Globule-Stretch Transition of a Self-attracting Chain in the Repulsive Active Particle Bath

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1. Radial distribution function (RDF)

To calculate the number of neighboring active particles, n_a, surrounding the chain, we firstly calculated the radial distribution functions (see Fig.S1) of active particles around the chain beads. F_a=5 and the concentration ϕ of active particles varies from 0.02 to 0.2. It's found that the first trough of RDFs is around 1.6 σ. We used it as the cut-off distance for calculating the n_as.

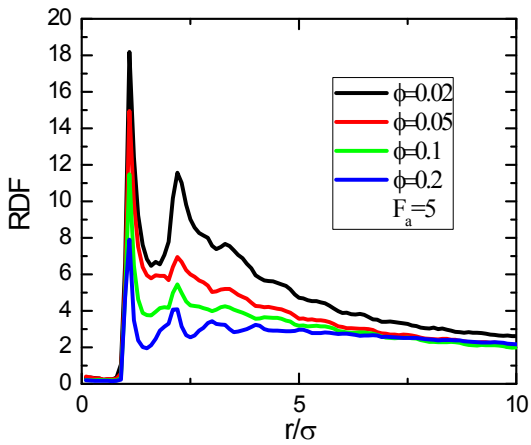

Fig.S1: The radial distribution functions of SPPS around chain beads for various particle concentration with propelling force F_a =5 and chain length N =100.

2. Evolution of the pair interaction energy between the chain beads

The interaction energy between chain beads are calculated in the evolution of the chain from the globule state to the stretch state for F_a=7.5 and from the stretch state to the globule state for F_a=0.5. The results are shown in Fig.S2. The attractive energy barrier is about 350K_BT. Such high-energy nonequilibrium state is sustained through the large energy input in propelling the SPPs and the transfer of the energy through the particle-bead interactions.

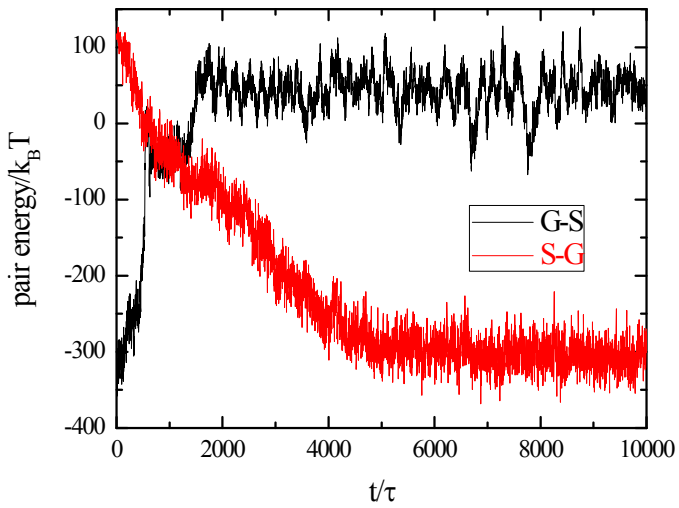

Fig.S2: The pair interaction energy of the chain beads as a function of time. The black line is for the G-S process with F_a=7.5, while the red line is for the S-G process with F_a=0.5. (The chain length N_p = 100, D_r =10^{-3} and ϕ= 0.05.)

3. Schematic calculation of the free energy barrier between the globule and stretch conformations

Even though it's not clear how to quantify the dynamic barrier during the conformation changes of the chain, it's useful to do quasi-static calculations on the free energy barrier between the globule and stretch conformations. We calculate the potential of mean force (PMF) along the reaction coordinate, Rg, by umbrella sampling method and Weighted Histogram Analysis Method (WHAM) [1–3] in the situation of F_a=0 (passive) and ϕ = 0.05. Figure S3 shows that the PMF increases about 120K_BT as Rg increases from 4.3σ (globule state) to 16.2σ (stretch state). Such large free energy barrier is overcome by active motions of the propelling particles.

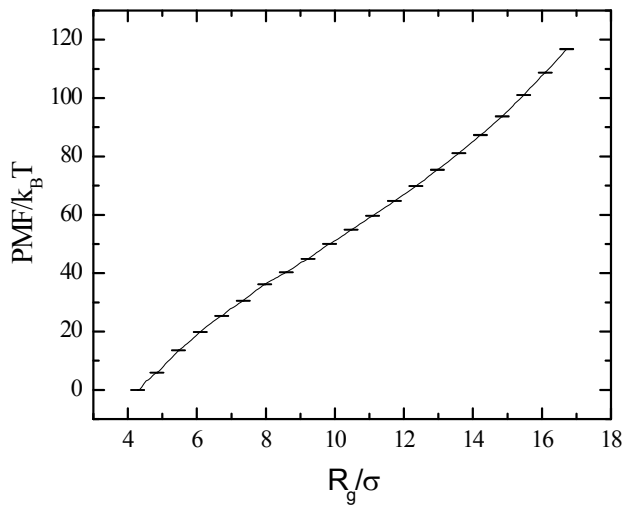

Fig.S3: Potential of mean force as a function of R_g. (The chain length N_p = 100 and ϕ= 0.05.)

References

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(2) B. Roux, The calculation of the potential of mean force using computer simulations, *Comput. Phys. Commun.*, 1995, 91, 275–282.

(3) http://membrane.urmc.rochester.edu/content/wham/.