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**Rapid Configurational Fluctuations in a Model of Methylcellulose** XIAOLAN LI, KEVIN DORFMAN, University of Minnesota - Twin Cities — Methylcellulose is a thermoresponsive polymer that undergoes a phase transition at elevated temperature, forming fibrils of a uniform diameter. However, the gelation mechanism is still unclear, in particular at higher polymer concentrations. We have investigated a coarse-grained model for methylcellulose, proposed by Larson and coworkers, that produces collapsed toroids in dilute solution with a radius close to that in experiments. Using Brownian Dynamics simulations, we demonstrate that this models dihedral potential generates "flipping events", which helps the chain to avoid kinetic traps by undergoing a sudden transition between a coiled and a collapsed state. If the dihedral potential is removed, the chains cannot escape from their collapsed configuration, whereas at high dihedral potentials, the chains cannot stabilize the collapsed state. We will present quantitative results on the effect of the dihedral potential on both chain statistics and dynamic behavior, and discuss the implication of our results on the spontaneous formation of high-aspect ratio fibrils in experiments.

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