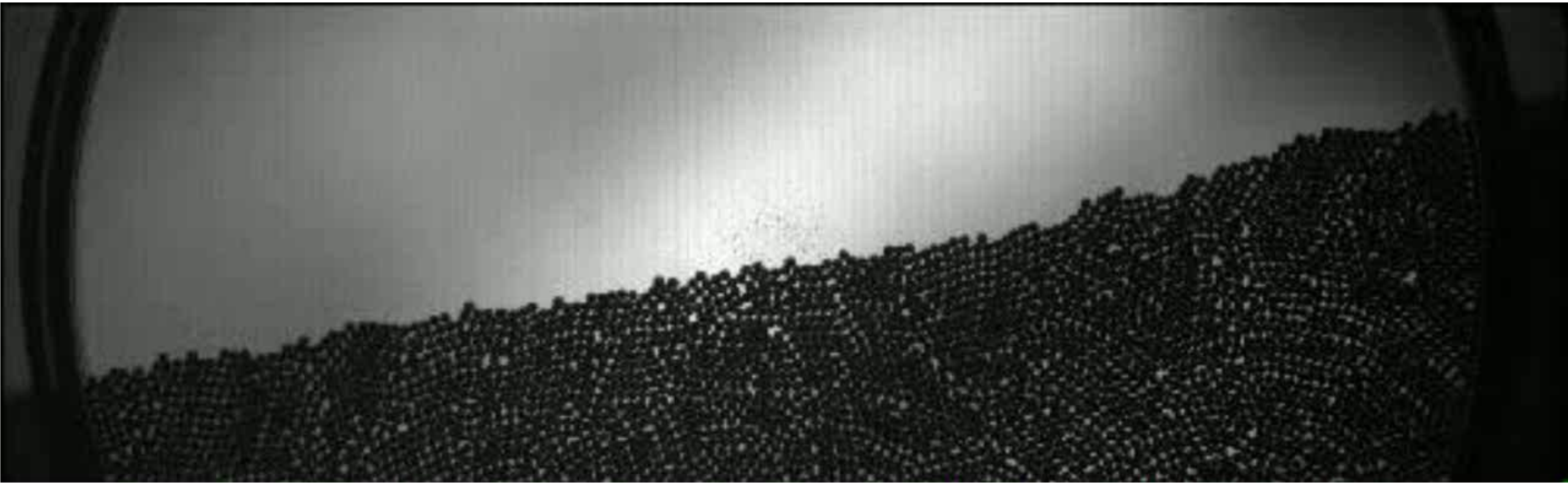
Drum diameter=125 spheres diameter.

The drum is half filled with more than 8000 spheres.

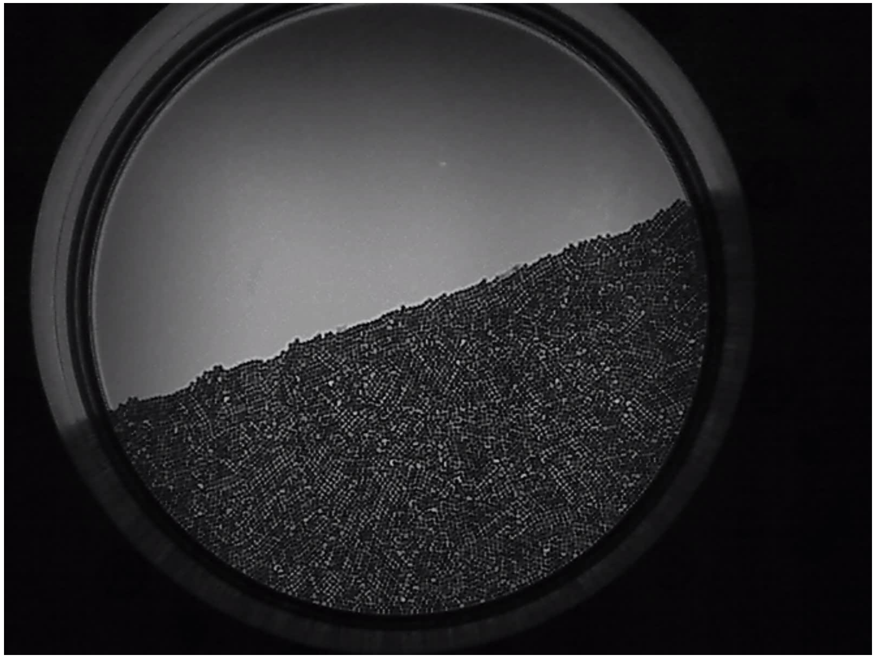
Small Avalanche

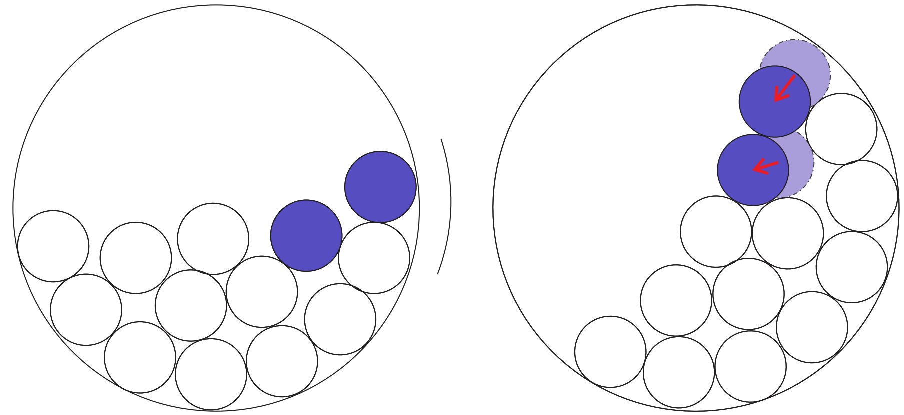


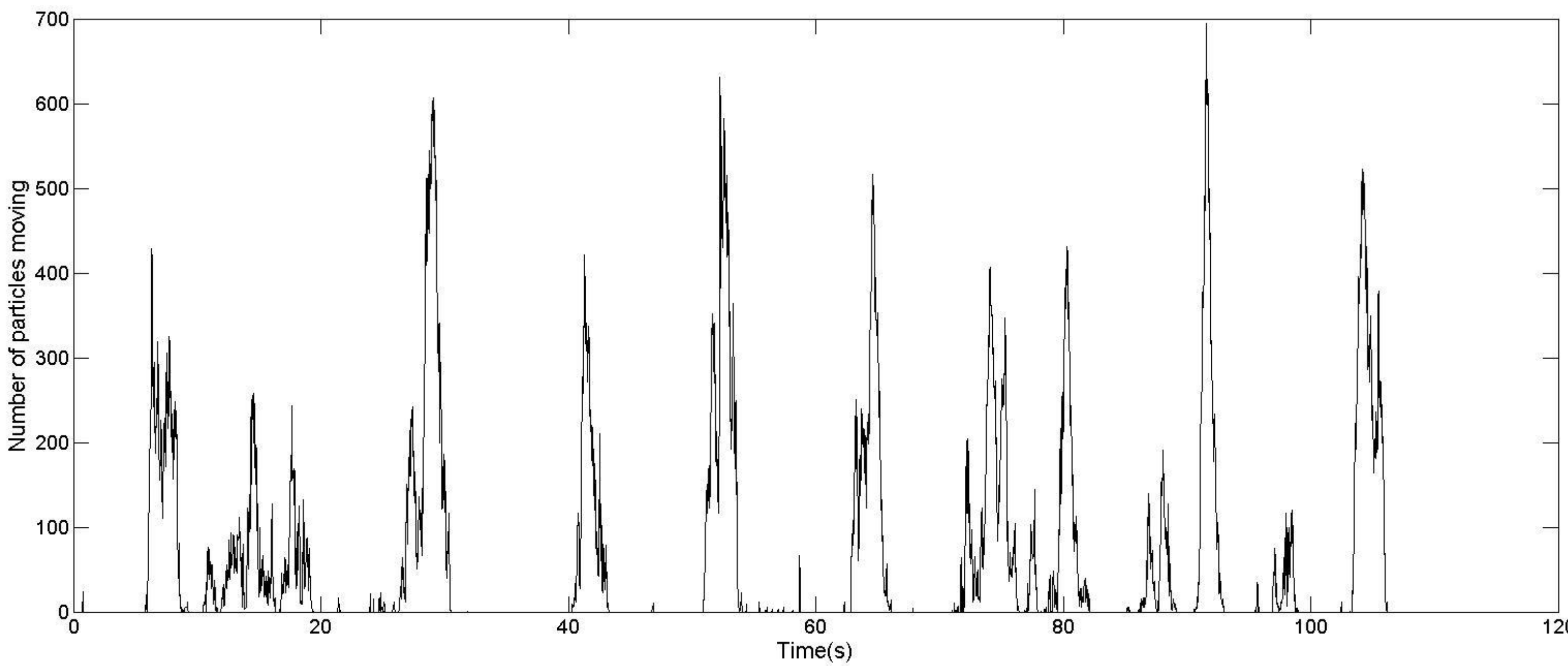
Large Avalanche

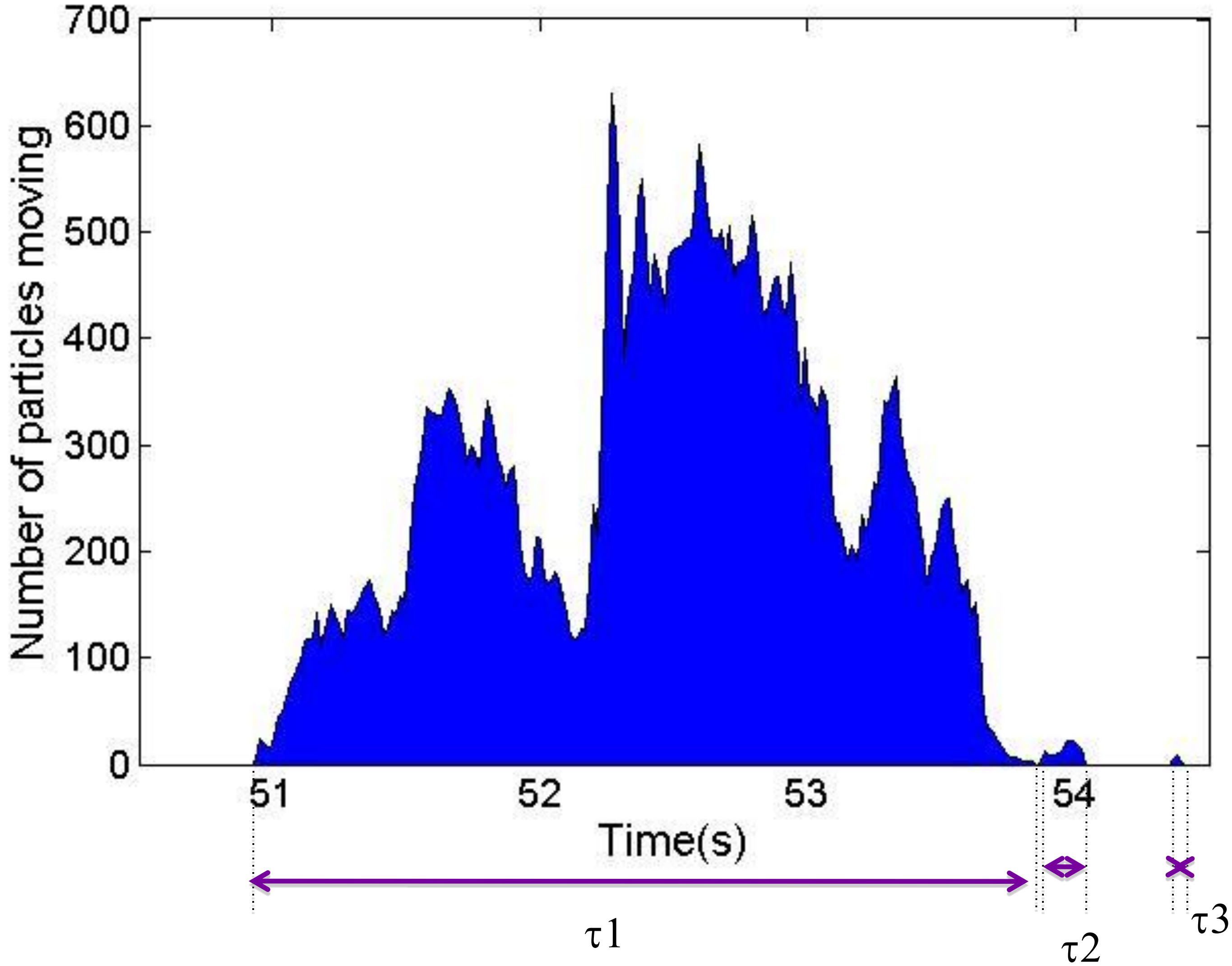


g

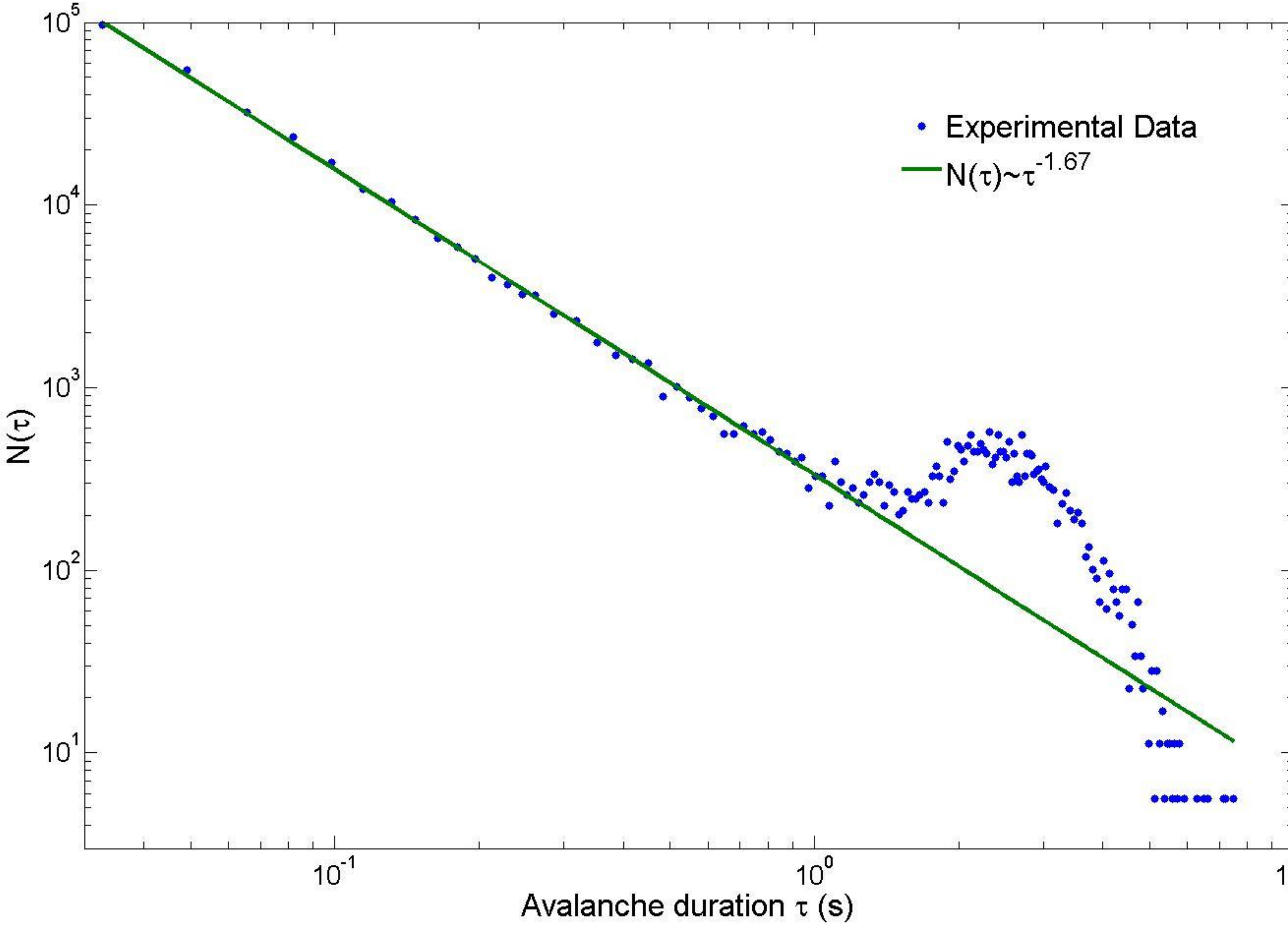




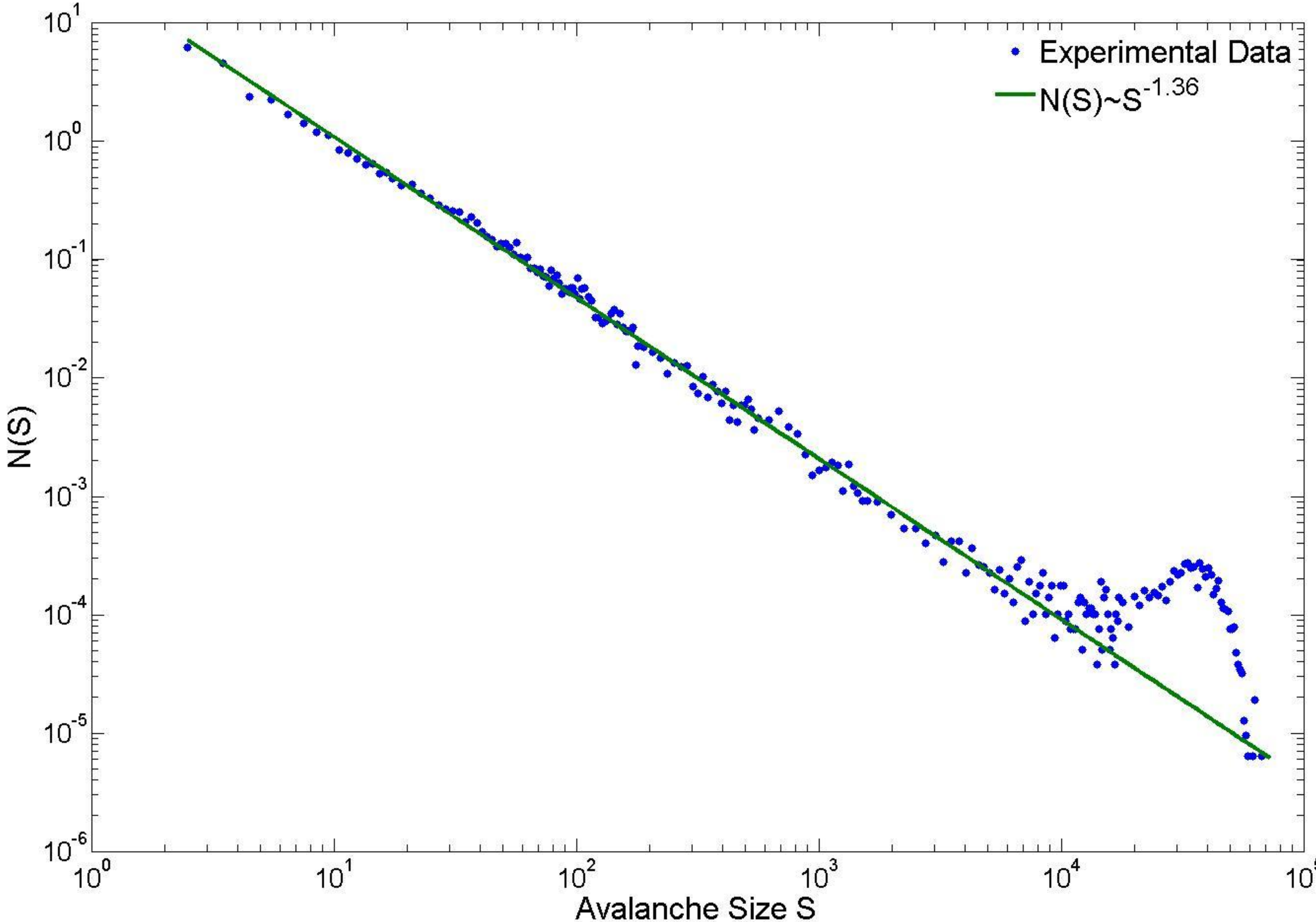

Number of particles moving
Time(s)
0
100
200
300
400
500
600
700
0
20
40
60
80
100
120



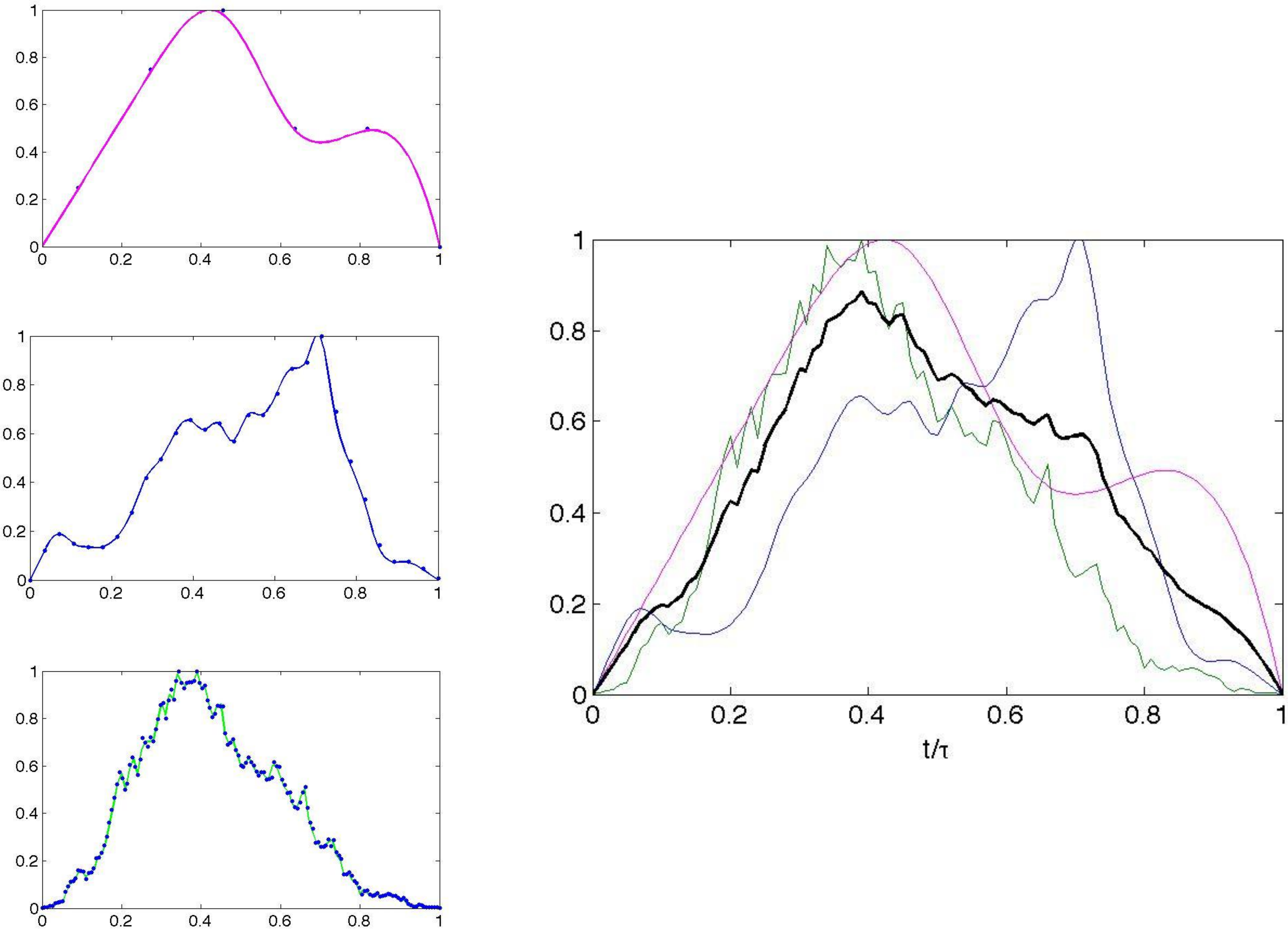
700
600
500
400
300
200
100
0
Number of particles moving
51
52
53
54
Time(s)
τ1
τ2
τ3



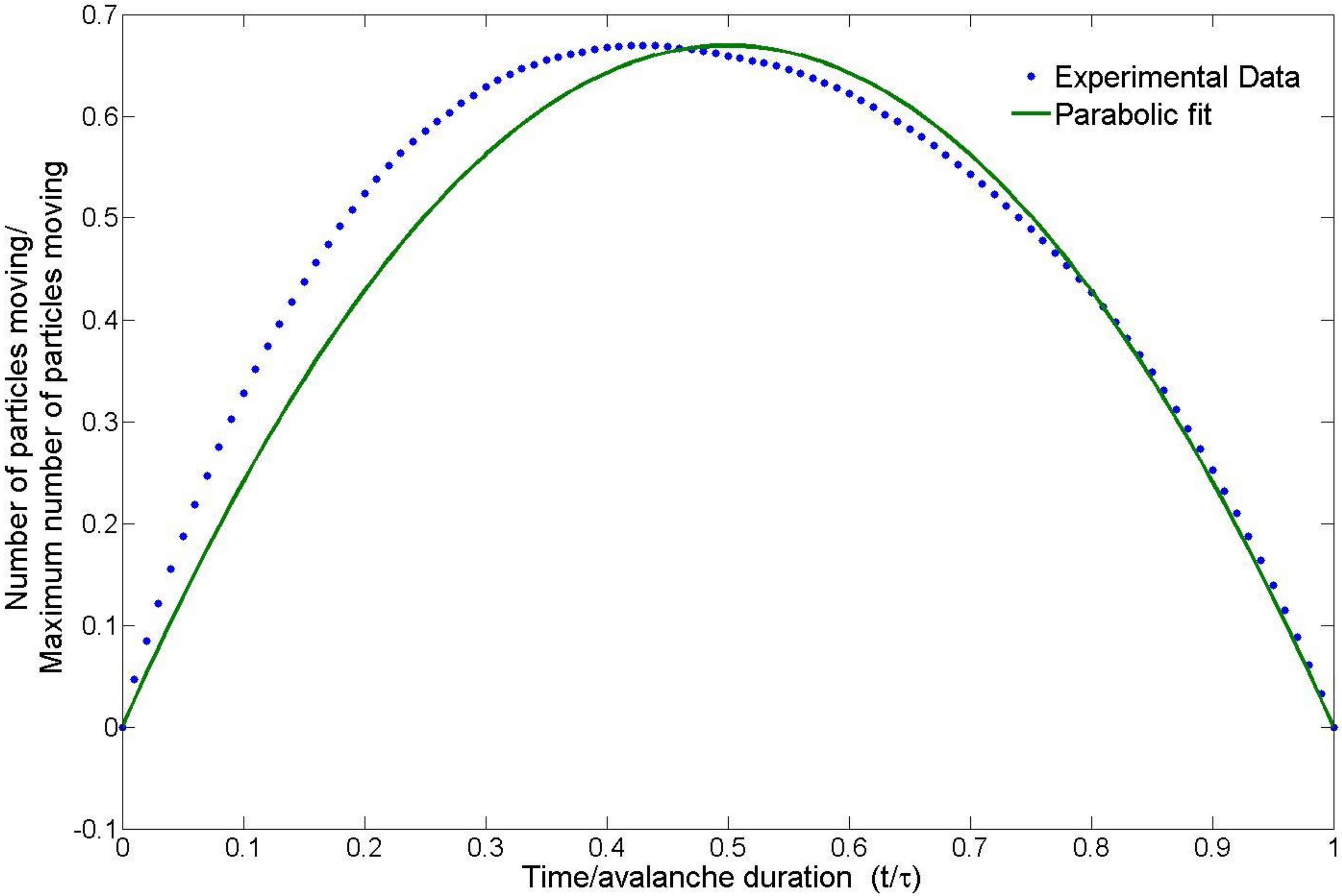
Experimental Data
N(τ)~τ^-1.67
N(τ)
Avalanche duration τ (s)
10^5
10^4
10^3
10^2
10^1
10^-1
10^0
10^1



Experimental Data
N(S)~S^-1.36
N(S)
Avalanche Size S
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^0
10^1
10^2
10^3
10^4
10^5



0
0.2
0.4
0.6
0.8
1
t/τ



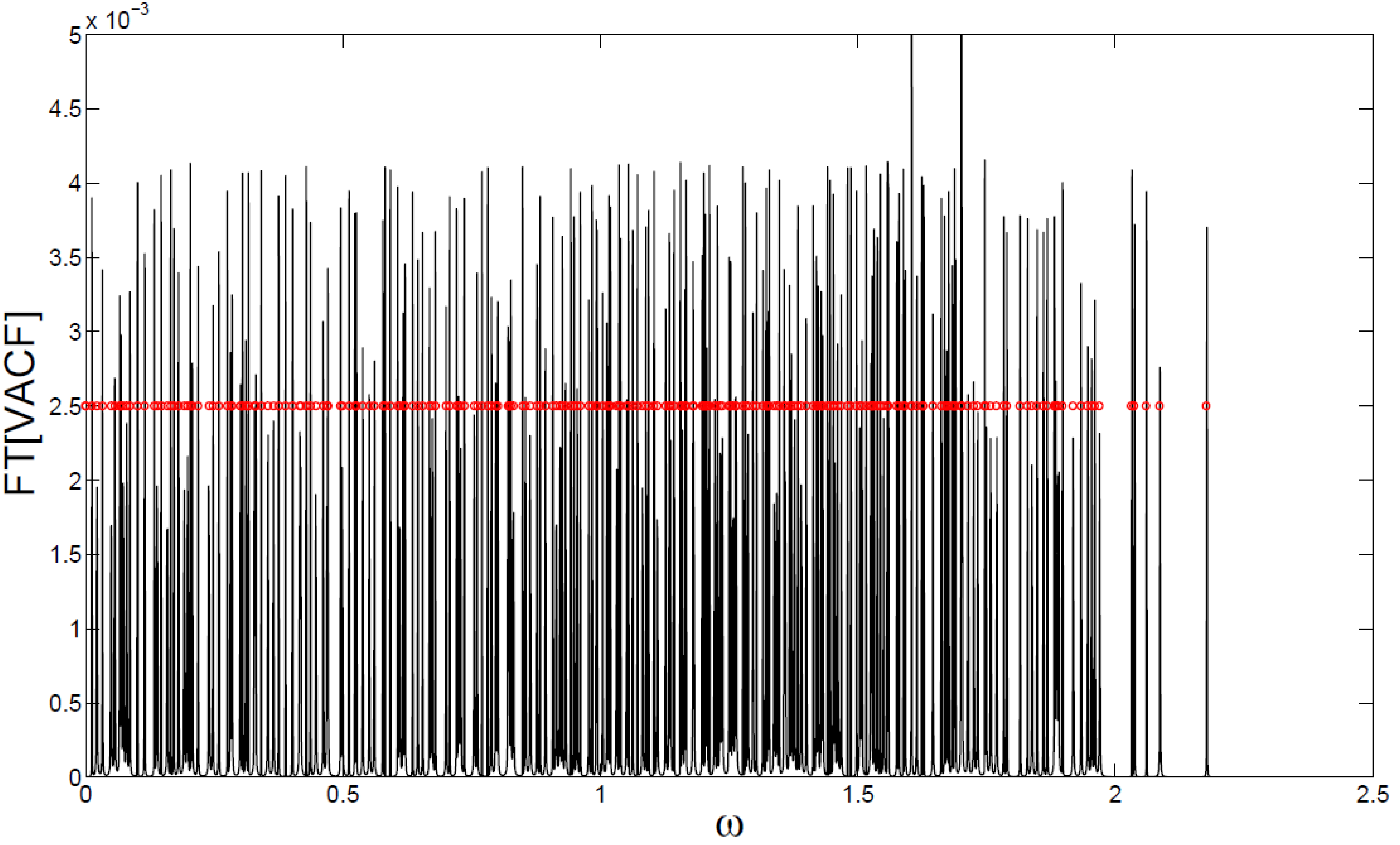
Experimental Data
Parabolic fit
Number of particles moving/
Maximum number of particles moving
Time/avalanche duration (t/τ)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Comparison of Experiment.

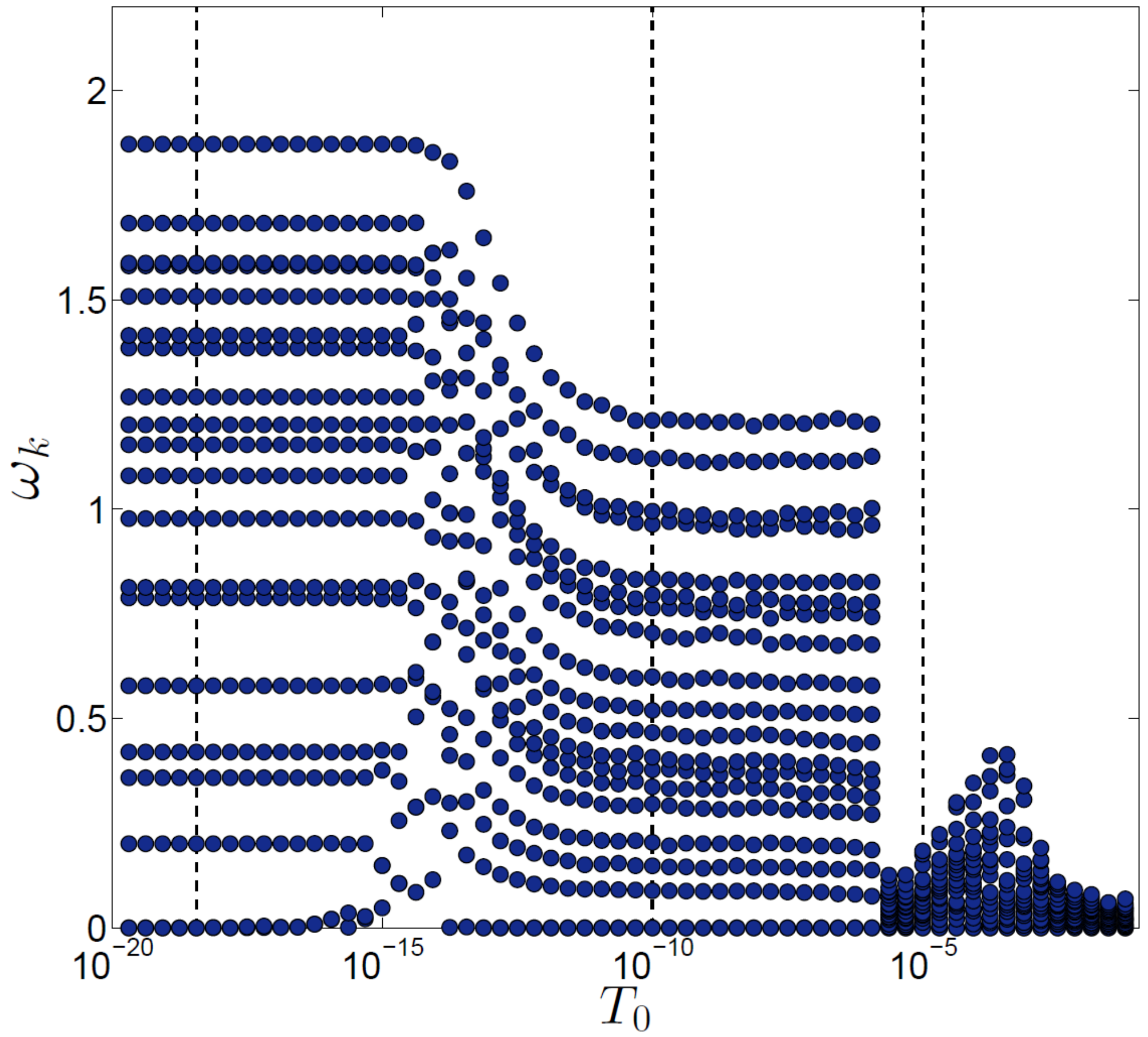
Universal Quantities for densely packed grains	Mean Field Theory	Granular Shear experiment	Our Rotating drum
Avalanche size distribution $D(s) = s^{-\tau}$	1.5	1.5	1.36
Avalanche duration distribution $D(T) = T^{-\alpha}$	2	2 or exponential	1.67
Averaged Source function	Symmetric (parabola)	Symmetric (parabola)	Asymmetric
Quasi-Periodic event statistics	sometimes	sometimes	Not for slow rotations.

The End

Density of States N=128



Temperature dependence of ω_k

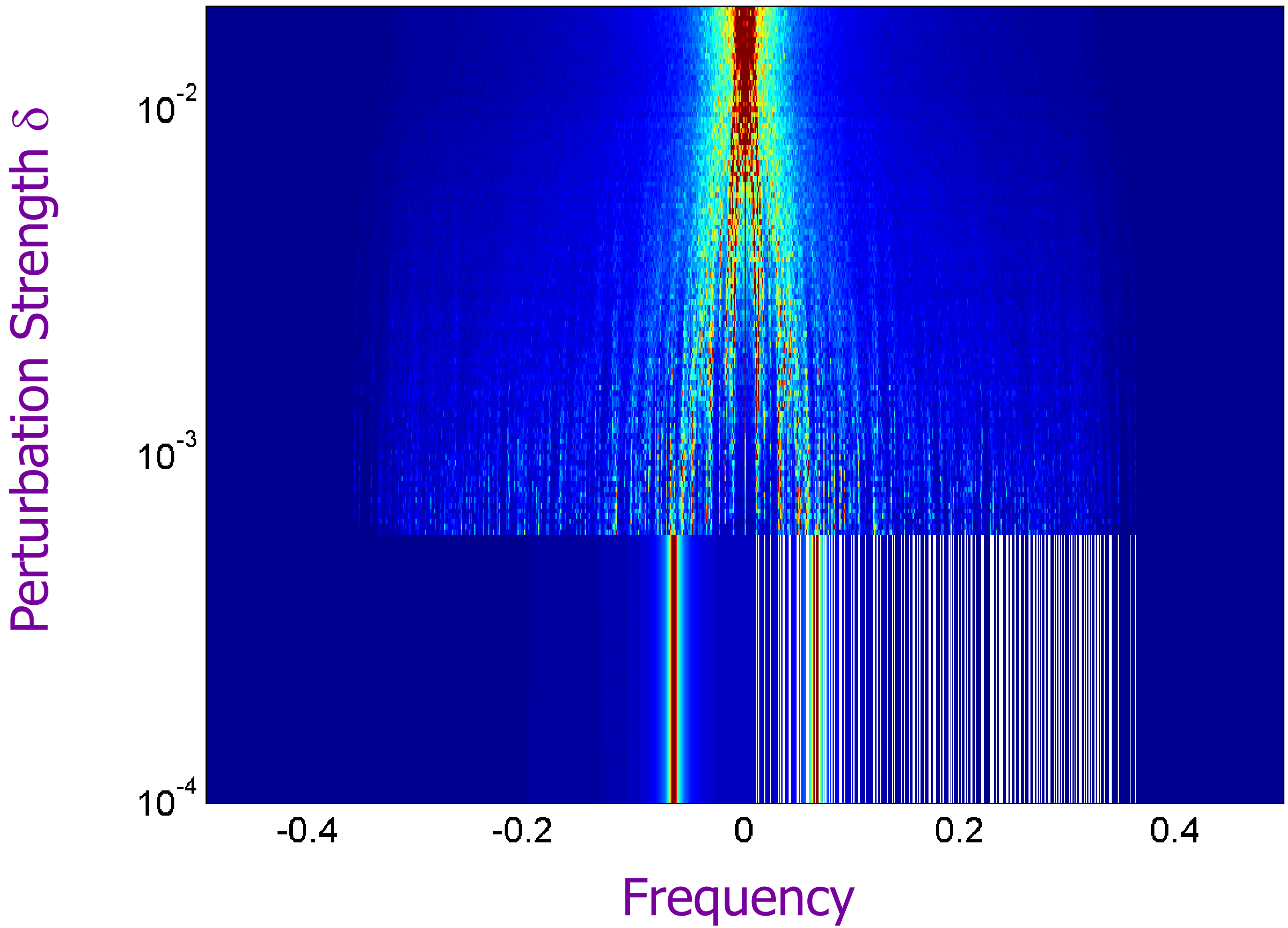


Testing Harmonic Approximation

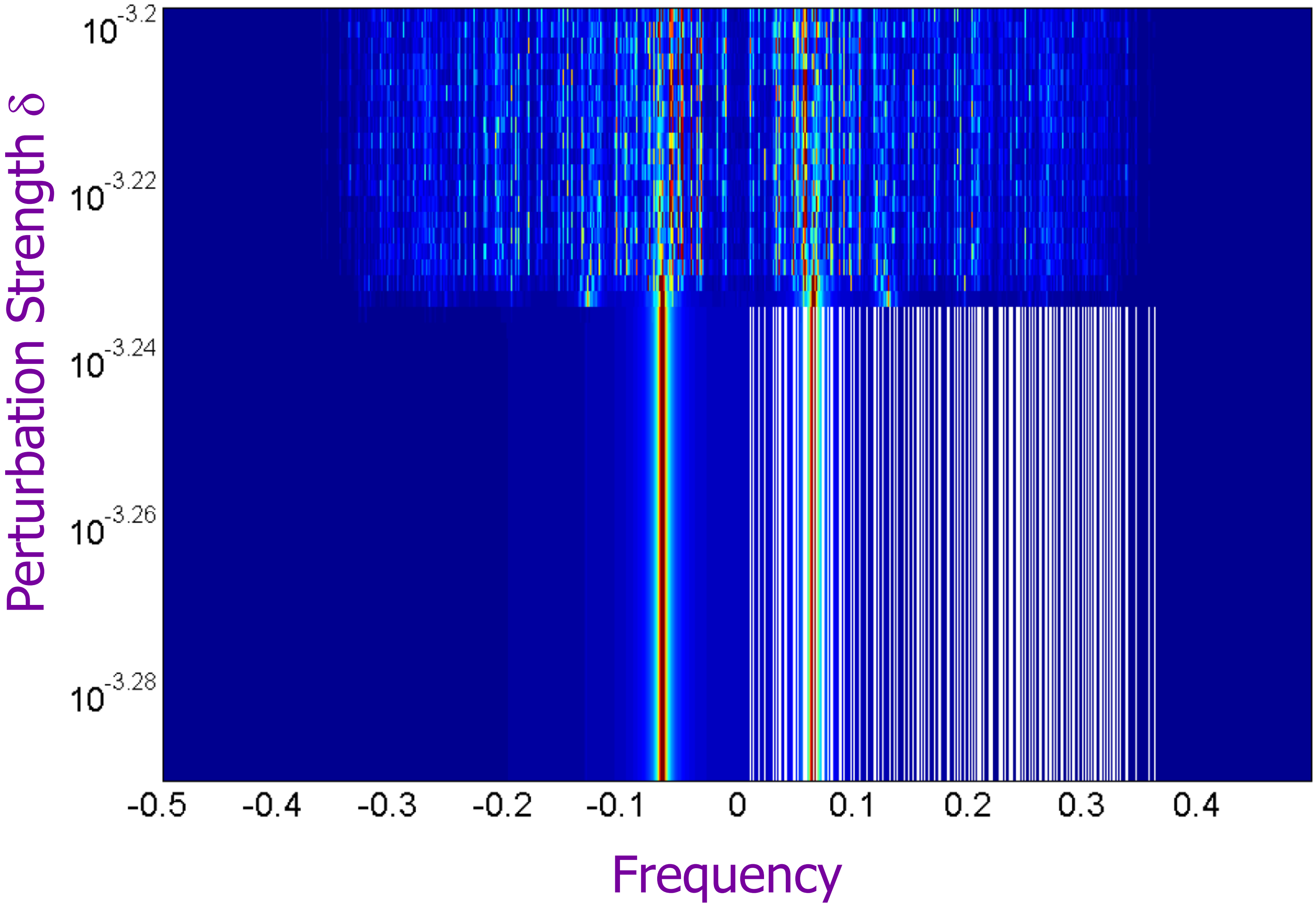
2D Molecular Dynamics

- 2D frictionless bidisperse mechanically stable disk packings.
  - Jammed (ϕ_J).
  - Wide range of $\Delta\phi=\phi-\phi_J$
- Apply perturbations with amplitude δ
  - along eigen-direction from the dynamical matrix.
- **Measure system response:**
  - at constant energy.
- Harmonic system will remains in the original eigenmode of the perturbation.

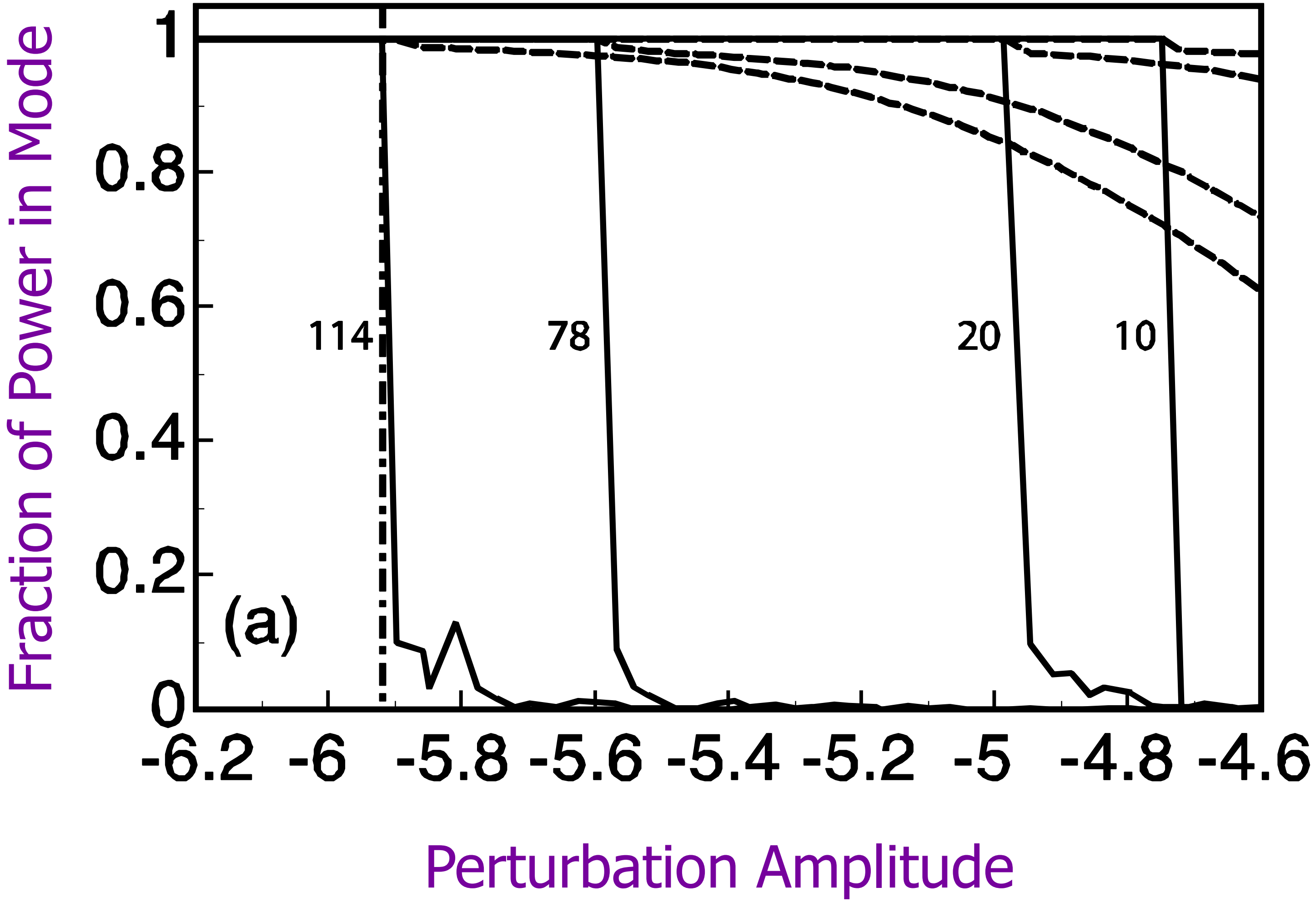
Fourier Spectrum



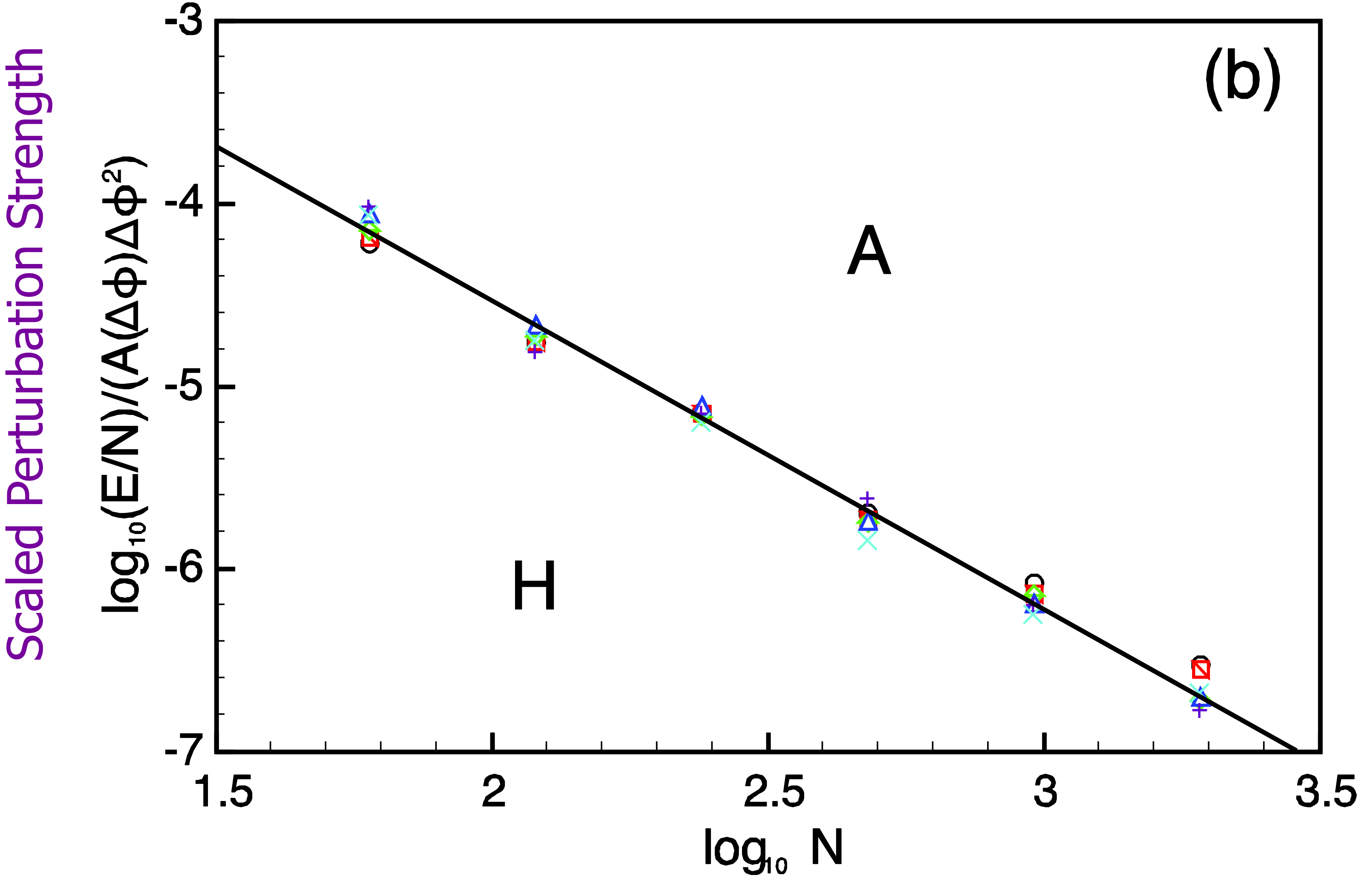
Fourier Spectrum

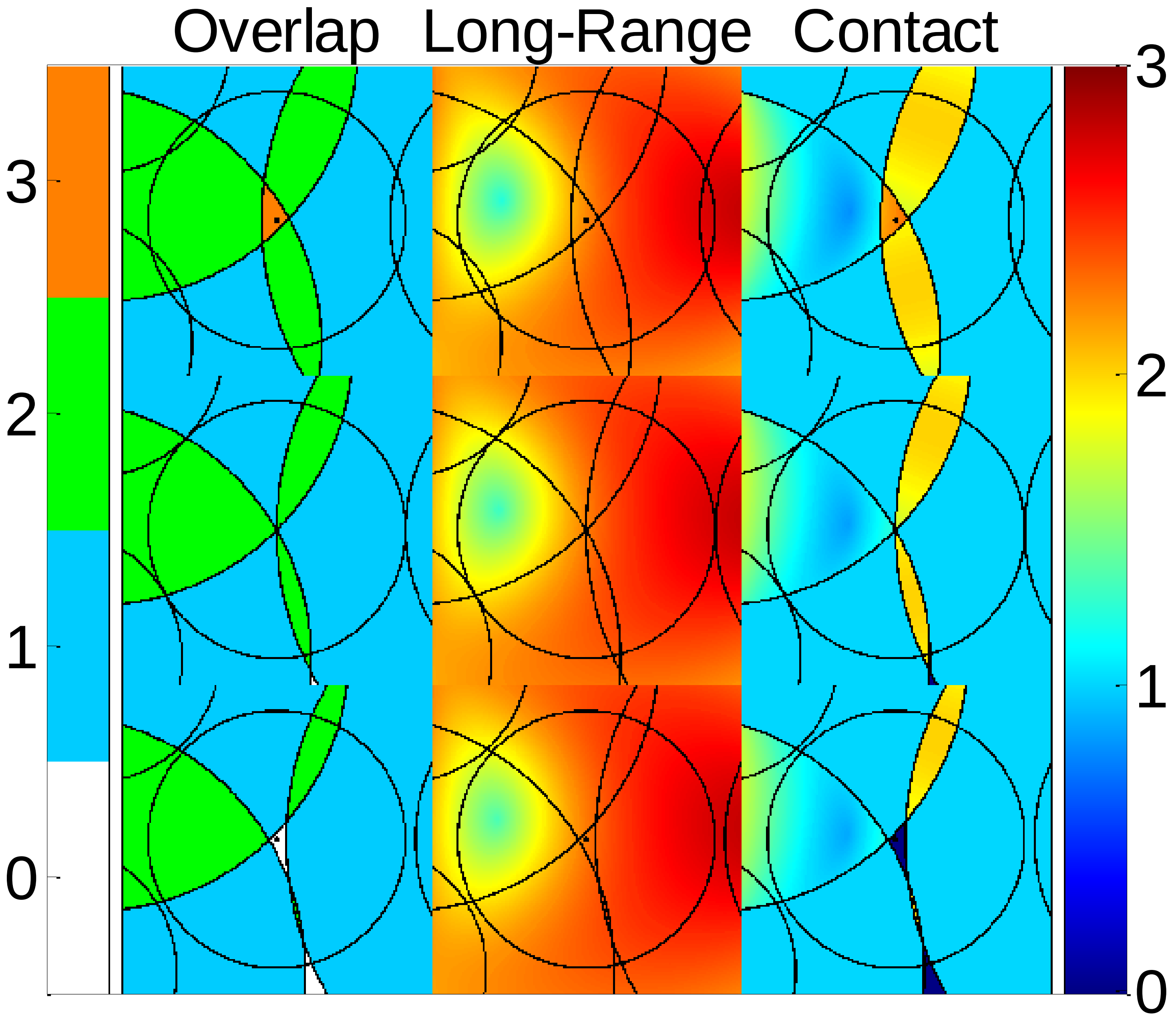


Amplitude of Several Fourier Modes



Inherently Anharmonic




Overlap
Long-Range
Contact
3
2
1
0
3
2
1
0

Effects of Nonharmonic Behavior

Simulation

- Heat Capacity.
- Density of States $D(\omega)$:
  - response to external perturbation.
  - thermal transport

Experiment

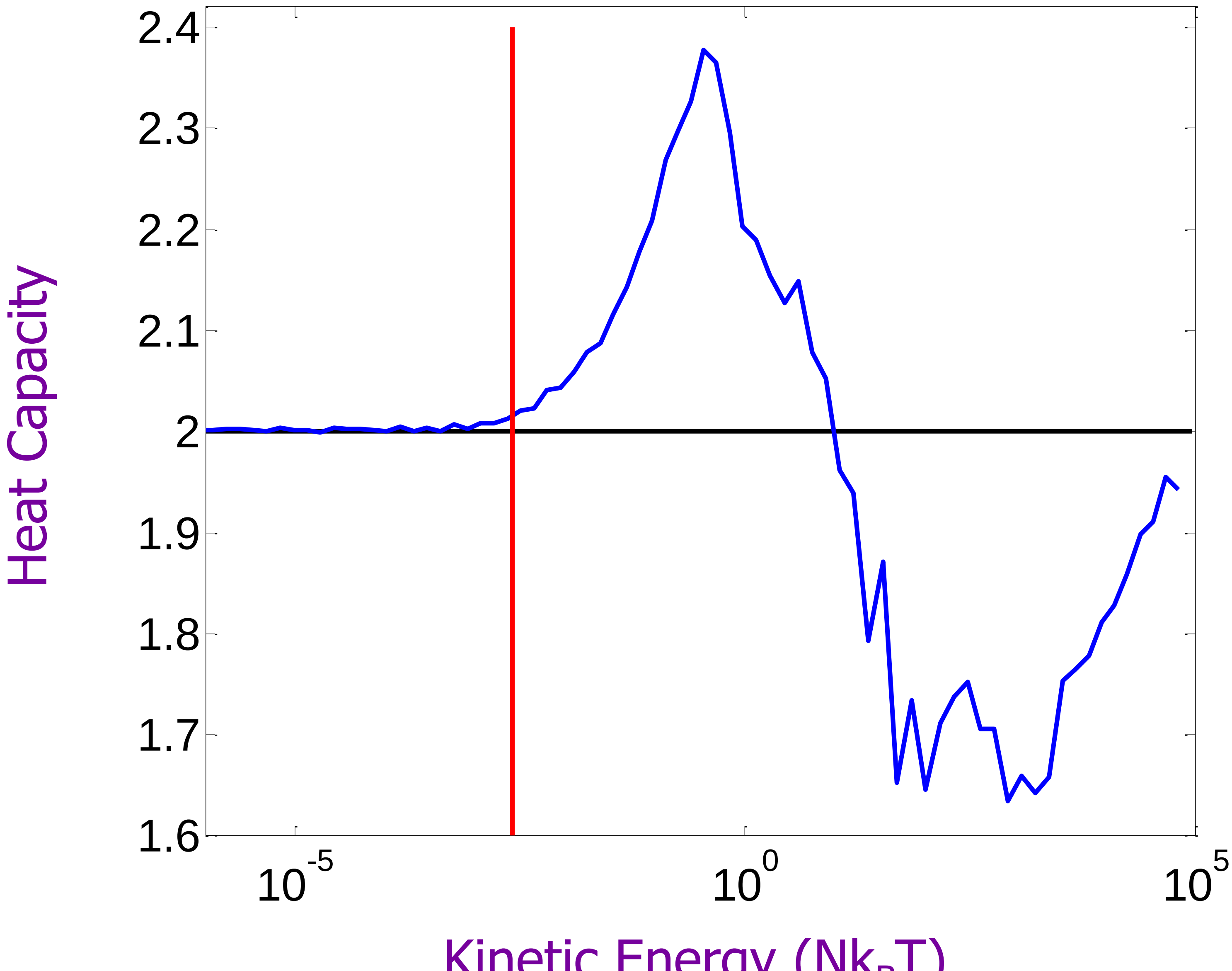
- Do “real” systems show nonharmonic behavior?

Example Effect: Heat Capacity of Granular Solids (Packings)

$$C_V = \frac{\Delta T}{Q} = 2Nk_B$$

$$\hat{C}_V = \frac{C_V}{Nk_B} = 2$$

Heat Capacity



Displacement matrix – the 'true' vibrational DOS

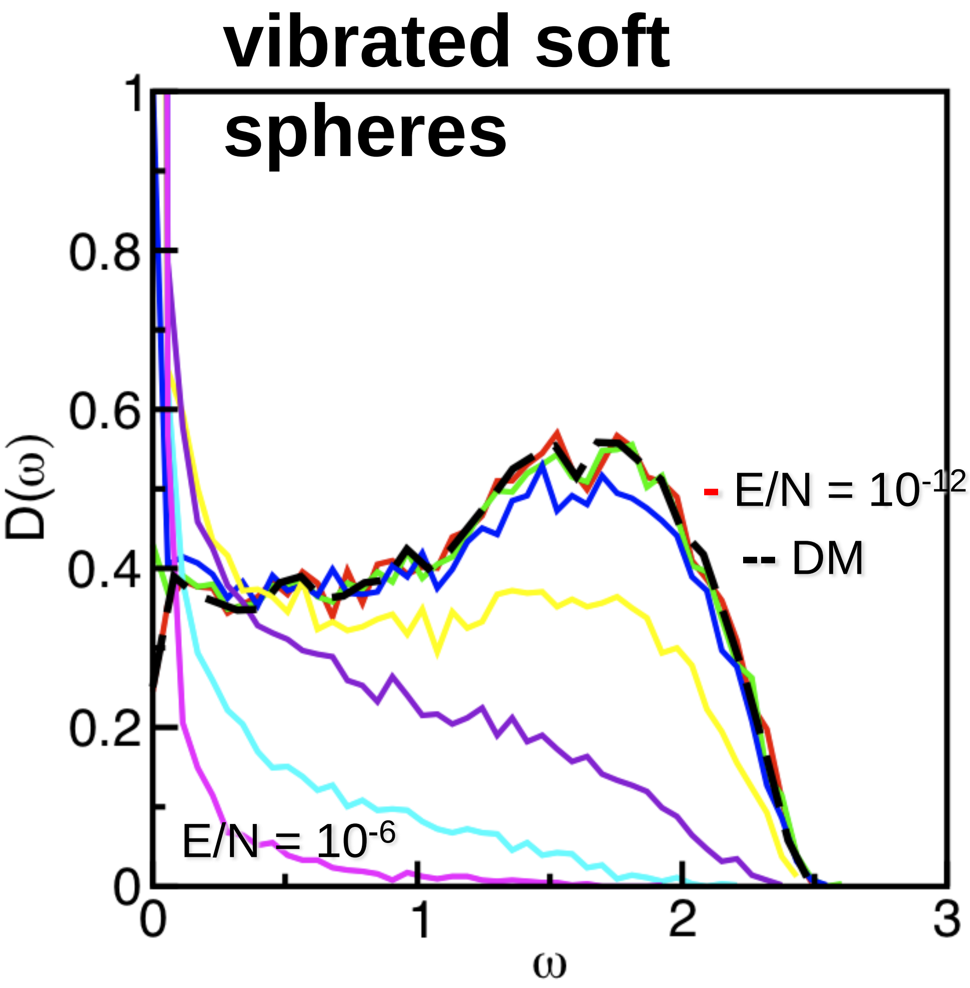
Dynamical matrix: $M_{kl} = \left.\frac{\partial^2 V}{\partial r_k \partial r_l}\right|_{\vec{r}=\vec{r}_0}$

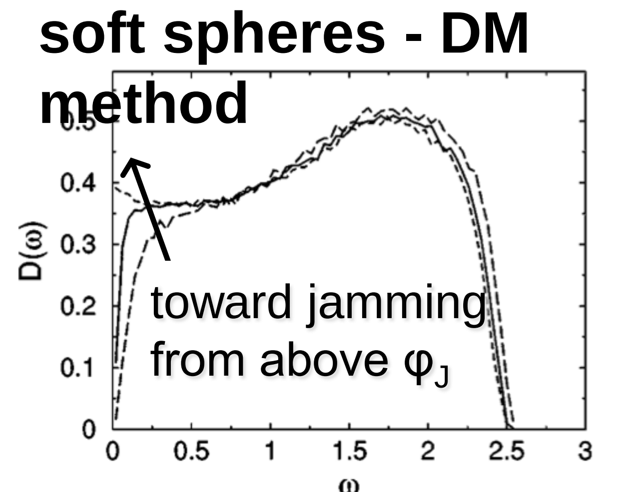
Displacement matrix: $C_{kl} = \langle (r_k - r_k^0)(r_l - r_l^0) \rangle_t$

In harmonic approximation: $M = T \times C^{-1}$

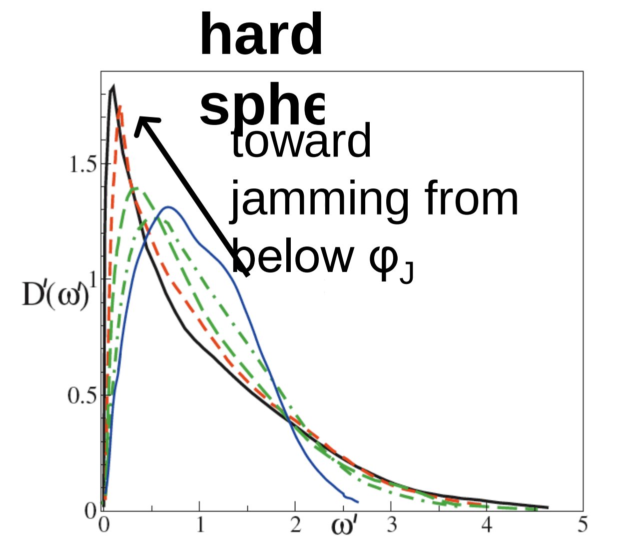
Granular solid: modes of M & C will differ due to nonharmonicities. How much?

Vibrational DOS for granular solids





O'Hern, Silbert, Liu, Nagel, PRE 68 011306 (2003)

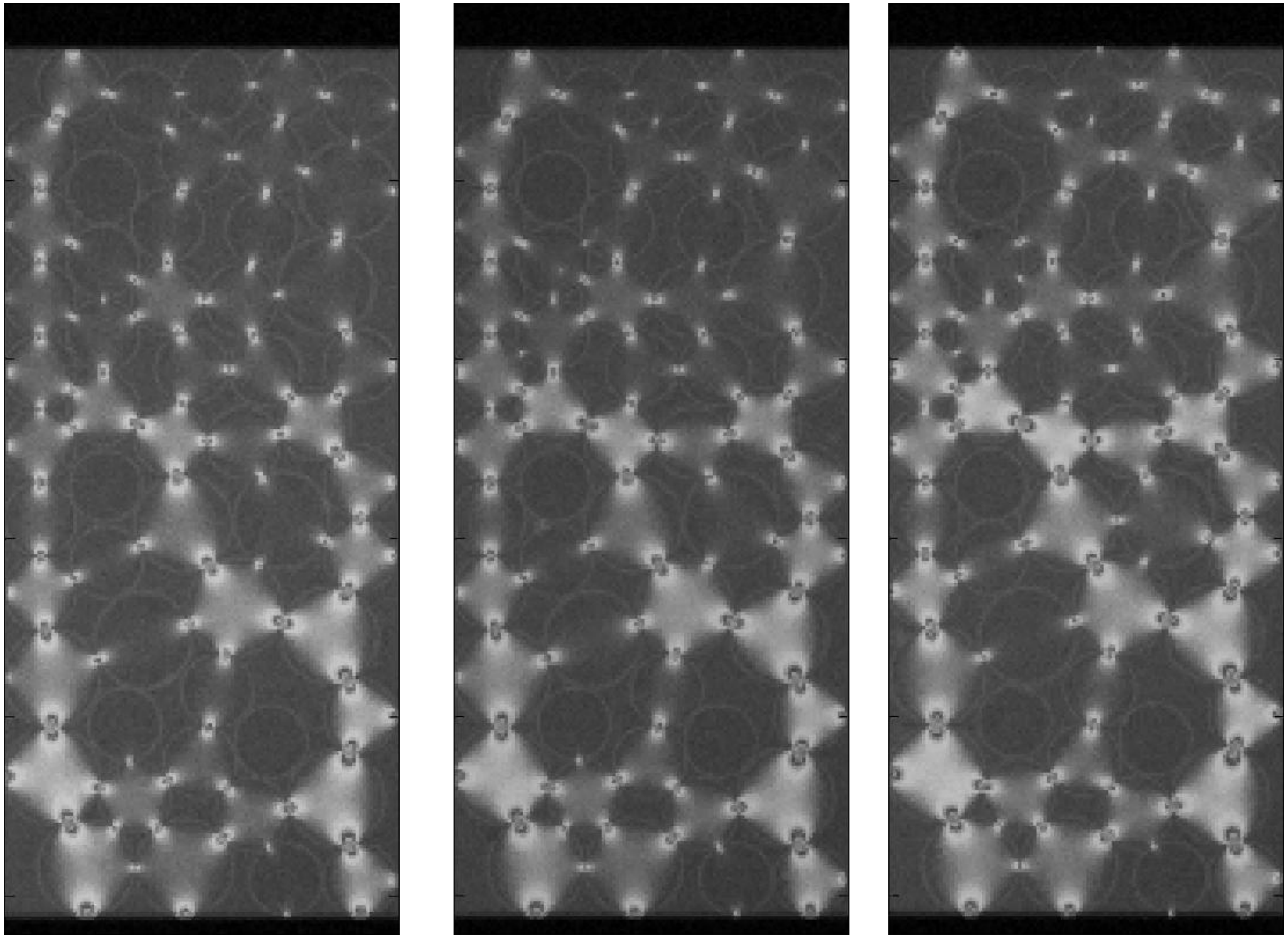


Brito & Wyart, J. Chem. Phys. 131, 24504 (2009)

Carl Schreck: J13.00002: Vibrational density of states for granular solids

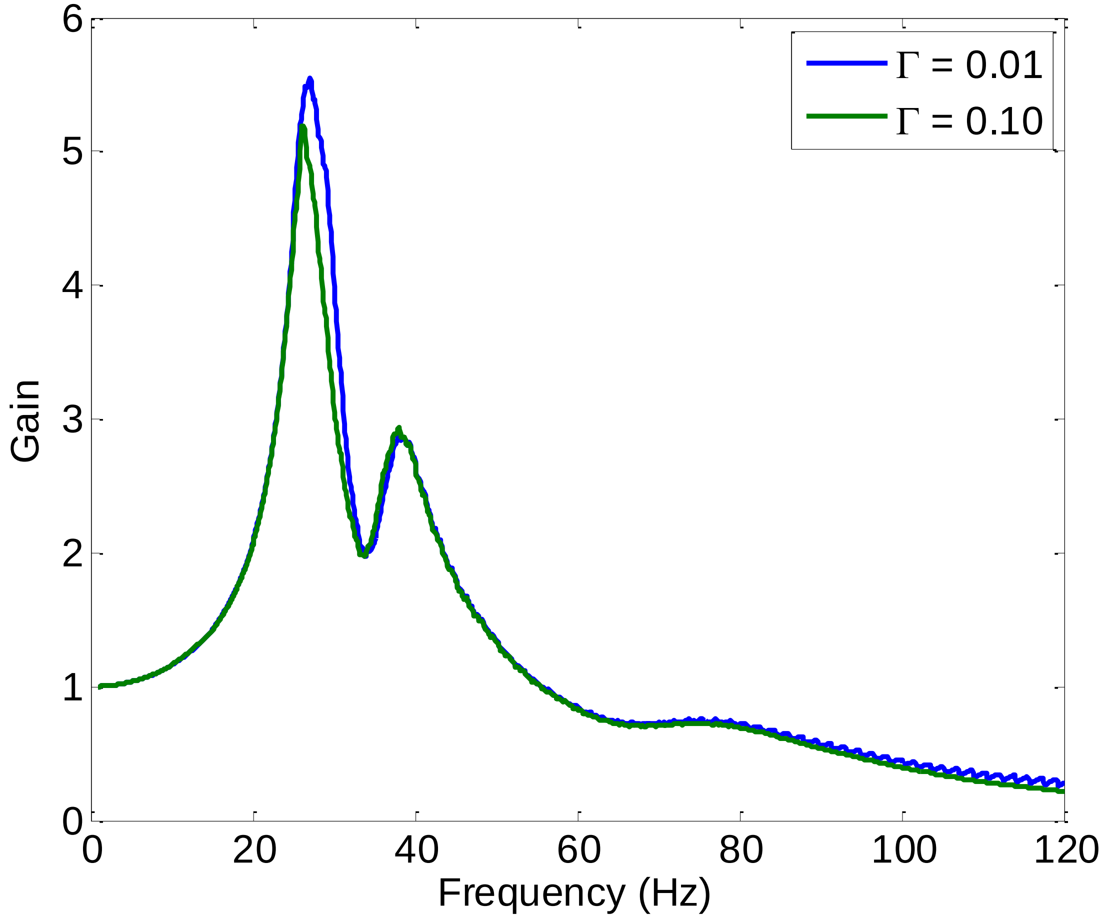
Experiments: "Real" systems

Driving Γ: 0.01 g 0.10 g 0.50 g

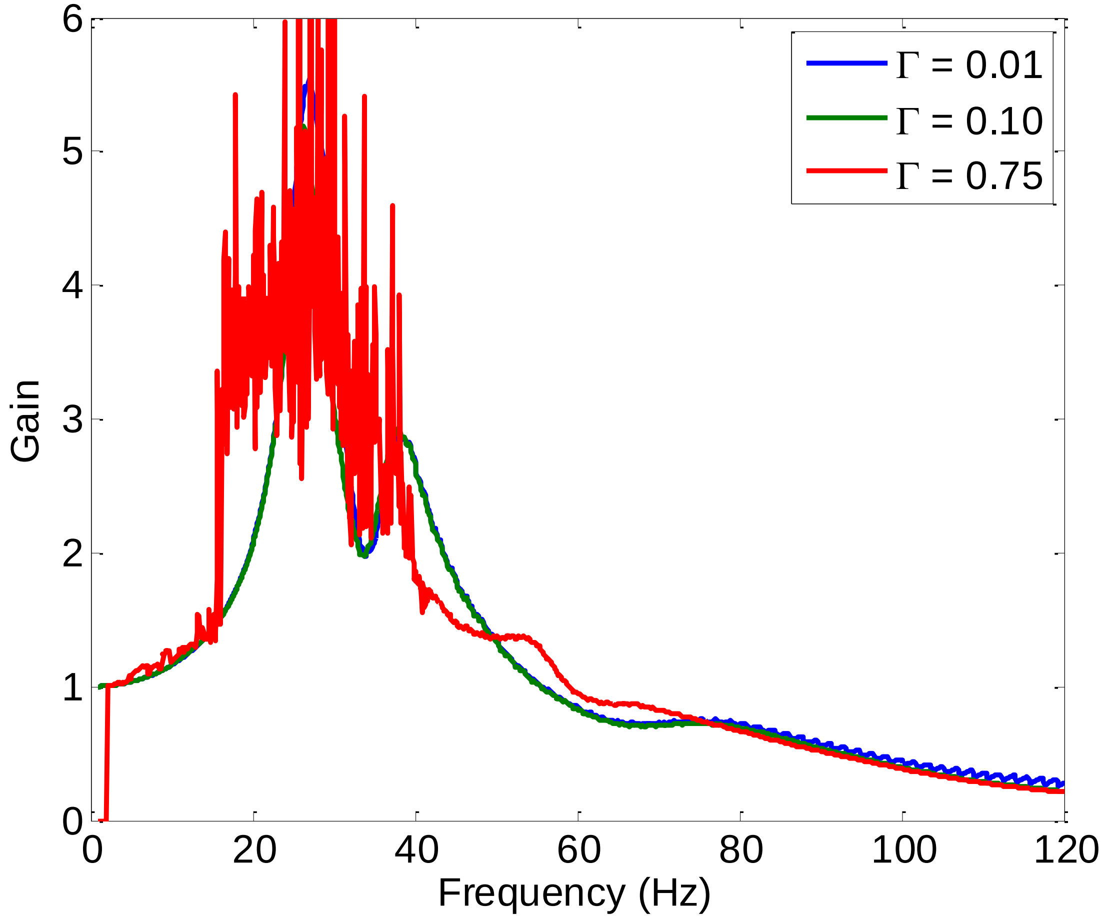


- 53 Photo elastic particles
- (41) 3/8"
- (12) 1/2"
- Constant pressure weight: 10 x M_s
- Sinusoidal Drive
- Max Acceleration: $\Gamma = A\omega^2/g$
- Brightness ~ proportional to stress

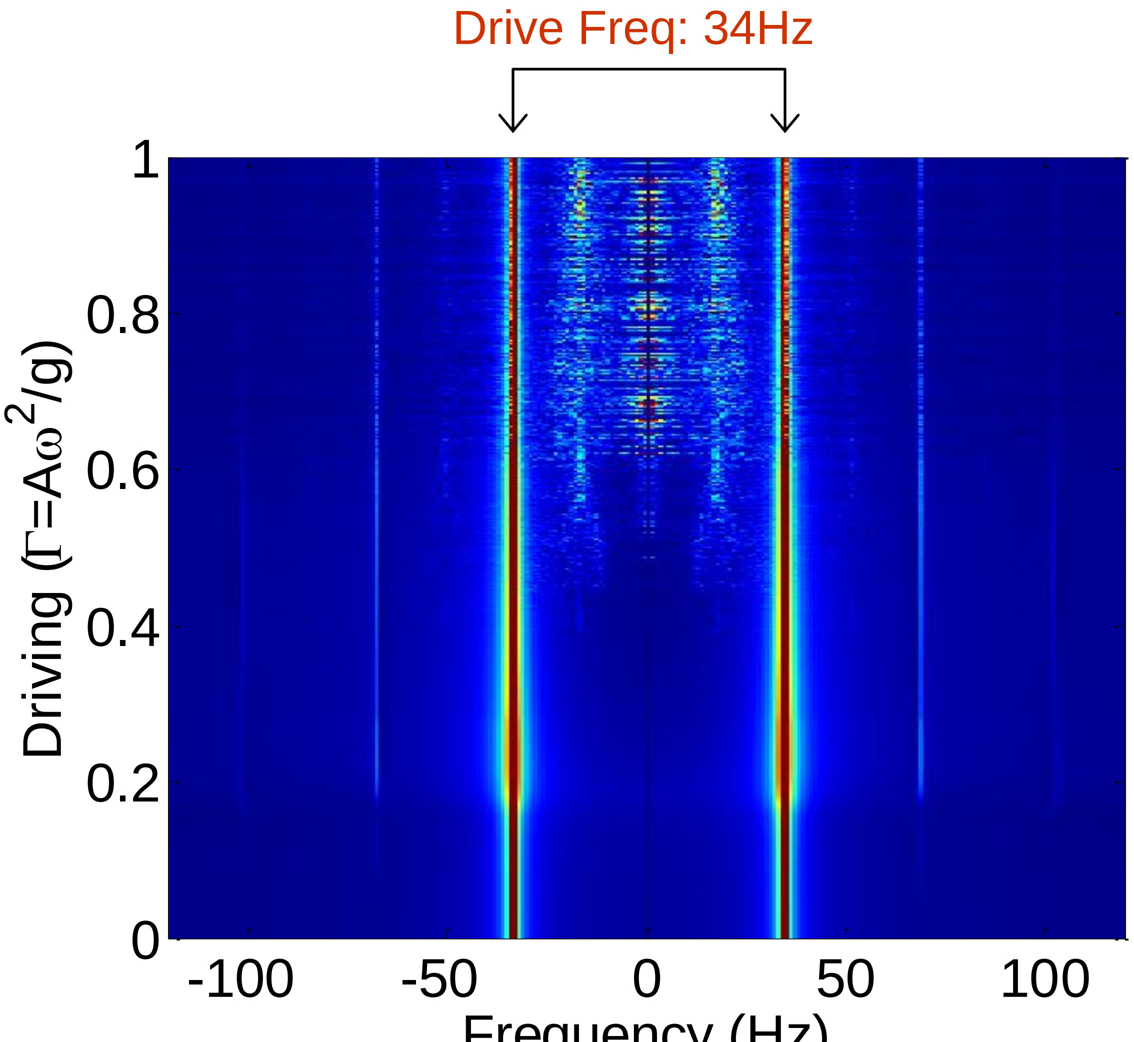
Frequency Response



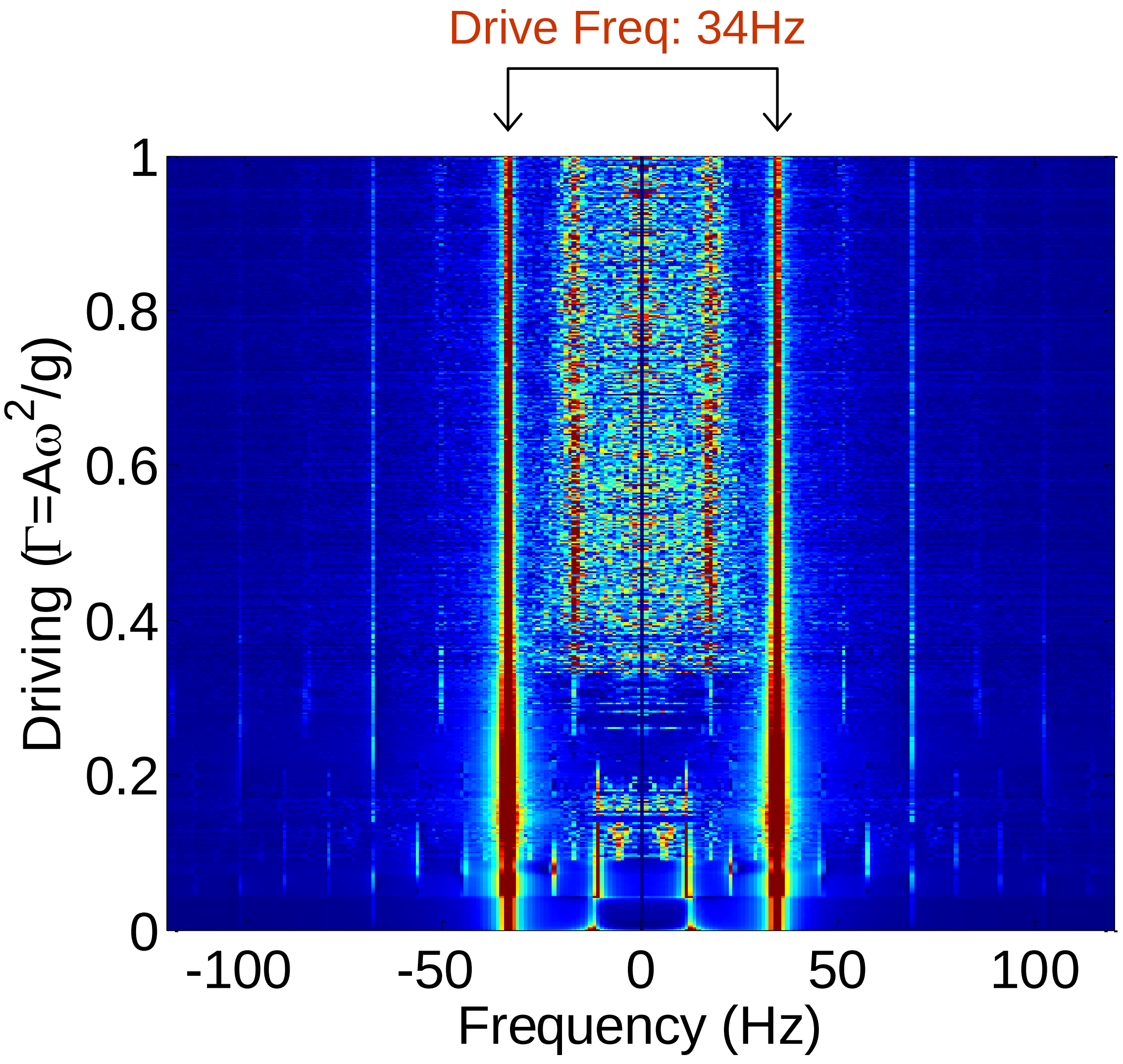
Frequency Response



Frequency Response vs. Driving Amplitude



Frequency Response vs. Driving Amplitude
(Low Pressure)



Conclusions

Simulation

- 2D frictionless bidisperse mechanically stable packings.
- Perturbations δ along eigen-directions:
  - fluctuations abruptly spread to all discrete harmonic modes at δ_c.
  - Above δ_c all harmonic modes disappear into a continuous frequency band.
- δ_c scales with $\Delta\phi/N$:
  - No linear vibrational response as $N \to \infty$. regardless of $\Delta\phi$.
  - No linear vibrational response as $\Delta\phi \to 0$ for all N. (Jamming)
- Nonharmonic behavior dramatically affects all aspects of system response:
  - heat capacity, density of states, elastic moduli, and energy propagation.

Experiments

- Dramatic change in disturbance propagation:
  - Frequency Response becomes erratic and time-dependent.
  - Fluctuations explode to a band of frequencies, even with constant frequency driving.
  - Critical Amplitude decreases with confining pressure.

Final Conclusions

The Dynamical Matrix

Rarely Matters