Ensemble inequivalence and negative extensibility/compressibility in semiflexible polymers with fluctuating bending stiffness

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Many semiflexible polymers exhibit fluctuations in the local bending stiffness along their contour. This may be due to intrinsic conformational changes (e.g., denaturation bubble formation in double stranded DNA, helix-coil transition in polypeptides, or reversible bundling of parallel aligned F-actin filaments) or to the reversible adsorption and desorption of molecules from the polymer's environment. In this presentation, we analyse the tensile elasticity of a strongly stretched wormlike chain which consists of N concatenated segments, where each segment can be in one of two states, A and B, which differ in bending stiffness. We call this model the reversible wormlike chain (rWLC) model. In the Gibbs (fixed-force, isotensional) ensemble, we obtain analytic expressions for the force-extension relation and the mean fraction of B segments. We show that, under certain conditions, there is a tension-induced crossover from a mostly A to a mostly B rWLC. In the Helmholtz (fixed-extension, isometric) ensemble, we obtain analytic expressions up to a summation. We show that, for finite N, there is significant ensemble inequivalence. Remarkably, in the Helmholtz ensemble, the rWLC can exhibit negative extensibility and multiple peaks. In addition, we consider a grafted rod-like semiflexible filament with two-state bending stiffness and we analyse its response to a point force exerted on the tip or to a confining wall. We show the ensemble inequivalence in the force-extension relation and the emergence of negative extensibility/compressibility for this system.