Granular Materials Laboratory

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Novel plasticity of purely repulsive solids near jamming

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Purely Repulsive Jammed Solids

2D Molecular Dynamics

- 2D frictionless bidisperse mechanically stable disk packings.
  - 50:50 mixture, \( D_L / D_S = 1.4 \)
  - Jammed (\( \phi_J \)), 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

\[ F = -K\delta \]

\[ F = 0 \]

Double Sided Springs

\[ F = -K\delta \]

\[ F = K\delta \]
Normal Modes in Disorder System

Displacements:
\[ U_n = X_n - X_n^0 \]

Dynamical Matrix:
\[ \kappa_{nk} = \nabla_n \nabla_k V(X_n^0) \]

Newton’s Law:
\[ m\ddot{U}_n \approx \sum_{k=1}^{2N} \kappa_{nk} U_k \]

Solution:
\[ U_n = \sum_{k=1}^{2N} A_k \hat{\epsilon}_{kn} \cos(\omega_k t + \varphi_k) \]
Vibrational Density of States
Vibrational Density of States

Dynamical Matrix:
\[ \kappa_{nk} = \nabla_n \nabla_k V(X_n^0) \]

Covariance Matrix:
\[ \tilde{\kappa}_{nk} = C_{nm}^{-1} V_{mk} \]
\[ C_{nm} = \langle U_n U_m \rangle \]
\[ V_{nm} = \langle V_n V_m \rangle \]

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 $\Delta \phi = 10^{-6}$, $N = 10$, $T = 10^{-13}$
Density of States $\Delta \phi = 10^{-6}$, $N=10$, $T=10^{-8}$
Density of States $\Delta \phi = 10^{-6}$, $N=10$, $T=10^{-3}$
Density of States $\Delta \phi = 10^{-6}$, $N = 10$
Density of States $N=10$

Elastic Solid

$N^\alpha$

$\tilde{d}(\omega)$

Log(Temperature)
Stress vs. Strain

Purely Repulsive

vs.

Double-Sided
Stress vs Strain
Stress vs Strain $T=0$

![Graph showing stress vs strain with a linear relationship between stress and strain.](image-url)
Jamming Density ($\phi_J$) vs Strain

Area Fraction ($\phi$) vs Strain ($\gamma$)
Jamming Density ($\phi_J$) vs Strain

Density $\phi_J$
Stress vs Strain $T > 0$

Stress $\sigma_{xy}$

Strain $\varepsilon_{xy}$

$10^{-7}$

$10^{-4}$
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

$\omega = 0.01 \text{ degrees/s}$

Drum diameter = 125 spheres diameter.

The drum is half filled with more than 8000 spheres.
Small Avalanche
Large Avalanche
## Comparison of Experiment.

<table>
<thead>
<tr>
<th>Universal Quantities for densely packed grains</th>
<th>Mean Field Theory</th>
<th>Granular Shear experiment</th>
<th>Our Rotating drum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Avalanche size distribution [ D(s) = s^{-\tau} ]</td>
<td>1.5</td>
<td>1.5</td>
<td>1.36</td>
</tr>
<tr>
<td>Avalanche duration distribution [ D(T) = T^{-\alpha} ]</td>
<td>2</td>
<td>2 or exponential</td>
<td>1.67</td>
</tr>
<tr>
<td>Averaged Source function</td>
<td>Symmetric (parabola)</td>
<td>Symmetric (parabola)</td>
<td>Asymmetric</td>
</tr>
<tr>
<td>Quasi-Periodic event statistics</td>
<td>sometimes</td>
<td>sometimes</td>
<td>Not for slow rotations.</td>
</tr>
</tbody>
</table>
The End
Density of States $N=128$
Temperature dependence of $\omega_k$
Testing Harmonic Approximation

2D Molecular Dynamics

- 2D frictionless bidisperse mechanically stable disk packings.
  - Jammed ($\phi_J$).
  - Wide range of $\Delta \phi = \phi - \phi_J$
- Apply perturbations with amplitude $\delta$
  - 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

Frequency

Perturbation Strength $\delta$

$10^{-3.2}$

$10^{-3.22}$

$10^{-3.24}$

$10^{-3.26}$

$10^{-3.28}$

-0.5 -0.4 -0.3 -0.2 -0.1 0 0.1 0.2 0.3 0.4
Amplitude of Several Fourier Modes

Fraction of Power in Mode

Perturbation Amplitude

(a)
Inherently Anharmonic

Scaled Perturbation Strength

\[ \log_{10} \left( \frac{(E/N)}{(A(\Delta \phi)^2)} \right) \]

against

\[ \log_{10} N \]
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)

\[ C_V = \frac{\Delta T}{Q} = 2Nk_B \]

\[ \hat{C}_V = \frac{C_V}{Nk_B} = 2 \]
Displacement matrix – the ‘true’ vibrational DOS

Dynamical matrix \( M_{kl} = \frac{\partial^2 V}{\partial r_k \partial r_l} \bigg|_{\vec{r} = \vec{r}_0} \)

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 nonharmonicitites. How much?
Vibrational DOS for granular solids

**vibrated soft spheres**

- $E/N = 10^{-12}$
- $E/N = 10^{-6}$

**soft spheres - DM method**

- Toward jamming from above $\phi_J$

**hard spheres**

- Toward jamming from below $\phi_J$

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

Experiments: “Real” systems

Driving $\Gamma$:

- 0.01 g
- 0.10 g
- 0.50 g

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

![Frequency Response Diagram](image)

- Blue line: $\Gamma = 0.01$
- Green line: $\Gamma = 0.10$
- Red line: $\Gamma = 0.75$

The diagram shows the frequency response of a system with varying damping factors $\Gamma$. The y-axis represents gain, and the x-axis represents frequency (Hz).
Frequency Response vs. Driving Amplitude

Drive Freq: 34Hz
Frequency Response vs. Driving Amplitude (Low Pressure)

Drive Freq: 34Hz
Conclusions

### Simulation

- **2D frictionless bidisperse mechanically stable packings.**
- **Perturbations $\delta$ along eigen-directions:**
  - Fluctuations abruptly spread to all discrete harmonic modes at $\delta_c$.
  - Above $\delta_c$ all harmonic modes disappear into a continuous frequency band.
- $\delta_c$ 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