Self-Entanglement of a Long Polymer Chain

Diddo Diddens[1], Albert Johner[1], Sergei Obukhov[2], Joerg Baschnagel[1]

[1] Institut Charles Sadron, Equipe TSP, 23 Rue du Loess, BP 84047, 67034 Strasbourg
[2]Department of Physics, University of Florida, P.O. Box 118440, Gainesville, FL, USA
diddo.diddens@ics-cnrs.unistra.fr

We study the effective interaction between the two halves of a long polymer chain under ✈-conditions by both Monte Carlo and Molecular Dynamics simulations. It is well known that in good (poor) solvents, different chain segments repulse (attract) each other, whereas these two opposing effects roughly cancel in the vicinity of the ✈-point. However, the *topological* self-interaction of long polymer chains under these conditions is less clear, which motivated our present analysis.

In a first step, we analyze structural properties such as the number of monomeric contacts between the two halves of the chain. Subsequently, we focus on the dynamical processes leading to the separation of the two halves after cutting the chain in the middle. This question is relevant for stimuli-responsive materials, in which e. g. the central bond of a long polymer chain is cleaved photochemically. Another motivation stems from biological issues such as the enzymatic cutting of long DNA/RNA strands in crowded media, which also involves the disengagement of distinct parts of long polymer chains. Finally, we will also discuss the separation of other architectures such as two polymers tethered together at their centers.