Abstract Submitted
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Phase transitions of a semi-flexible polymer chain[1] KATHERINE STARR, MARK TAYLOR, Dept. of Physics, Hiram College — Polymeric materials are of importance in many areas, ranging from biomedical engineering to materials science. Many of the useful properties of these materials are related to the microscopic shape or conformation of the individual polymer molecules. For example, a polymer molecule may be in an expanded or compact conformation and, depending on local conditions, may undergo a transition between these two states. Here we study the effects of inherent chain stiffness on this collapse transition. We use a pearl-necklace model in which chain stiffness is related to bond length. We have carried out computer simulations of these model chains using the Wang-Landau algorithm to determine the density of states g(E) of the polymer. From g(E) we can compute the partition function and thus all thermodynamic properties of the chain. We present results for a range of chains length, stiffness, and bead-bead interaction range. For stiff chains the polymer collapse transitions is found to be first order (i.e., there is a free energy barrier separating the two coexisting conformations). Decreasing the chain stiffness leads to a second order (continuous) collapse transition. We are able to distinguish between these two types of transitions using either a canonical or microcanonical analysis.

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