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Tube Geometry and Brownian Dynamics in Semiflexible Polymer Networks

Jens Glaser[1], *Masashi Degawa*[2], *Inka Lauter*[2], *Rudolf Merkel*[2] *and Klaus Kroy*[1]

[1]Leipzig University, Institute for Theoretical Physics, Vor dem Hospitaltore 1, 04103 Leipzig, Germany, E-Mail: jens.glaser@uni-leipzig.de

[2]Research Center Jülich, Institute for Bio- and Nanosystems: Biomechanics (IBN4), 52425 Jülich, Germany

1. Introduction

Solutions of stiff biopolymers have unique properties which rely on the fact that the filaments are neither completely rigid nor completely flexible. A successful description of their equilibrium properties is based on the concept that topologically excluded volume resulting from hard-core interactions with the surrounding solution confine each polymer to an effective tube-like cage. The tube model for stiff polymers is a generalization of the original tube model of flexible polymers introduced by Doi and Edwards. The tube radius plays a central role for the phenomenology of stiff polymer solutions. In the literature [1-2], its scaling behavior with concentration as well as exact prefactors have been derived using mean-field theory and simulation.

Generalizing Onsager's ansatz for hard cylinders, we propose a theory of polymers represented as effective particles interacting via an effective soft potential accounting for the topological restriction encountered by the polymers.

2. Results

As a result, the distribution of tube radii in a semidilute solution is predicted. The analytical results are validated by Brownian dynamics computer simulations of the distribution functions. The center-of-mass diffusion of the polymers in semidilute solution is observed to undergo a slowing down with a crossover to a lower diffusion exponent due to entanglement constraints.

Experimental results on the distribution of tube radii in solutions of the semiflexible biopolymer F-actin are also presented. These are obtained by confocal laser scanning microscopy. The experiments additionally allow for spatially resolving the variation of the tube radius along the tube backbone, which can be compared to the theory.

3. Conclusion

By combining theory, simulation and experiment we are able to provide a consistent description of the tightly entangled state of semiflexible polymer solutions and in particular the distribution of tube diameters and the Brownian dynamics of the filaments. The results should apply to a wide range of systems, including biopolymers, but also

synthetic polysaccharide gels as well as carbon nanotubes, which are accessible experimentally by microrheological methods and direct observation.

References

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