Dynamics of auto-motile filament propelled by self-generated solute gradient

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Abstract

An auto-motile semi-flexible active polymer shows varieties of dynamical states depending upon the flexibility and activity of the filament. The activity in the filaments incorporated by inserting chemically active dimers, consists catalytic (C) and non-catalytic (N) bead, at regular intervals along the chain. The chemical reactions at the catalytic bead of the dimer produces a self-generated concentration gradient and gives sufficient fuel to exhibit self-propulsion for the filament. When one end of this filament is clamped, the filament shows cilia like beating.

Motivation and Aim

- Active transport performed by molecular motor is a commonly observed mechanism in biological system.
- Family of kinesines and dyneins, actively transport vesicles are the examples of above.
- E-coli bacteria also undergo propulsion by similar mechanism with the help of their flagella.
- In a recent experiment, synthetic bio-compatible polymeric motors show highly efficient mode of transportation and drug delivery.
- Molecular motor distributed along the polymer length and hence exhibits cilialike beating is a common mechanism, observed in nature. Microtubule is such an example.

Modeling of self-propelled polymer with the distribution of 'active' component along its length.

To study the dynamics of spontaneous beating of polymer.

Mesoscopic Dynamics

Polymer Model

Coarse grained model of polymer with Nb beads.

Total potential energy of the system is, $V(\mathbf{r}^{N_b}, \mathbf{r}^{N_s}) = \mathbf{V}_p(\mathbf{r}^{N_b}) + \mathbf{V}_{bs}(\mathbf{r}^{N_b}, \mathbf{r}^{N_s})$

Total Polymer potential, $V_p(\mathbf{r}^{N_b}) = \sum_{i=1}^{N_b-1} \mathbf{V}_{sp}(q_i) + \sum_{i=1}^{N_b-2} \mathbf{V}_{be}(q_i, q_{i+1}) + \frac{1}{2}\sum_{i,j=1}^{N_b} \mathbf{V}_{LJ}(r_{ij})$

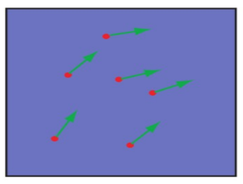
Where V_{sp} is the spring potential, V_{be} is the bending potential and V_{LJ} is the Lenard-Jones potential.

Polymer-beads solvent potential is, $V(\mathbf{r}^{N_b}, \mathbf{r}^{Ns}) = \frac{1}{2}\sum_{i=1}^{N_b}\sum_{j=1}^{N_s} \mathbf{V}_{LJ}(r_{ij})$

Solvent Dynamics : Multiparticle Collision Dynamics

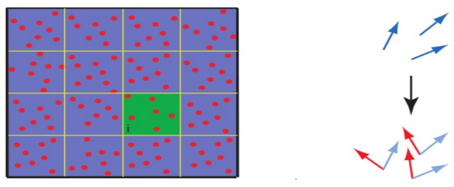
It is a two step process.

Streaming



$$r_i(t+h) = r_i(t) + V_i(t+h)$$

Collision



Center of mass velocity per cell

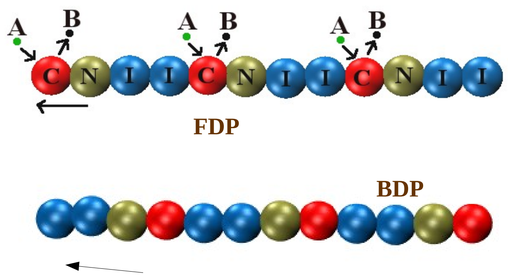
$$\bar{V}_i(t) = \frac{1}{n_i}\sum_{j\in C_i}^{n_i} V_j(t)$$

Rotation of relative velocity by angle

$$V_i' = \bar{V}_i + D(\alpha)(V_i - \bar{V}_i)$$

Self-Propelled Active polymer

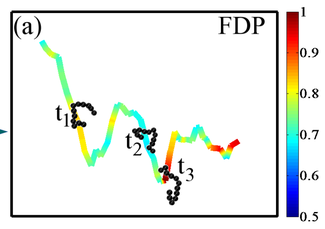
Trajectory

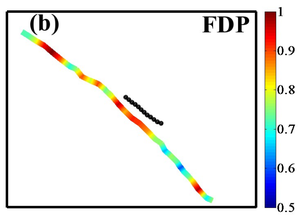


Instantaneous configuration of active polymer shows two different direction of propulsion.

- To characterize the stiffness of active polymer, we define a ratio, $\xi = \frac{l}{\sigma}$
- Here kuhn length and diameter of the bead is defined by l and σ
- In our case, for flexible limit, $\xi \approx 4.0$
- In our case, for stiff polymer limit, $\xi \approx 15.0$

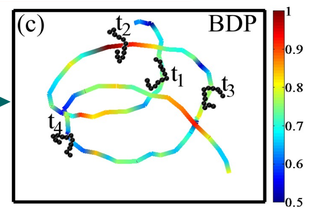
Snaking motion of FDP in less stiff polymer limit





Translational motion of FDP in stiff polymer limit

Rotational motion of BDP in less stiff polymer limit

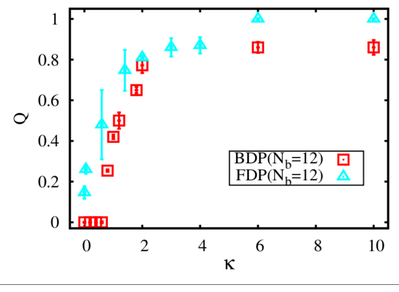


Depending upon the rigidity and the filament configuration, polymer exhibits three distinct types of spontaneous motion.

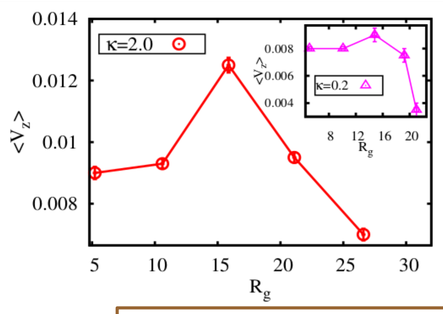
Defining order parameter, Q to characterize different mode of filament trajectories

$$Q = \frac{1}{C_0 T_{tot}}\left|\int_0^{T_{tot}} \mathbf{V}_{cm} dt\right|$$

Q = 0.0 ; Rotational Motion.
Q = 1.0 ; Translational Motion.
0.0 < Q < 1.0 ; Snaking Motion.

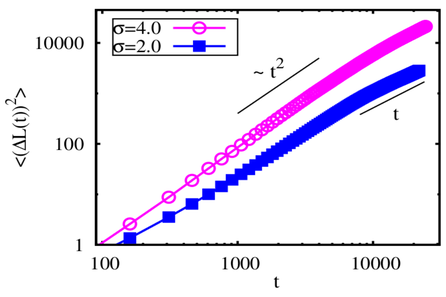


Self-Propelled Motion and Effect of Hydrodynamic Interaction



- Directed velocity is a non monotonic function of filament size.
- There is an optimal size for which highest directed velocity can be achieved.

- **Polymer with smaller monomer size shows diffusive nature at longer time scale.**
- **Polymer with bigger monomer size shows ballistic behavior.**



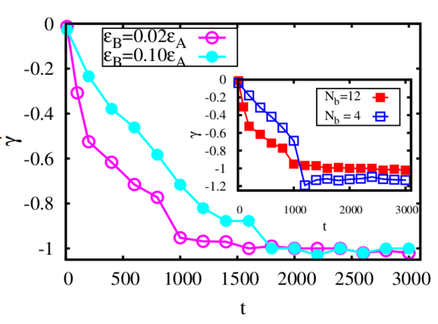
Excess-Kurtosis

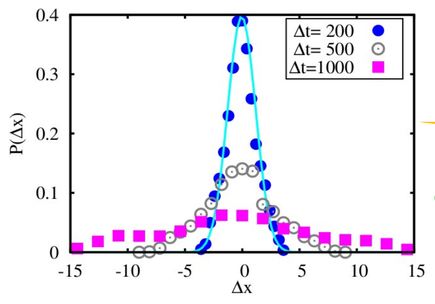
To know more deeper phenomena about self-propelled motion of active polymer, we define **"Excess-Kurtosis"**.

It is a fourth moment of particle displacement, defined as , $\gamma = \frac{\langle(\Delta x)^4\rangle}{\langle(\Delta x)^2\rangle^2} - 3$

Non-zero value of excess-kurtosis indicates non-Gaussian nature.

More deviation from γ = 0.0 for the filament with higher activity at shorter times showing increased non-Gaussianity.



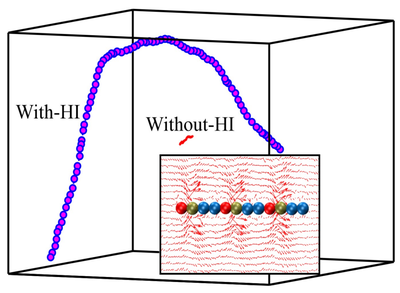


Probability at Short time scale

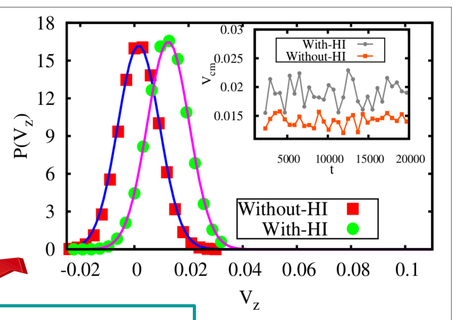
Shows Gaussian nature, depicting domination of random motion.

- **Simple diffusive motion corresponds to Gaussian distribution all the time.**
- **Large time scale the distribution changes to non-Gaussian, indicating self-propelled motion of the polymer.**

Effect of Hydrodynamic Interaction



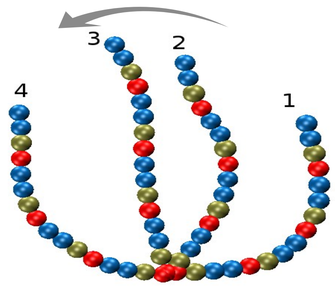
Without-HI slows down the directed motion as well as shows pronounced reorientation of the polymer.



- With HI polymer directed velocity, Vz=0.0125.
- Without-HI polymer directed velocity, Vz=0.001

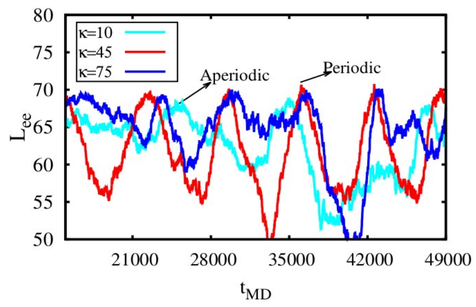
Spontaneous Beating of Active Polymer

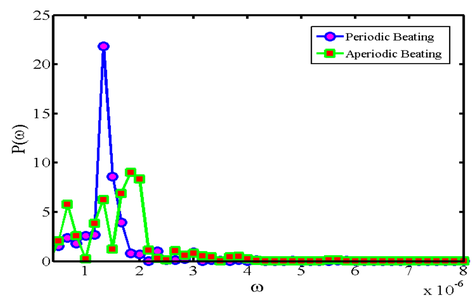
Nature of Beating



Overview of the spontaneous oscillation of clamped filament for Nb = 16. The arrow shows the direction of the beating.

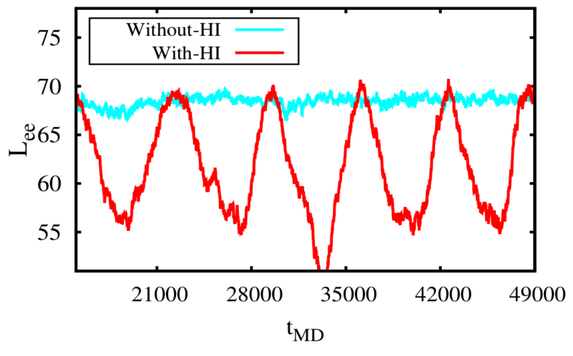
For a particular active force, periodic nature of beating depends upon the bending force of the polymer.





- **Sharp peak in power spectrum density clearly depicts periodic nature for $\kappa = 10$**
- **For $\kappa = 45$ Broadened frequency in power spectrum density indicates aperiodic nature of beating.**

Role of hydrodynamic-interaction (HI) has great importance. Without-HI, polymer does not show beating.



Conclusion

- Chemically active semi-flexible polymer, propelled by self-generated solute gradients, is a good candidate to explain the directed propulsion mechanism of the lab made synthetic polymer nanorockets.
- Our model of auto-motile active polymer is simple and easy to observe in experiment and has a potential to perform given task (cargo transport).
- When clamped this self-propelled polymer exhibits cilia like beating and hence able to capture basic mechanism behind it.

References

[1] Coarse-grained simulations of an active filament propelled by a self-generated solute gradient. D. Sarkar and S. Thakur Phys. Rev. E. **93**, 032508 (2016).
[2] Insight into the mechanism of spontaneous beating of active filament. (Manuscript under preparation).