Absorbing phase transition on particle trajectories in oscillatory sheared systems near jamming

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Reversible - irreversible transition in particle trajectories

Low density colloids ($\varphi = 0.20$) driven by oscillatory shear:

Reversible - irreversible transition in particle trajectories

-- The active (irreversible) particles’ number

Continuous transition.

-- This absorbing phase transition is classified as Directed Percolation (DP) class ($\beta_{DP} = 0.58$):

* Contact process [Hinrichsen 2000]
* Turbulent transition [Sano 2016]
* Turbulent transition in liquid crystal [Takeuchi 2007]

Soft Glasses driven by oscillatory shear

**PNIPAM**

\( \varphi = 0.67 \)

Continuous transition: Conserved Directed Percolation (DP) class.

Requirements for DP absorbing phase transition:

- ✓ Existence of just one absorbing phase.
- ✗ No long range interactions.
- ✗ No heterogeneity.
- ✓ One component order parameter.


Much higher density system should not satisfy the requirements.

What happens then?

-- To give the clear numerical evidences for reversible-irreversible transition in high density jammed solids.
Numerical method for oscillatory shear

-- 3D overdamped athermal particles
(Lees- Edward boundary condition)

\[ \xi_s \left[ \frac{\partial \mathbf{r}_i}{\partial t} - \dot{\gamma}(t) y_i \mathbf{e}_x \right] + \sum_j \frac{\partial U(r_{ij})}{\partial \mathbf{r}_i} = 0 \]

-- Interaction potential (Harmonic sphere)

\[ U(r_{ij}) = \frac{\epsilon}{2} \left( 1 - \frac{r_{ij}}{a_{ij}} \right)^2 \Theta(a_{ij} - r_{ij}), \]

-- Strain evolution with oscillation

\[ \dot{\gamma}(t) = \gamma_0 \omega \sin(\omega t) \]
\[ \gamma(t) = \gamma_0 [1 - \cos(\omega t)], \quad \text{Quasi static situation:} \]

\[ \omega = \frac{2\pi}{T} \quad T = 10^4 \tau_0. \]
Conditions of numerical simulations

-- Particle number:

\[ N = 300, 1000, 3000, 10000 \]

-- Particle composition:

\[ N = N_1 + N_2 \]
\[ N_1 : N_2 = 1:1 \]
\[ \sigma_1 : \sigma_2 = 1:1.4 \]

-- Packing fraction:

\[ \varphi = 0.80 \quad \text{cf: } \varphi_J = 0.647 \]

-- Initial conditions: Random configurations.

\[ N = 300 : 10 \]

-- Ensemble

\[ N = 1000 : 5 \quad \text{independent runs are performed for averaging.} \]
\[ N = 3000 : 5 \]
\[ N = 10000 : 4 \]

-- Simulation time: \[ 4000T \]
Movie: Oscillatory shear dynamics

\[ N = 10000 \]
\[ \gamma_0 = 0.05 \]
Movie: Oscillatory shear dynamics (Stroboscopic)

\[ \gamma_0 = 0.05 \]

Every one cycle stroboscopic motions.

The particle motions change discontinuously.
Reversible-irreversible transition

Irreversible

\[ t = t_0 + T \]

Reversible (Absorbing phase)

\[ t = t_0 + \frac{T}{2} \]

\[ t = t_0 + T \]

Discontinuous

\[ \omega = \frac{2\pi}{T} \]
Displacement for 1 period

Displacement for 1 cycle:

$$\Delta r(t, T) = \frac{1}{N} \sum_j |\vec{r}_j(t + T) - \vec{r}_j(t)|$$

$$\omega = \frac{2\pi}{T}$$

Absorbing phase transition is observed at $\tau_d$. 
Discontinuous transition for one cycle displacement

Averaged 1 cycle displacement: \( \left\langle \Delta r(T) \right\rangle \)

Finite size scaling:

Reversible and irreversible branches are distinct. **First order transition.**

Large system size limit: \( \gamma_c \approx 0.0885 \)
This system shows yielding transition.

\[ \gamma(t) = \gamma_0 \left[ 1 - \cos(\omega t) \right], \]

\[ \sigma(t) = -\sigma_0 \cos(\omega t + \delta) \]

\[ G'(\omega) + iG''(\omega) = \frac{\sigma_0}{\gamma_0} e^{i\delta} \]

Elastic limit: \( \gamma_{pl} \approx 0.09 \)
Comparisons of characteristic strain amplitudes for several system sizes

The dynamic transition point $\gamma_c$ is close to the yielding transition point of the stress maximum $\gamma_{pl}$, not $\gamma_x$. 
-- Overcoming the energy barrier of stress maximum corresponds to the activation process for configuration change.

First-order transition in particle trajectories.
Summary (1)

- Oscillatory driven dense particles show discontinuous reversible - irreversible phase transition at high density for $\varphi > \varphi_J$.
- The transition takes place at yielding transition point of stress maximum.

How does the transition behaviour change in a region between low and high densities?
Model and method

✓ System
  2 dimensional overdamped harmonic spheres.

✓ Simulation size
  \[ L = 20\sigma \]

✓ Particle composition
  \[ N = N_1 + N_2 \]
  \[ N_1 : N_2 = 1 : 1 \]
  \[ \sigma_1 : \sigma_2 = 1 : 1.4 \]

✓ Initial condition
  Random configurations.

✓ Simulation time
  4000T

✓ 5 independent runs are performed for averaging
Displacement per cycle

\[ \Delta r(t, T) \triangleq \frac{1}{N} \sum_j |r_j(t + T, T) - r_j(t, T)| \]
Stroboscopic movie for one cycle displacements (high density)

\[ \varphi = 0.901, \gamma_0 = 0.10 \]

Every 1 cycle

\[ L = 20 \sigma \]
Displacement per cycle

\[ \Delta r(t, T) \triangleq \frac{1}{N} \sum_j |r_j(t + T, T) - r_j(t, T)| \]

\[ \phi = 0.715 \]

\[ \gamma_0 = \{0.220, 0.260, 0.300, 0.340, 0.380\} \]

Continuous transition
Stroboscopic movie for one cycle displacements (low density)

\[ \varphi = 0.715, \gamma_0 = 0.14 \]

Every 1 cycle

1 + \log(<\Delta r>/7)

\[ (<\Delta r> = 10^0) \]

\[ (<\Delta r> = 10^{-7}) \]
Displacement for 1 cycle (near jamming)

Displacement per cycle

$$\Delta r(t, T) \triangleq \frac{1}{N} \sum_{j} |r_j(t + T, T) - r_j(t, T)|$$

Reentrant absorbing phase transition

$\phi = 0.750$
Phase diagram: one cycle displacement

Displacement per cycle

Reversible

Irreversible

$1 + \log \langle \Delta r \rangle / 7$
Phase diagram: one cycle displacement

Displacement per cycle

Discontinuous absorbing phase transition
Phase diagram: one cycle displacement

Displacement per cycle

Continuous absorbing phase transition
Phase diagram: one cycle displacement

Reentrant absorbing phase transition
Phase diagram: one cycle displacement

Transition behaviour changes near $\phi_J$
Contact bonds percolation

\[ \phi = 0.715 \quad \gamma_0 = 0.140 \]

\[ \phi = 0.767 \quad \gamma_0 = 0.340 \]

\[ \phi = 0.901 \quad \gamma_0 = 0.120 \]

Z = 0.7

Z = 2.1

Z = 4.7

Short range

Continuous
Contact bonds percolation

\[ \phi = 0.715 \quad \gamma_0 = 0.140 \]

\[ \phi = 0.767 \quad \gamma_0 = 0.340 \]

\[ \phi = 0.901 \quad \gamma_0 = 0.120 \]

Long range bonds are Percolated

Discontinuous

Z: Coordination number
Relationship between transition behaviour and Coordination number

- \( Z \approx 1 \): Continuous
- \( Z \approx 3 \): Marginal
  Random loose packing or shear jam [Sastry2016]
- \( Z \geq 4 \): Discontinuous
• By changing packing fraction from low to high density, we find that the reversible-irreversible transition’s behaviors change dramatically at jamming transition point.

• The mechanism of the discontinuous to continuous crossover is attributed to the contact bonds’ percolation.