Coarsening and Aging of Lattice Polymers

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Abstract

The nonequilibrium properties of homopolymeric collapse were investigated using Monte Carlo simulations of the interacting self-avoiding walk (ISAW) in three dimension with short nearest neighbor (NN) and longer range next-nearest neighbor (NNN) interactions. Recently, the scaling behavior of the average cluster size as well as aging was investigated using an off-lattice polymer model by applying methods from domain coarsening phenomenons to polymers [1, 2]. We extend this work to lattice polymer models in order to be able to simulate longer polymers and define properties that are dependent on the underlying structure, like the equal-time two point correlation function.

1. Introduction

- bad solvent (high temperature) → polymer is extended coil
- good solvent (low temperature) → configuration globular
- interacting self-avoiding walk on a simple cubic lattice:

$$H = -\frac{1}{2}\sum_{\substack{i\neq j\\ i\neq j\pm 1}} w(r_{ij})$$

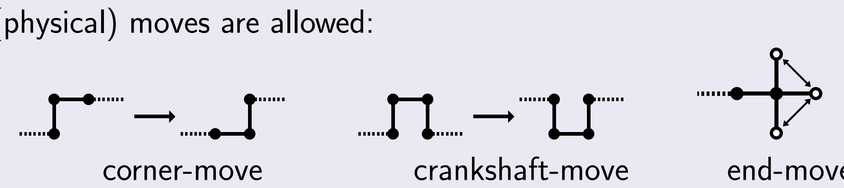
- Nearest-Neighbor (NN) interaction

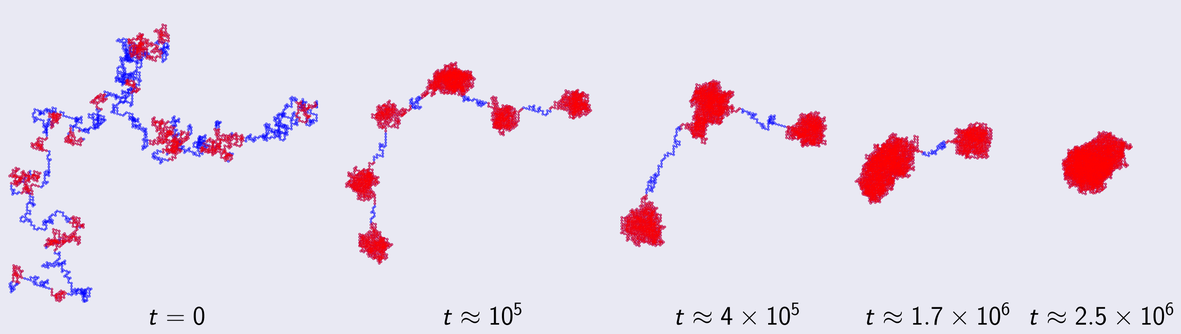
$$w(r_{ij}) \equiv \begin{cases} 1 & \text{for } r_{ij} = 1 \\ 0 & \text{for } r_{ij} \neq 1 \end{cases}$$

- Next-Nearest Neighbor (NNN) interaction

r_{ij}	$w(r_{ij})$
1	0.7
$\sqrt{2}$	0.48
$\sqrt{3}$	0.3
2	0.1

- interested in the kinetics of polymer collapse → induced by a temperature quench
- standard Metropolis Monte-Carlo simulation
  - only local (physical) moves are allowed:





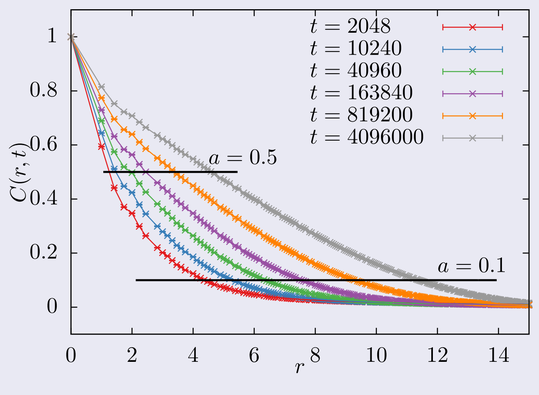
2. Cluster Growth in the Nearest Neighbor Model

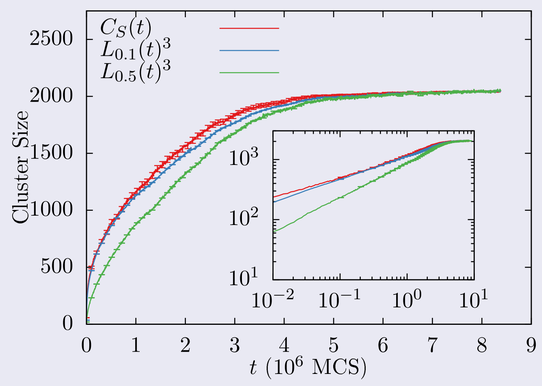
- equal-time two point correlation function

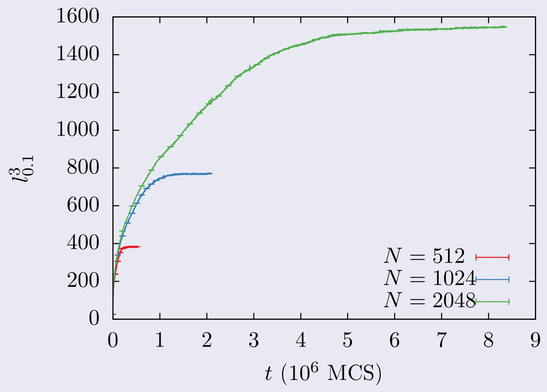
$$C(t, R) = \langle \rho_i(t, R) \rangle$$

$$\rho_i(t, R) = \frac{1}{m_R}\sum \kappa(t, r_i + R)$$

- κ is unity if there is a monomer at a position and zero otherwise
- m_R number of possible lattice points at distance R







- power law cluster growth

$$C_S(t) \propto t^{\alpha}$$

- $C(t, R) \rightarrow$ characteristic length ℓ_a of ordered structures:

$$C_S(t) \propto \ell_a(t)^3$$

- $\Rightarrow \alpha = 0.38$ is considerably smaller than in the off-lattice model ($\alpha = 1$)

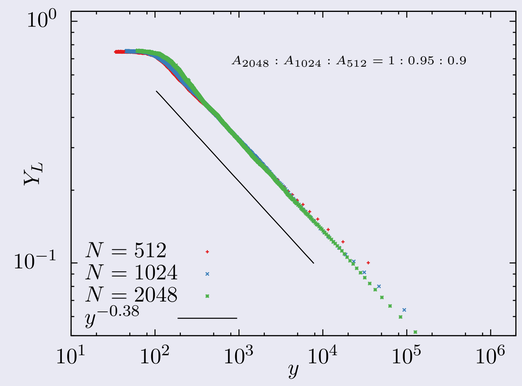
3. Finite-Size Scaling of the Cluster Growth

- finite size scaling function:

$$\ell^3_{0.1}(t) = N Y_L(y)$$

$$y = (N/\ell^3_{0.1})^{1/\alpha} = N^{1/\alpha}/A_N^{1/\alpha} t$$

- data collapse with power law decay; exponent $-\alpha$



4. Aging

- probed by two-time correlation function

$$C(t, t_w) = \langle O_i(t) O_i(t_w) \rangle - \langle O_i(t) \rangle \langle O_i(t_w) \rangle$$

with order parameter:

$$O_i = \begin{cases} 1 & \text{if monomer } i \in \text{cluster} \\ 0 & \text{if monomer } i \notin \text{cluster} \end{cases}$$

- scaling with respect to $t/t_w \rightarrow$ scaling with respect to cluster size?

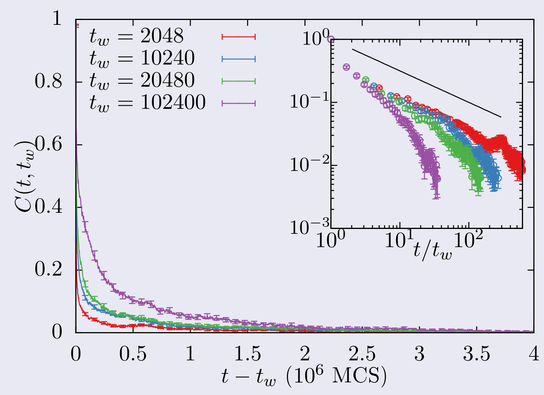
$$C(t, t_w) \propto \frac{\ell^3_{0.1}(t)}{\ell^3_{0.1}(t_w)}^{-\lambda_c}$$

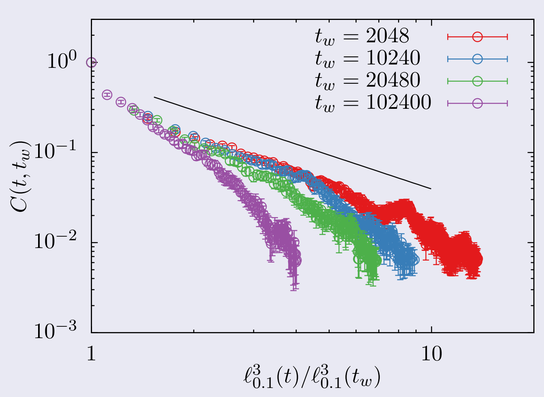
with the dynamic aging exponent λ_c

- bound of expected values for λ_c

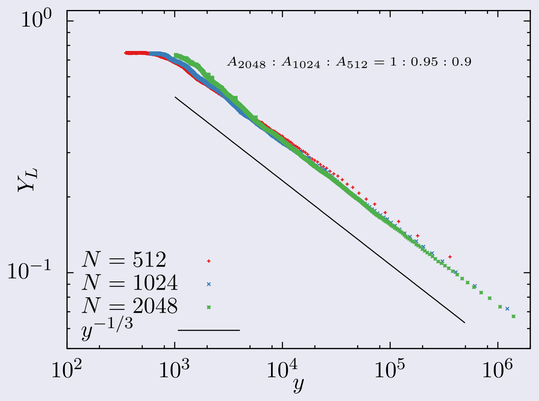
$$0.762791 \leq \lambda_c \leq 1.525582$$

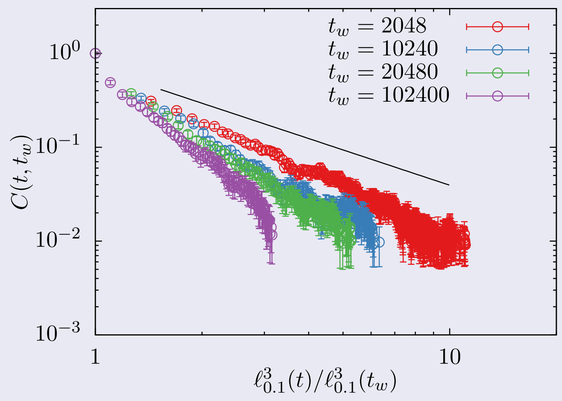
- in agreement with the off-lattice model, $\lambda_c = 1.25$ was found





5. Next-Nearest Neighbor Model





- exponent $\alpha = 1/3$ similar to the NN model
- dynamic aging exponent $\lambda_c = 1.25$

References

- S. Majumder and W. Janke, EPL (Europhysics Letters) **110**, 58001 (2015).
- S. Majumder and W. Janke, Physical Review E **93**, 032506 (2016).

Acknowledgments

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Conclusion

We found a power-law growth of ordered structures (or clusters) during the collapse of lattice polymers. The found exponent $\alpha (= 0.38$ in the NN model and $= 1/3$ in the NNN model) was considerably smaller than the growth exponent previously reported ($\alpha = 1$) for off-lattice models. In addition we investigated aging and found the same dynamic aging exponent as in the off-lattice model for both interaction ranges ($\lambda_c = 1.25$).

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