Elasticity of bistable flexible and semiflexible polymers

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In this talk, I will present recent progress in the theoretical investigation of the elasticity of various bistable polymer systems.

First, I will introduce a minimal model for a semiflexible polymer with locally fluctuating bending stiffness (arising, for example, from local conformational changes or from the attachment and detachment of ligands): the reversible freely jointed chain (rFJC). This model consists of a freely jointed chain with two-state hinges—open or closed. In the latter case, a longer elementary rod is formed. The conformational properties (emergent persistence length, mean-square end-to-end distance, and mean-square transverse deflection), as well as the bending response in the Gibbs ensemble, are calculated. The disorder associated with the bistable hinges is treated as annealed. A quenched version of this disorder is also analyzed, and the difference in the bending response between the two cases is discussed [1-3].

Another system with locally fluctuating bending stiffness is the reversible wormlike chain (rWLC), a concatenated sequence of wormlike blocks with fluctuating bending stiffness. For a finite number of blocks, we show that the rWLC exhibits different elastic responses depending on whether the force or the extension is the control parameter (i.e., Gibbs vs. Helmholtz ensemble inequivalence) [4,5].

In the case of flexible polymers, we consider the tensile elasticity of two bistable systems: a loop–linear polymer and a zipping–unzipping polymer. In all of these cases, we find significant ensemble inequivalence (Gibbs vs. Helmholtz) [6].

We also consider a polymer necklace in the thermodynamic limit, consisting of a sequence of concatenated reversible zipped and unzipped (bubble) blocks under tension. In the flexible case, this corresponds to a modified version of the classic Poland–Scheraga model of DNA melting. For Gaussian bubbles, we obtain a continuous phase transition, as expected. The novelty lies in the fact that the way we model the zipped segments (rod vs. Gaussian chain with a larger Kuhn length) significantly affects the temperature–tension phase diagram. For a semiflexible necklace under strong tension, no phase transition is observed; instead, we show that there is a crossover from a weakly bound to a strongly bound state [6,7].

References:

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