Vibrations in jammed solids: Beyond linear response

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Nonlinear Effects in Granular Solids

Nonlinear vibrational properties of granular solids – Vibration dampening, solitary modes, dispersion, deviations from elasticity theory

Non-linear effects in real granular packings:

- Breaking existing and forming new contacts
- Non-linear interactions (Hertzian)
- Sliding and rolling friction
- Energy dissipation

See Carl Schreck’s poster for details on Hertzian interactions

Isolate the effects of fluctuations in the network of contacts!
Absence of Linear Response

Dynamical Matrix:

\[ V(r_{ij}) = \frac{\epsilon}{2} \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right)^2 \Theta \left( 1 - \frac{r_{ij}}{\sigma_{ij}} \right) \]

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

Diagonalize the dynamical matrix to access eigenfrequencies:

\[ \hat{e}_i, i \in \{1, \ldots, 2N\} \]

\[ \lambda_i = m\omega_i^2 \]
Absence of Linear Response

Temperature allow particle to explore its surrounding on a distance $\delta$:

$$\frac{1}{2}k\delta^2 = T \quad \delta = \sqrt{\frac{2T}{k}}$$

Apparent diameter of a particle: $\sigma^{\text{eff}} = \sigma - \delta$

$$\phi^{\text{eff}} = \phi \left(1 - \frac{\delta}{\sigma}\right)^2$$

Need to increase the volume fraction to rejam the system at a given $T$:

$$\phi = \frac{\phi_J}{\left(1 - \sqrt{\frac{2T}{k\sigma^2}}\right)^2}$$
Absence of Linear Response

$\phi = \frac{\phi_J}{\left(1 - \sqrt{\frac{2T}{k\sigma^2}}\right)^2}$
Generating Jammed Packings

Mechanically stable packing

\[ \Delta \phi > 0 \]

Local minima

\[ \Delta \phi = 0 \]

\[ \Delta \phi < 0 \]

degenerate minima

\[ V(\vec{r}) \]

\[ r \leftrightarrow \] grow

\[ r \rightarrow \] shrink

\[ \sigma \]

\[ 1.4\sigma \]
Beyond the Harmonic Approximation…

- Molecular Dynamics Simulation
- Constant energy
- Linear Spring Repulsion
- Frictionless
- No dissipation
- At $t=0$, add temperature

\[ N = 20 \]
Non-harmonicity in Disordered Solids

**Protocol:**
- Perturb along eigenmode by $\delta$
- Let the system evolve at constant energy
- Study the FT of the particle motion

$N = 12$
$\Delta \phi = 10^{-5}$
mode = 6

First contact breaks!

Beyond the Harmonic Approximation…

Under *harmonic approximation*:

\[ M = k_B T C^{-1} \]

\[ V = \frac{1}{N} \langle \nu \nu^T \rangle \]

\[ V = k_B T I \]

**Solution 1:** probing the correlation of particles displacements via

\[ M = VC^{-1} \]

**Solution 2:** looking for vibrational frequencies emerging in the Fourier Transform of the velocity autocorrelation function via

\[ d(t) = \sum_{i=1}^{N} \frac{\langle \mathbf{v}_i(t) \cdot \mathbf{v}_i(0) \rangle_0}{\sum_{i=1}^{N} \langle \mathbf{v}_i(0) \cdot \mathbf{v}_i(0) \rangle_0} \]

\[ \tilde{d}(\omega) = \mathcal{F}[d(t)] \]
Assessing the Vibrational Frequencies

(a) $D(\omega)$ vs $\omega$

(b) $D(\omega)$ vs $\omega$

- $D(\omega)$: Distribution function of vibrational frequencies
- $\omega$: Angular frequency
- $\phi$: Phase
- $\phi_j$: Phase at temperature $T$
- Disordered Solid: Phase transition region

$logT$ vs $\phi_j$
Assessing the Vibrational Frequencies

Non trivial evolution of the covariance matrix prediction and Fourier transform of Velocity autocorrelation function w/ T
Temperature Dependence of the Frequencies

\[ \phi \]

Disordered Solid

\[ \phi_j \]

\[ \omega_k(T) = \omega_k^d + \frac{\omega_k^* - \omega_k^d}{\left(1 + l_c(\Delta\phi)/\sqrt{T}\right)\nu} \]
Temperature Dependence of the Frequencies

\( \phi \)

Disordered Solid

\( \phi_j \)

\( \log T \)

\( \omega_m \)

\( T_0 \)
Testing Resonance in the Modes

- Drive one particle
- Record average kinetic energy per particle in steady state

\[ \langle K_{pp} \rangle \]

\[ \log_{10}(\delta \omega)^2 \]

\[ N = 10 \]

\[ \Delta \phi = 10^{-8} \]
Rearrangement probability

100 snapshot over the course of the simulation
Introducing a new Phase Diagram

ICS = Iso-coordinated Solid
HCS = Hypo-coordinated Solid
HPL = Hard Particle Liquid
DL = Dense Liquid

\[ z_{\text{iso}} = dN - d + 1 \]
Density of States

![Graphs showing density of states for ICS, HPL, and HCS](image)
Conclusions & Future directions

- No linear response for a wide range of parameters
- Need of a new description for the vibrational dynamics of jammed packings
- Transition from resonant to non-resonant modes
- Investigating effect of friction, particle shape and order

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