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Simulation of Thick Polymers

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We simulate $3d$ flexible off-lattice ring polymers of length L up to $L = 4000$ for various values of the global radius of curvature $R_{grc} = 0.25, 0.48, 1.0$ and $R_{grc} = 2.0$. We utilize two different ensembles: one with a δ-function constraint on the radius, and another one with a θ-function. For both cases global radius of curvature provides a valid regularisation of polymers with thickness $D = 2R_{grc}$. The Flory type critical exponent ν_{SAW} of self avoiding non-interacting rings at $D = 2$ is determined to be $\nu_{SAW} = 0.5869(5)$ from the radii of gyration chain length L-scaling, while other D-values produce consistent results. We also study low temperature configurations of marginally compact Lennard Jones homo-polymers on a ring and identify some conformational simplices.

1 Introduction

The mechanism by that proteins fold into their biologically active form is despite decades of research still not resolved. Most of the ongoing work focuses on the sequence specifity of the final structure, i.e. emphasizes the differences of proteins to polymers. For instance, in the funnel picture[1] it is assumed, that the energy landscape of a functional protein resembles a funnel leading to the biologically active structure, while a random chain leads to the rough energy landscape of spin glasses. Only recently, a different approach has been considered. Banavar et. al.[2–4] have claimed that ground state conformations of *short* and *thick* homo-polymers exhibit only a finite set of conformational simplices i.e., helices, sheets and some others, which are independent from the actual form of the employed chain interactions. In light of the claims by Banavar et. al. it seems to be useful to study in more detail the physics of thick polymers.

2 Models

A natural starting point are homo-polymers i.e., $3d$ off-lattice chains with a constant finite thickness D: tubes. We will consider non-interacting flexible tubes - without stiffness -, and in a more ambitious approach: thick homo-polymers with an attractive interaction on the chain. Tubes are regularised with the help of a new quantity: the *global radius of curvature*[5]. The partition function of thick polymers is denoted $Z(D)$ or $Z(R_0)$ with $D = 2R_0$ and is obtained upon inserting a θ-function constraint

$$\sum_{conf} 1 \rightarrow \sum_{conf} \theta(R_{grc} - R_0) \qquad (1)$$

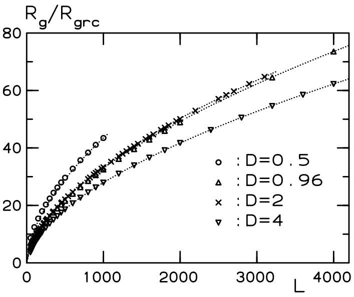

Figure 1. All $R_g := \sqrt{R_g^2}$ data of eq.(4) in units of R_{grc} at $R_{grc} = 0.25, 0.48, 1.0$ and $R_{grc} = 2.0$ with $D = 2R_{grc}$ as a function of L. The scaling curves use $\nu_{SAW} = 0.5874$ and are adjusted to match the data points at largest L. Around $D \approx 1 - 2$ the polymer swelling just is $\mathrm{const}D$.

into the partition function. For the interacting Lennard Jones homo-polymers we have

$$Z_{LJ}(R_0) = \sum_{rings} \delta(R_{grc} - R_0) e^{-\frac{1}{T}\sum_{i<j+1} V_{LJ}(r_{ij})} \tag{2}$$

where T is the temperature. The Lennard Jones potential has the form

$$V_{LJ}(r_{ij}) = 4((\frac{1.6}{2^{1/6} r_{ij}})^{12} - (\frac{1.6}{2^{1/6} r_{ij}})^{6}). \tag{3}$$

It has a minimum value of $-1.$ at $r_{min} = 1.6$.

3 Scaling of Thick Ring Polymers

In the Monte Carlo simulation we measure the mean radius of gyration R_g squared, which is defined as

$$R_g^2 = \frac{1}{L} < \sum_i (\vec{x}_i - \vec{x}_{cms})^2 > . \tag{4}$$

We display in Fig.1 all of our R_g simulation data in units of R_{grc}. The curves in the plot correspond to the finite length scaling forms $R_g \propto L^{\nu_{SAW}}$ with a fixed value $\nu_{SAW} = 0.5874$. None of the data sets at either value of R_{grc} is consistent with a Gaussian behavior at $\nu = 0.5$. A detailed analysis of effective exponents yields

$$\nu_{SAW} = 0.5869(5), \tag{5}$$

which puts non-interacting tubes into the universality class of self-avoiding walks.

4 Interacting LJ Homopolymers

We also explore the properties of near ground state conformations of interacting flexible thick tubes at a value $R_{grc} = 1.4$. Here we display in Fig.2 near ground state configurations for interacting Lennard Jones ring homo-polymers at length $L = 95$.

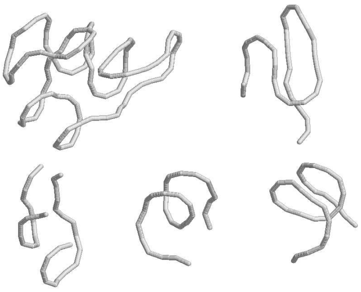

Figure 2. Near ground state conformations of a single Lennard Jones ring homo-polymer from $T = 0.1$ simulations at $R_{grc} = 1.4$ for $L = 95$. The left top corner (at position 1) displays the complete ring, while as counted from left to right , and from top to bottom, positions $2, 3, 4$ and 5 display sub-structures of the same ring.

5 Concluding Remarks

There exists the conjecture, that ground state - or near ground state - chain configurations of short thick tubes with attractive homo-polymer interactions would fold only into a finite set of conformational simplices. The degree of universality in these structures is currently under investigation.

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