Conformational transitions in semiflexible polymers: numerical simulations

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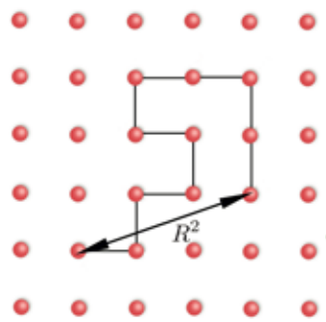
Abstract

We study the conformational properties of semiflexible polymers within the lattice model of self-avoiding random walks (SAW) with bending energy ε dependence on orientation between successive steps. We apply the pruned-enriched Rosenbluth method (PERM). Both the cases of bending preference $\varepsilon<0$ and unfavorableness $\varepsilon>0$ are analyzed, and details of ``coil-to-rod'' transition as well as transition into the ``superflexible'' state are discussed.

Introduction

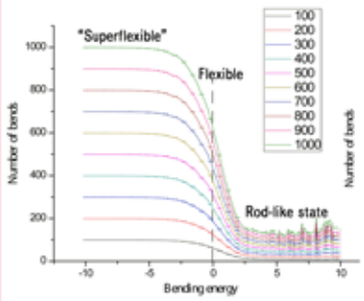


SAW on a latice

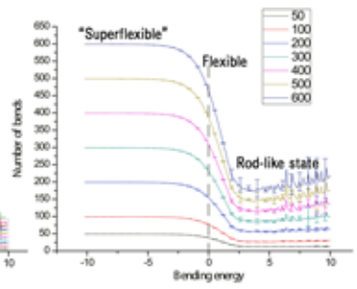
$$R^2 \sim N^{2\nu}$$

Chain in d=2 received in simulations

Conformational transitions

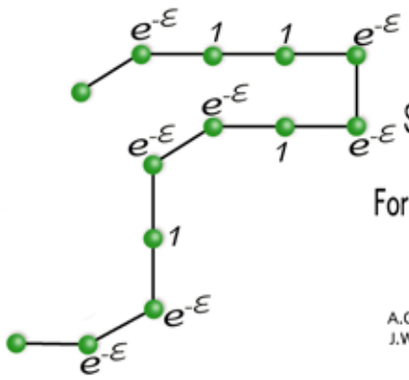


d=2



d=3

Model



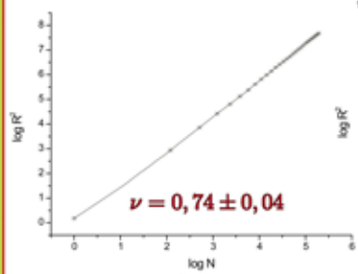
$$W \sim e^{-\varepsilon}$$

SAW on a d=2 or d=3 latice

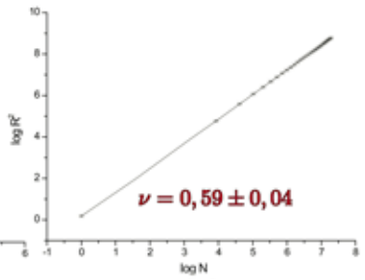
For each bending the energy penalty ε is paid

A.Giacometti, J.Phys.A **25** (1992) 2753
J.W.Halley, Phys.Rev.B **31** (1985) 293

Scaling laws



d=2



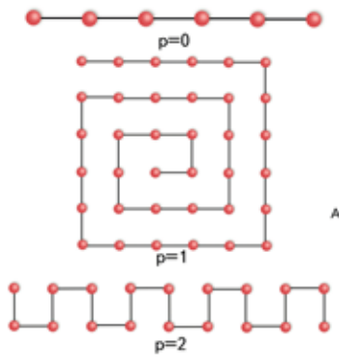
d=3

$\varepsilon=0$

$\nu = \frac{3}{4}$ B. Nienhuis, Phys. Rev. Lett. **49** (1982)

$\nu = 0,5882$ R. Guida and J. Zinn Justin J. Phys. A **31** (1998)

Nearest neighbours contacts



$$p = 2d - 1 - z(d)$$

$z(d)$ is a SAW fugacity

p – nearest neighbour contacts

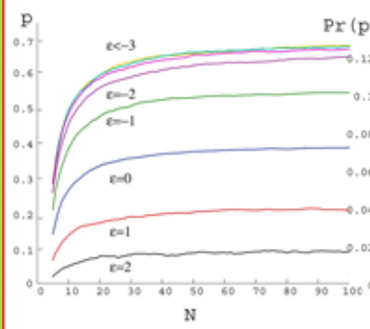
$z(d=2) = 2.6385 \pm 0.0001$

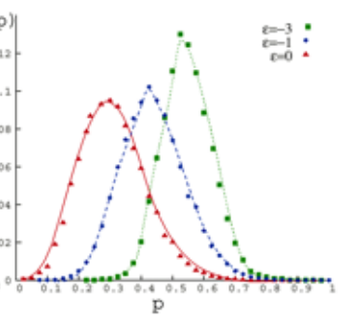
A.J. Guttman and J. Wang, J. Phys. A **24** 3107 (1991)

$p = 0.361$

for the SAW in d=2.

Nearest neighbours contacts: our results



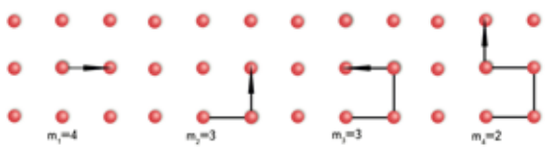


d=2

The method: PERM

For simulation we used the pruned-enriched Rosenbluth mrthod (PERM)

$$W_n \propto \prod_{i=1}^{n} m_i$$



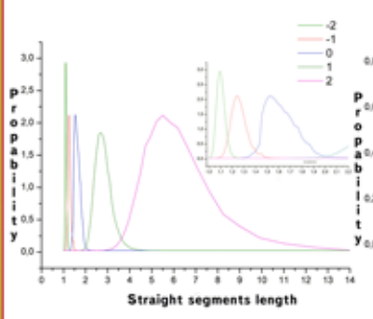
Population control parameters

$W_n^{>} = c^{>} Z_n$ "enrichment" $W_n = \frac{W_n}{2}$ and two chains are build

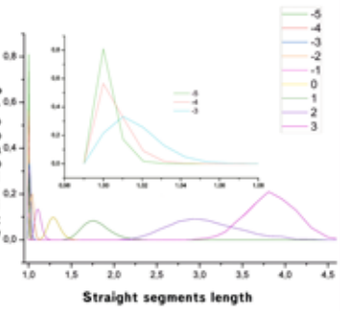
$W_n^{<} = c^{<} Z_n$ "pruning" $W_n = 2W_n$ with propability $\frac{1}{2}$

P.Grasberger, Phys. Rev. E **56**, 3682 (1996)
M.N. Rosenbluth, A.W. Rosenbluth, J. Chem. Phys. **23**, 356 (1955)
H.P.Hsu, V.Mehra, W.Nadler, P.Grasberger, J. Chem. Phys. **118**, 444 (2002)

Straight segments distribution



d=2



d=3

Conclusions

1. The Pruned-Enrichment method applied to study the structural transitions in semiflexible polymers.
2. The conformation transitions are analyzed changing the bending energy ε of subsequent monomer joints.
3. The shapes are analized using the parameter of nearest neigh bours contacts.
4. The distributions of straight segment lengthes are received.