A simple polymer in a spherical cage

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We study the change of the pseudo phase transition of a simple homopolymer inside a spherical confinement. Of particular interest is the shift of the collapse and freezing transitions with shrinking radius of the sphere. The polymer is a simple bead-stick model, where the distance between neighboring monomers is fixed, between three monomers in a row acts a bending potential and all non neighboring monomers interact via a Lennard-Jones potential. We use modern Monte Carlo methods to investigate the phase space of this model. Most of the results are obtained by parallel tempering simulations followed by a multi-histogram reweighting method combining a direct and a recursive procedure. To crosscheck our results, especially near the pseudo phase transition, we used a parallelized kind of the multicanonical simulation. To characterize the pseudo phase transition we analyse fluctuations of energetic and conformational observables. As zero order case the spherical cage is modeled only as a geometrical constraint without any interaction with the polymer. In further simulations we switched on a interaction between the polymer and the surface of the sphere and looked for effects induced by this interaction.