

Computer Simulations of semiflexible Polymers in Disordered medium

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Model

- hard disks (spheres) randomly distributed on a lattice in the continuum
- whereas the density is variable and can be greater than the percolation threshold

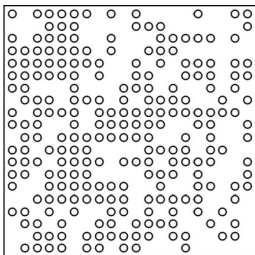


FIG. 1. Hard-disk disorder configuration with site occupation probability $p = 0.64$.

- additional alterable quantities are the diameter of the disks

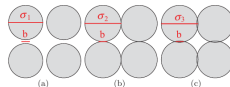


FIG. 3. (Color online) Sketch of the different disk sizes σ_i .

- and the stiffness of the polymere

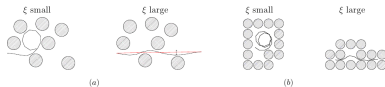


Figure 8. Sketch to elucidate the idea of softening and stiffening for persistent polymers at low (a) and high (b) occupation probabilities, respectively. The double-headed arrow indicates the width of the thermal fluctuations of the polymer.

Method

The method of investigation splits up into two simulations with different algorithms.

- creation of disordered sphere potential
- off lattice chain growth

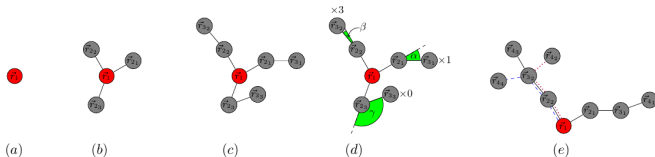


Figure 1. (a) \mathcal{M}_1 monomers at position \mathbf{r}_1 . The first monomer—here marked by the red filled circle—thus stands for \mathcal{M}_1 (3 in this example) different chains of zero length. (b) Each of the \mathcal{M}_1 chains is extended by one monomer. There are now $\mathcal{M}_2 = 3$ independent chains of length 1. Up to now, there is no energy term as there is no bending angle between neighboring bonds. (c) Each of the \mathcal{M}_2 chains is extended by one monomer. There are now $\mathcal{M}_3 = 3$ independent chains of length 2. (d) Now, energy comes into play as there is a bending angle between the first and second bonds of the polymers. Temperature T and coupling constant J are chosen such that they yield the weights that are given in the sketch ($\times 3$, $\times 1$, $\times 0$). Each of the chains is replicated according to its weight. Accordingly $\mathcal{M}_{3_{\text{new}}} = 4$. There are now four independent chains of length 2. (e) Each of these chains is extended independently by one monomer and bond. This procedure is iterated until the desired degree of polymerization is reached.