

Anisotropic diffusion of vibrated semi-flexible granular rods

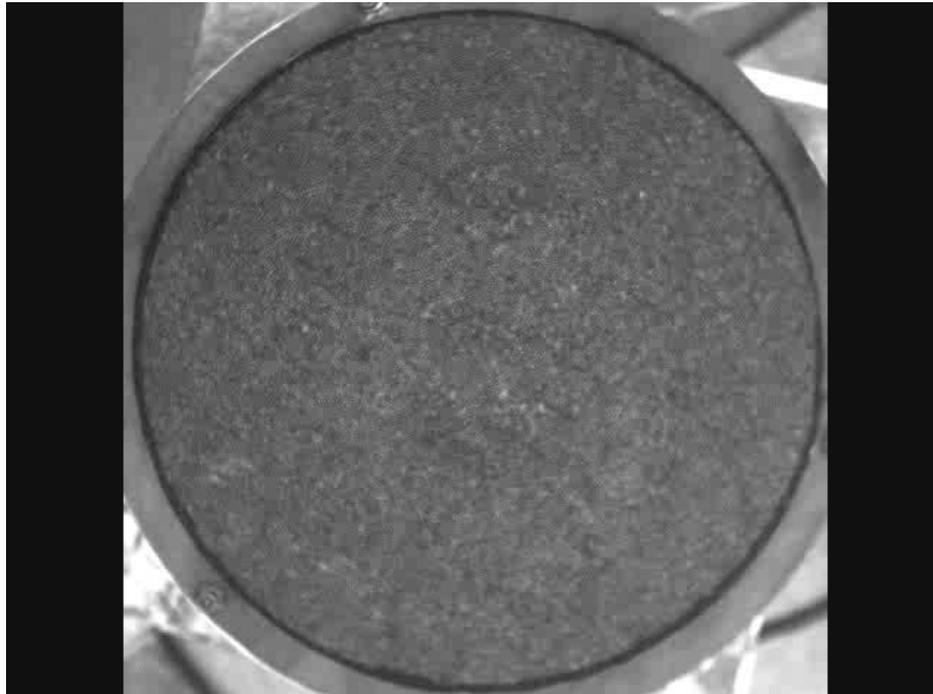


Vikrant Yadav & Arshad Kudrolli
Department of Physics
Clark University

Theoretical Background

What is Diffusion:

The process whereby particles of liquids, gases, or solids intermingle as the result of their **spontaneous movement** caused by **thermal agitation** and in dissolved substances move from a **region of higher to one of lower concentration**.¹



Diffusion and Random walks

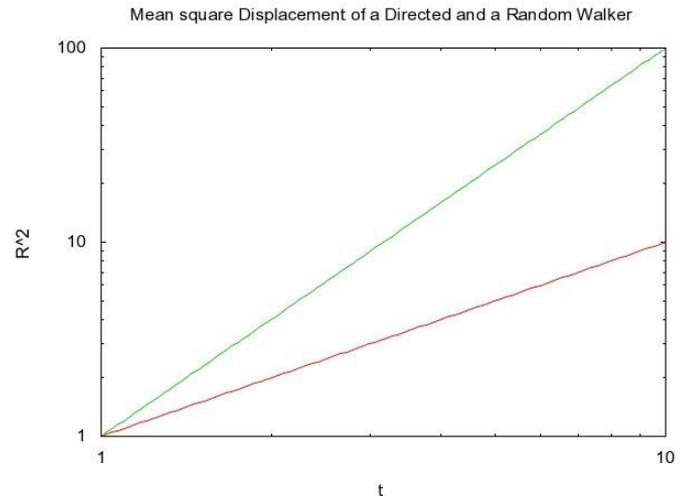
The process of diffusion can easily be modeled by a random walk. (?)

For a directed walker:

$$\vec{R} = \vec{V}t$$
$$\langle R^2 \rangle = |V^2|t^2$$

For a random walker:

$$\langle R^2 \rangle = 2nDt$$



Here n is the dimensionality of system and D is the Diffusion coefficient.

According to Einstein Relation

$$D = \frac{k_B T}{\zeta}$$

Where k_B is Boltzmann's constant, T is Temperature and ζ is friction coefficient.

Effect of Anisotropy

Motion of a nonspherical particle (in this case rodlike) can be decomposed along the direction of its long axis and along one perpendicular to it.

In general Friction along these 2 directions will not be same.

therefore, we get

$$D_{\parallel} = \frac{k_B T}{\zeta_{\parallel}} \quad , \quad D_{\perp} = \frac{k_B T}{\zeta_{\perp}}$$

From hydrodynamic calculations

$$\frac{D_{\parallel}}{D_{\perp}} = 2$$

This effect will not be visible in lab frame of reference as due to random rotations the diffusion looks isotropic at large time scales.

The same ratio is observed in 3-d as well as 2-d thermal systems.

Polymers

A polymer is composed of a large number of repeating structural units called monomers. They are formed when conditions required to add one chemical unit to a system is almost independent of its size.

e.g. nylon, PVC, DNA etc.

Structural properties of polymers were mainly studied by applying concepts of **self-avoiding random walk** to various models.

Dynamics of **thermal polymers** in a solution were studied in detail by, Doi & Edwards, de Gennes, Flory etc.

Structurally a polymer can be flexible or rodlike or anything in between.

If $t(s)$ and $t(s')$ are tangents to a polymer along its contour at s and s' respectively, then

$$\langle t(s) \cdot t(s') \rangle = e^{-|s-s'|/L_p}$$

Here L_p is the **Persistence length**.



Solution of Rigid Rodlike Polymers

Doi & Edwards worked out Dynamics of rigid rodlike polymers in a solution.

If L is the length of polymer and b is its diameter we can define 4 concentration regimes depending on number of polymers per unit volume ν

- 1) Dilute: $\nu \leq \frac{1}{L^3}$ (Polymers can rotate freely)
- 2) Semidilute: $\frac{1}{L^3} \leq \nu \leq \frac{1}{bL^2}$ (Rotation is severely restricted, static properties unaffected)
- 3) **Concentrated**: $\nu \geq \frac{1}{bL^2}$ ($D_{\parallel} = D_{\parallel 0}$, $D_{\perp} = 0$ i.e. the ratio $\frac{D_{\parallel}}{D_{\perp}}$ will diverge in this region.
- 4) Liquid Crystalline

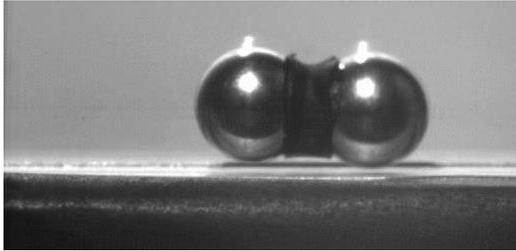
How closely can these systems can be modeled using Athermal granular chains?

Static Properties?

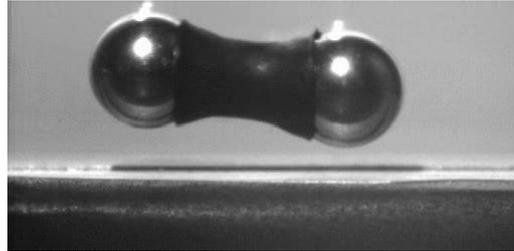
Dynamic Properties?

Novel patterns of motion in Nonspherical systems

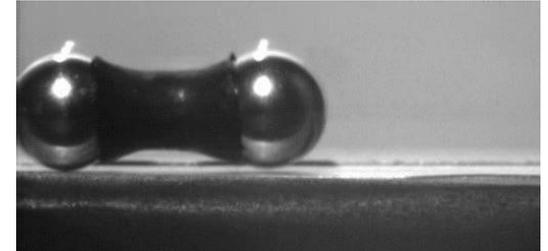
Dimers:



Flutter mode



Jump mode

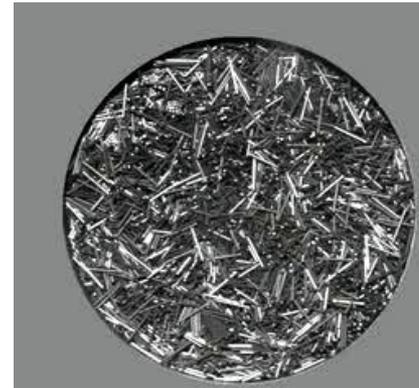


Drift mode

Rod like particles:



Vertically shaken rods



Vortex pattern

Motivation

- Diffusion of spherical particles as a function of area fraction has been widely studied. (Reis and Shattuck, PRL 2006)
- A natural extension is to look at diffusion of non-spherical systems e.g. Dimers (Atwell and Olafsen, PRE 2005)
- Our group has been widely interested in effect of dynamical properties of non spherical particles e.g. Vertically shaken rods (Blair et al., PRE 2003), Granular chains (Safford et al. , PRE 2009), Polar particles (Kudrolli, PRL 2010)
- Here, we discuss dynamics of Rod like granular chains
 - 1) Athermal, Out of equilibrium, Anisotropic Dynamics
 - 2) Can we apply equilibrium models of rod like polymers to gain an insight
- Why rod like polymers??
- Why semi-flexible granular chains??

Setup

Oscillator

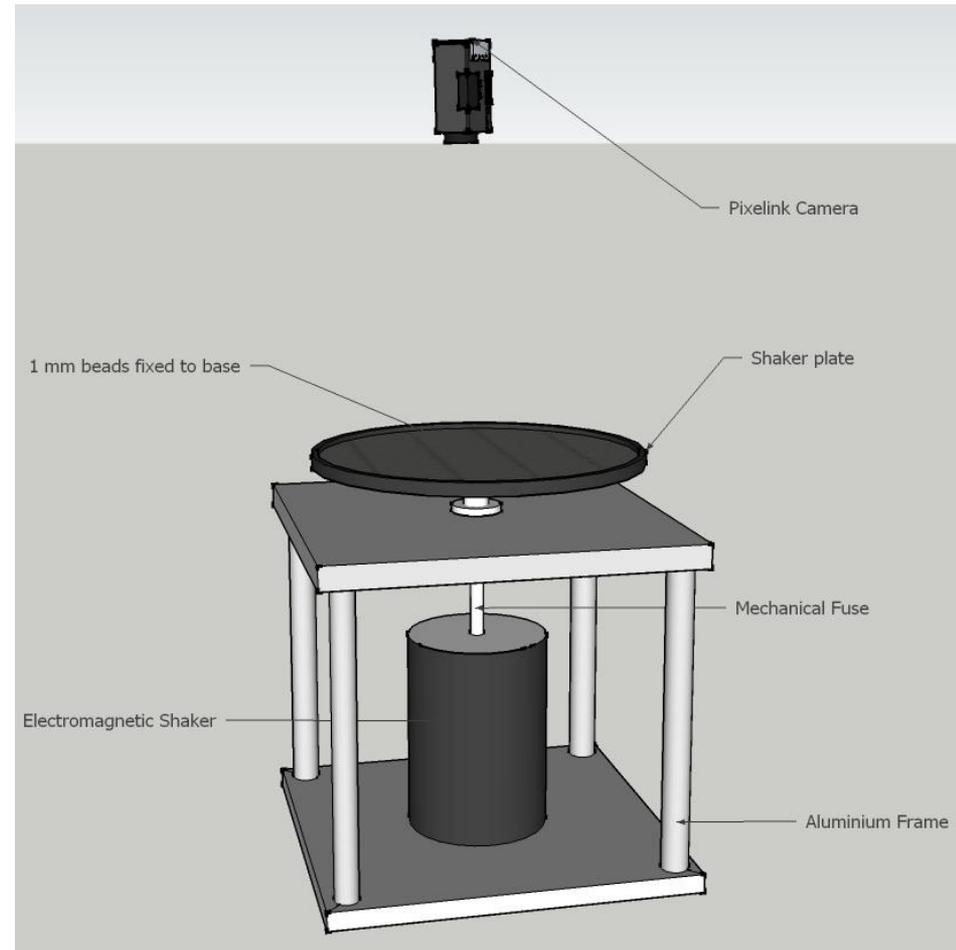
- 1) Frequency of vibration: 30 Hz
- 2) Effective acceleration = 3.0g
- 3) Diameter of beads fixed to base: 1 mm
- 4) Radius of Container: 142.5 mm

Granular Polymer

- 1) Diameter of beads: 3.125 mm
- 2) Length of polymer: 20.5 mm (long chain), 12.1 mm (short chain).

Imaging

- 1) 1000 × 1000 pixel (TIFF format)
Frame rate: 9.15 frames/second
- 2) 512 × 512 pixel (TIFF format)
1000 frames/second (High Speed imaging)



Control parameter

Area Fraction (ϕ):

$$\frac{n_{\text{bead}/\text{chain}} m_{\text{chain}} \pi r_{\text{bead}}^2}{\pi r_{\text{base}}^2}$$

Here

$n_{\text{bead}/\text{chain}}$ = number of beads per chain

m_{chain} = number of chains

r_{bead} = radius of bead on chain

r_{base} = radius of base fixed to shaker

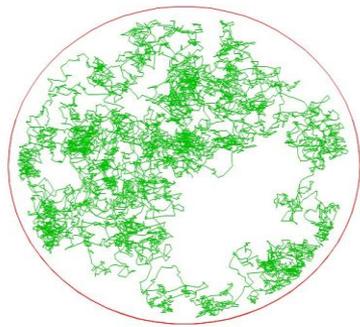
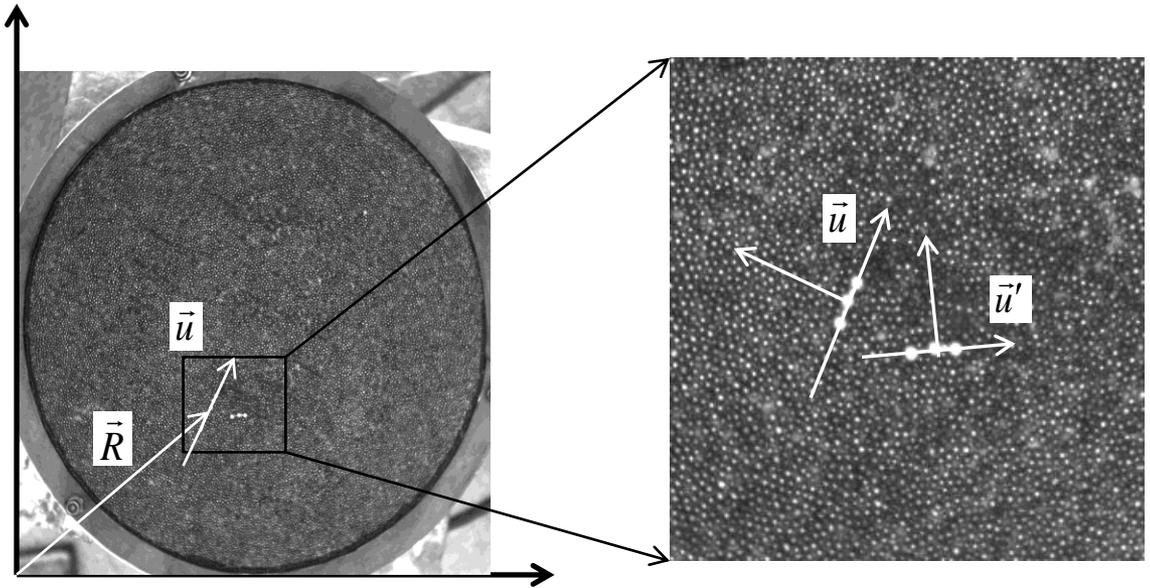
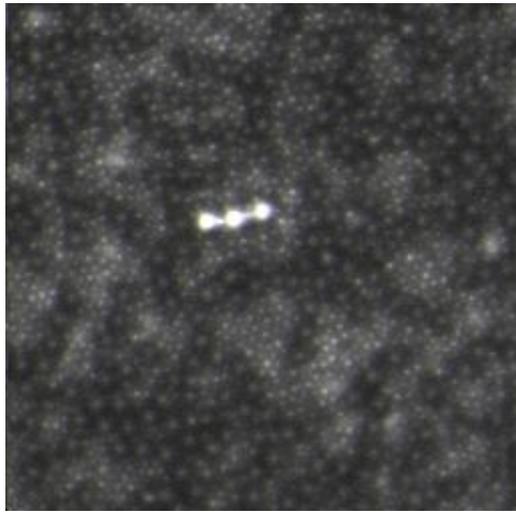


$$n = 3$$
$$L/b = 3.87$$

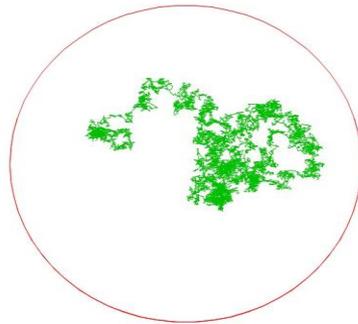


$$n = 5$$
$$L/b = 6.56$$

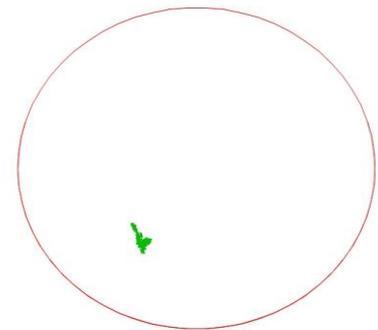
Motion in lab and body frame



$\Phi = 0.006$



$\Phi = 0.42$



$\Phi = 0.66$

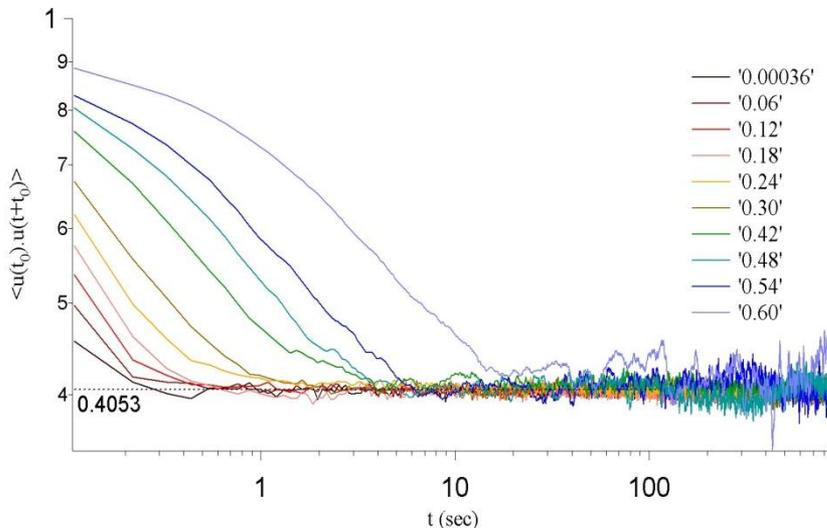
Direction Autocorrelation Function

$$\langle \vec{u}(t) \cdot \vec{u}(t + t_0) \rangle$$

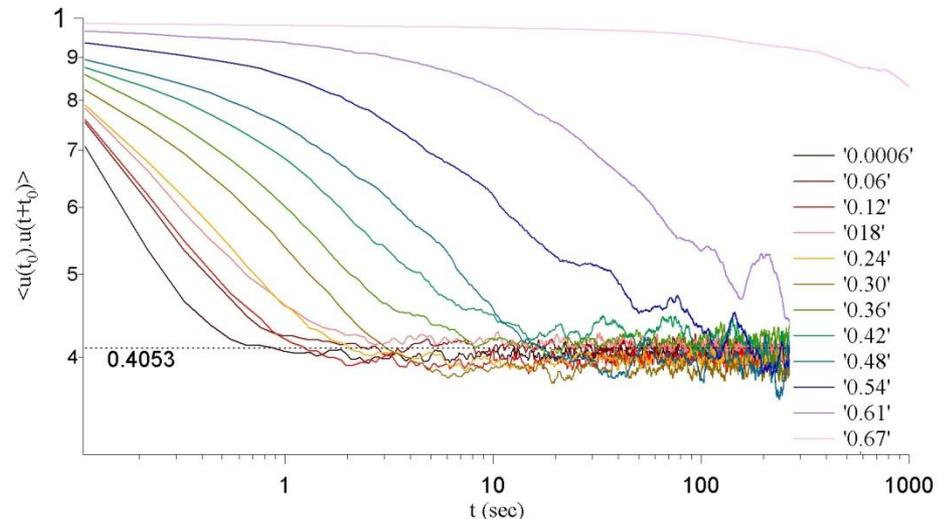
- In our case rods are indistinguishable from their earlier configuration after a rotation of 180 degree.
- In large time limit \vec{u} varies randomly from 0 to 180 degree.

$$\begin{aligned} \langle \vec{u}(t_0) \cdot \vec{u}(t + t_0) \rangle &= \langle \vec{u}(t_0) \rangle \cdot \langle \vec{u}(t + t_0) \rangle \\ &= 4/\pi^2 = .4052 \end{aligned}$$

L/b = 3.87

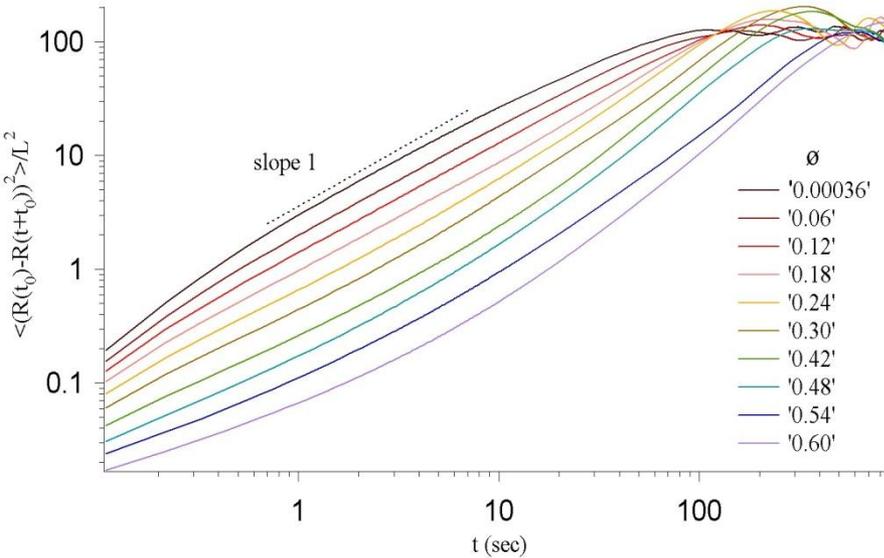


L/b = 6.56

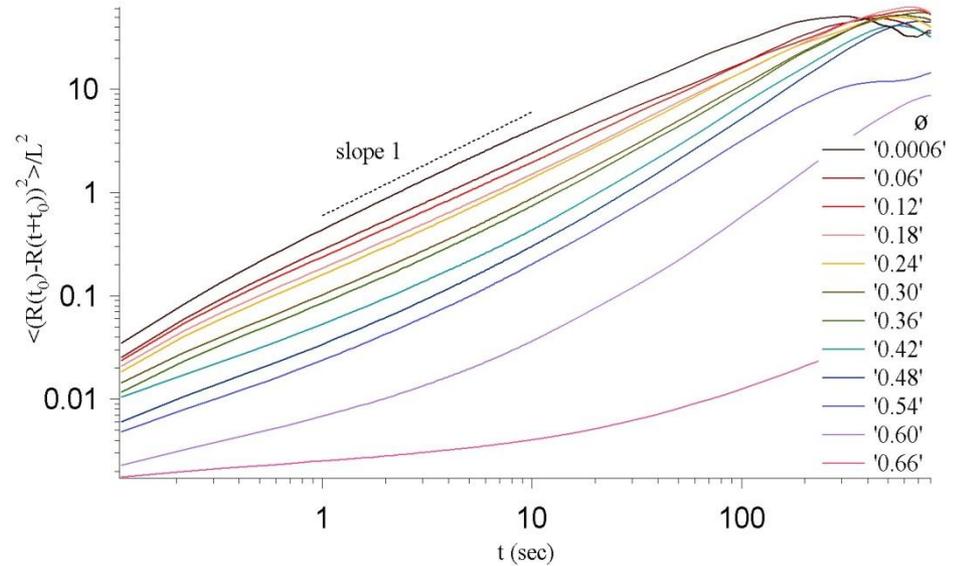


Scaled Mean Square Displacement in lab frame

$L/b = 3.87$



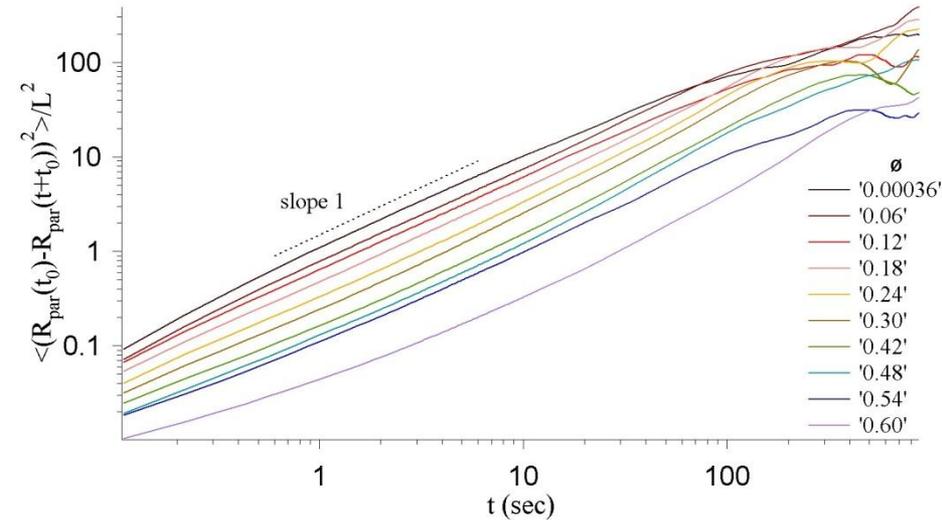
$L/b = 6.56$



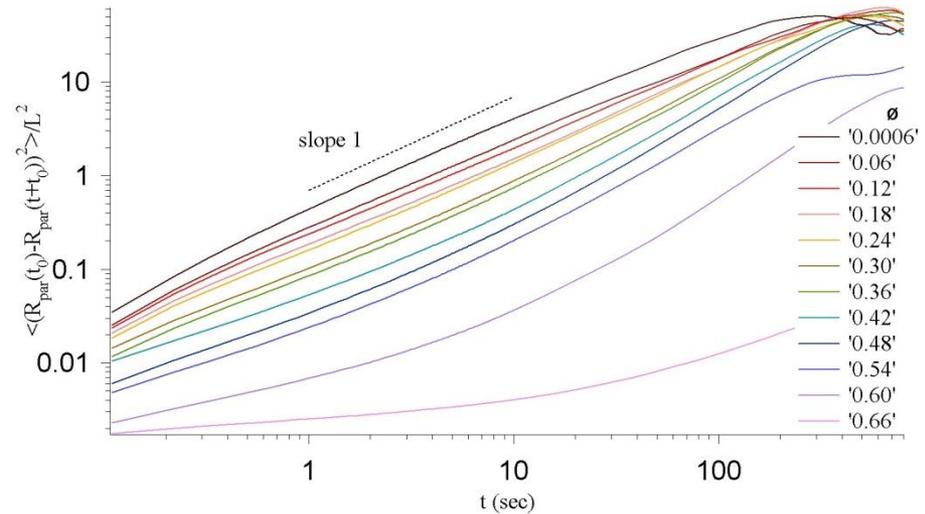
- At lowest densities system shows diffusive behavior
- As concentration of polymer increases system goes to sub-diffusive and tends to a jammed state
- The graph shows saturation near system boundaries

Scaled Mean Square Displacement in body frame along the length of polymer

$L/b = 3.87$



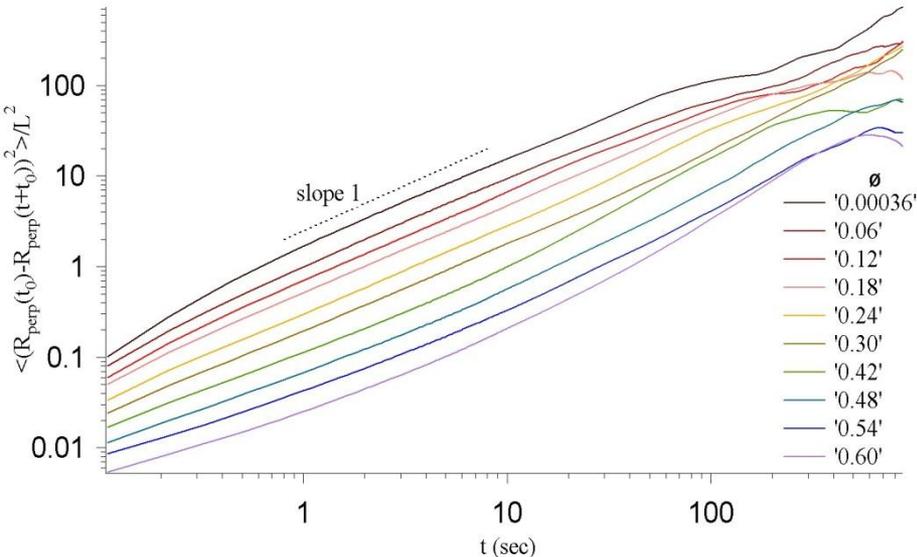
$L/b = 6.56$



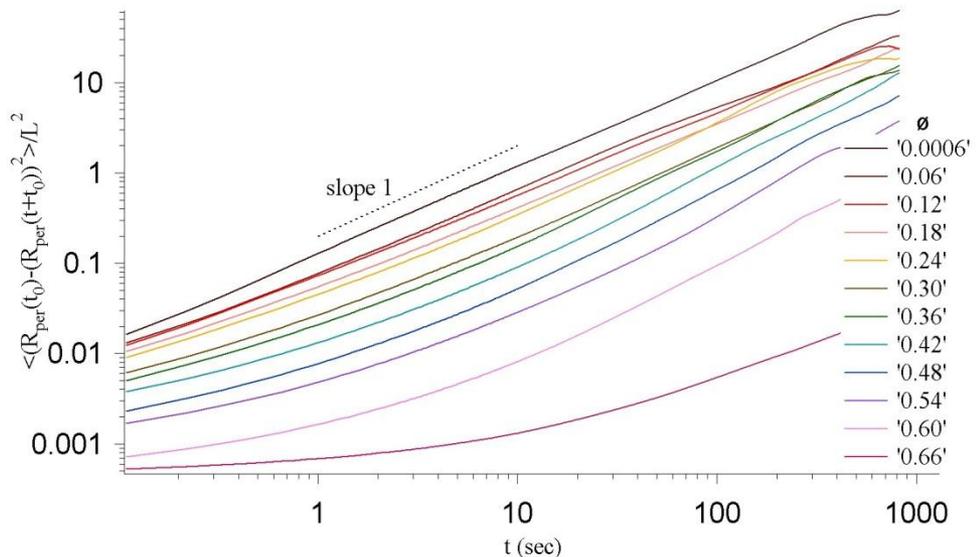
- We define a characteristic time T_{par} as the time scale over which polymer chain moves a distance equal to it's body length along the direction parallel to it.

Scaled Mean Square Displacement in body frame perpendicular to length of polymer

$L/b = 3.87$

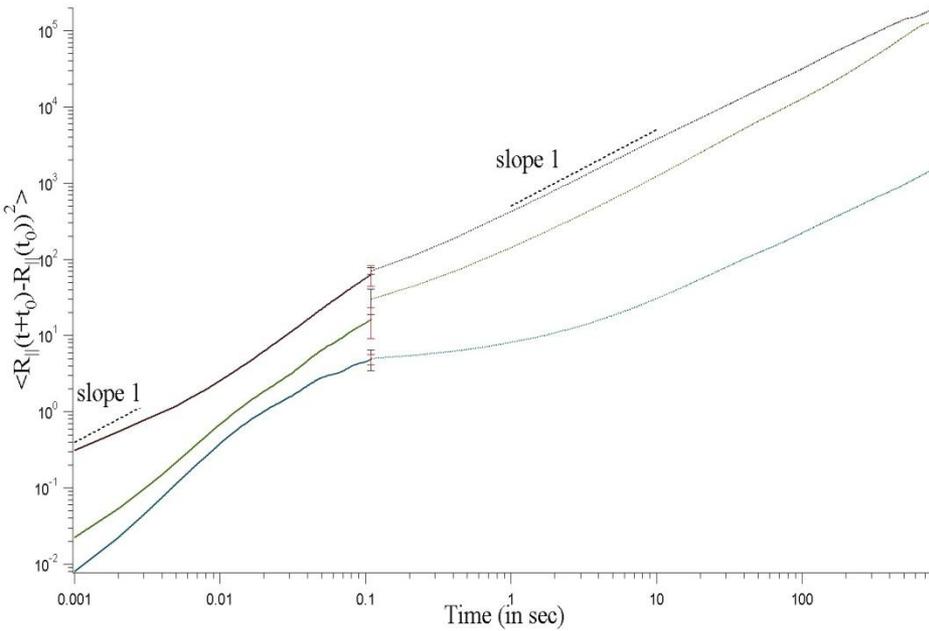


$L/b = 6.56$



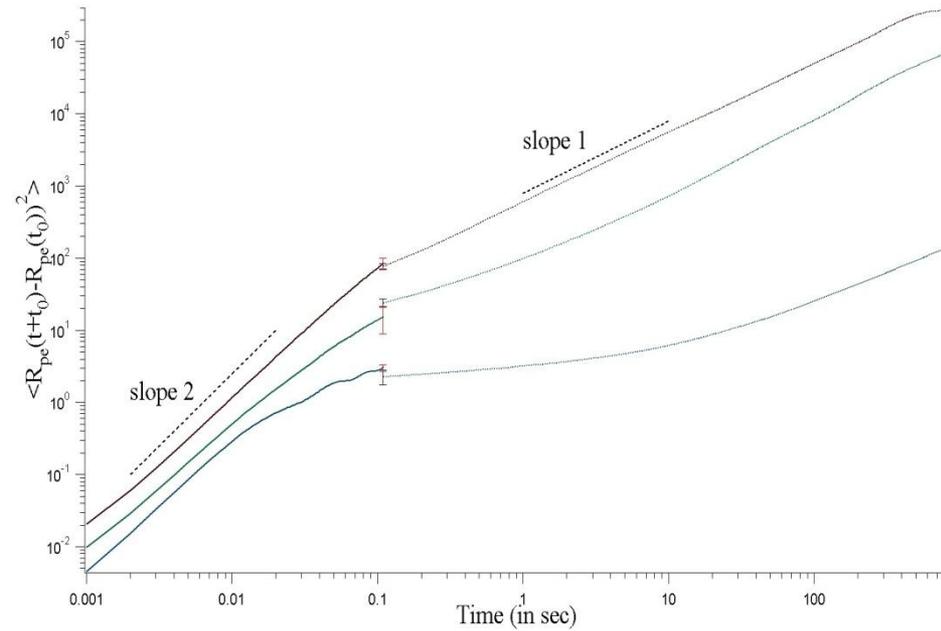
- Here we define a characteristic time T_{per} as the time scale over which polymer chain moves a distance equal to it's body length along the direction parallel to it.

Comparison of Root mean square displacement along parallel and perpendicular directions at smaller time scales for $\phi = 0.0006$, $\phi = 0.36$ and 0.66



Parallel

- Slope 1 at lower left end is due to collision among beads in same chain.
- Slope 1 at top is due to diffusion of chain.

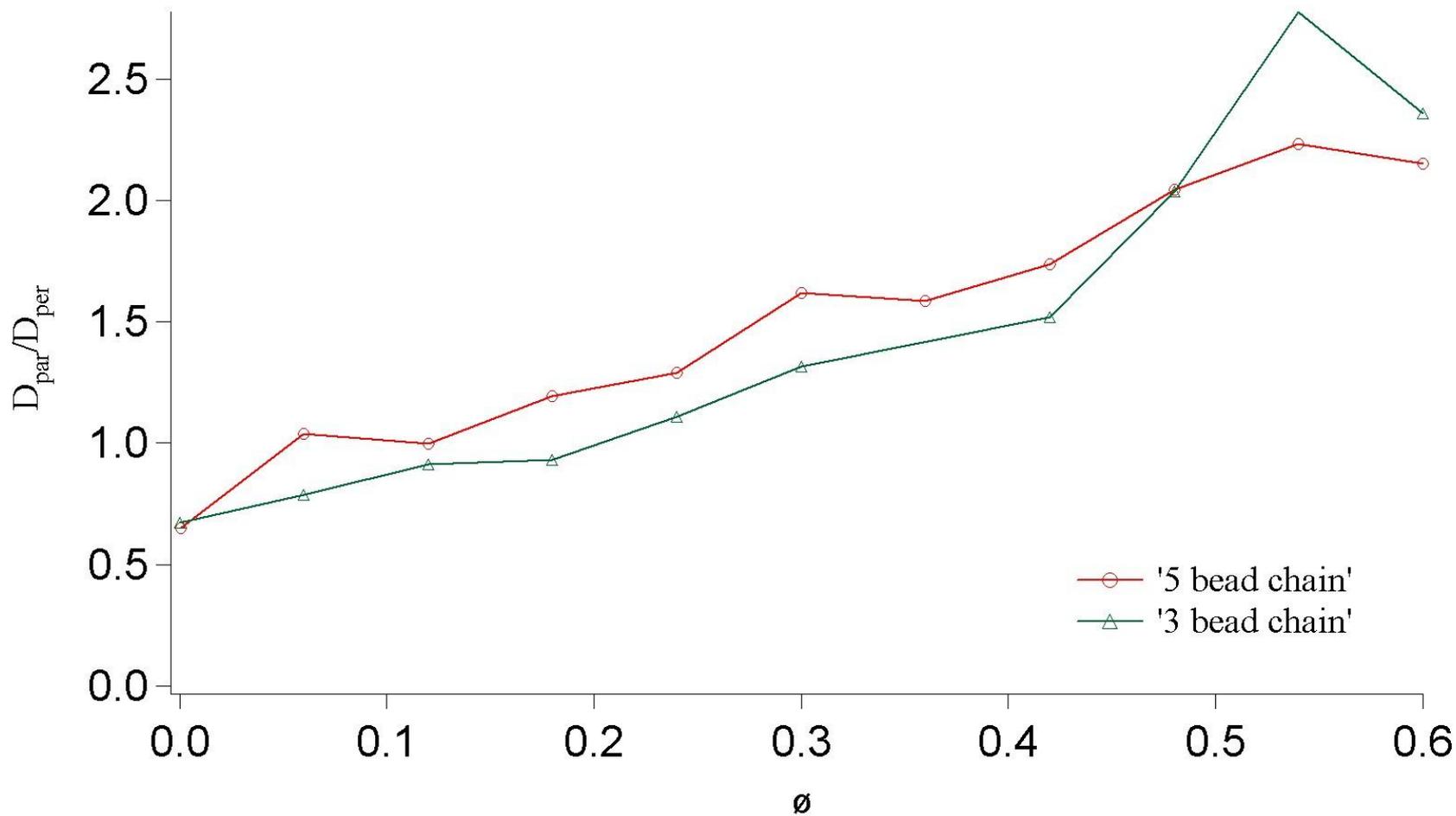


Perpendicular

- Slope 2 at lower end is due to ballistic motion.
- Slope 1 at top is due to diffusion.

Ratio of Diffusion in parallel and perpendicular direction for different chain lengths

$$\frac{D_{parallel}}{D_{perpendicular}} = \frac{T_{perpendicular}}{T_{parallel}}$$



Conclusion

- We observed anisotropy in diffusion of granular polymers.
- We observed that in dilute regime diffusion along the length of polymer is smaller than diffusion perpendicular to its length. This is different from analytic results earlier obtained for equilibrium polymers.
- We also observed that ratio of diffusion coefficients along directions parallel and perpendicular to length of polymer increases with an increase in area fraction. The Diffusion coefficients along parallel and perpendicular directions vanish simultaneously.