John von Neumann - Institut für Computing

Polymers Confined between Two Parallel Plane Walls

Hsiao-Ping Hsu and Peter Grassberger

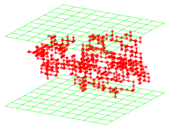
John-von-Neumann Institute for Computing, Forschungszentrum Jülich, Germany

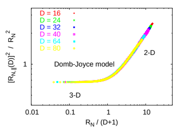
Model

Single $3d$ polymers confined to the region between two parallel walls are described by N-step walks on a simple cubic lattice confined to the region $1 \leq z \leq D$.

- Partition sum of Domb-Joyce model (DJ) ($N+1$ monomers):
  $$Z_N(w) = \sum_{\text{configs.}} w^k$$
  where $k = \sum_{i<j} \delta_{x_i,x_j}$ is the total number of pairs occupying the same site, and w is the Boltzmann factor.
- $w = 1 \rightarrow$ ordinary random walks (RW).
  $w = 0 \rightarrow$ self-avoiding random walks (SAW).
- DJ and SAW are in the same universality class as $N \rightarrow \infty$.
- There is a "magic" value $w^* \cong 0.6$, where corrections to scaling are minimal.

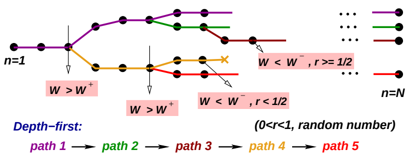
Hsu and Grassberger, J. Chem. Phys. 120, 2034 (2004).





Algorithm

Pruned-enriched Rosenbluth Method (PERM) with k-step Markovian anticipation



Grassberger, Phy. Rev. E 56, 3682 (1997)
Hsu et. al., Eur. Phys. J. B 36, 209 (2003)
Frauenkron et. al., cond-mat/9806321;
Pre. Rev. E 59, R16 (1999).
Caracciolo et al., J. Phys. A 32, 2931 (1999)

Scaling Predictions

I. Scaling law of fugacity μ:

$$(\mu_D - \mu_\infty) \sim aD^{-1/\nu_3} \text{ (large } D)$$

$\nu_3 = 1/2, \mu_\infty = 1/6$ (RW)
$\nu_3 = 0.58765(20), \mu_\infty = 0.2134910(3)$ (SAW)
$\nu_3 = 0.58765(20), \mu_\infty = 0.18812145(7)$ (DJ)

II. Monomer density $\rho(z)$: $\rho(z) \sim z^{1/\nu}$

- Relationship between density $\rho(z)$ (normalized to $\sum_y \rho(z) = 1$) and force $f = \frac{k_BT}{N}\frac{\partial \ln Z_N}{\partial D}$ (per monomer)
  $$\lim_{z\to 0} k\frac{\rho(z)}{z^{1/\nu_3}} = B\frac{f}{k_BT} = B\frac{a}{\nu_3\mu_\infty}D^{-1-1/\nu_3}.$$
  Here $k \approx (R_{\text{end-to-end}}/\sqrt{d})^{1/\nu_3}/N$ and B is a universal amplitude ratio.

  $B = 2$ (ideal chains)
  $B \approx 2(1 - b_1\epsilon) \approx 1.85$ $(d = 3)$ with $b_1 = 0.075$
  (chains with excluded volume, $d = 4 - \epsilon$)

Eisenriegler, Phys. Rev. E 55, 3116 (1996)

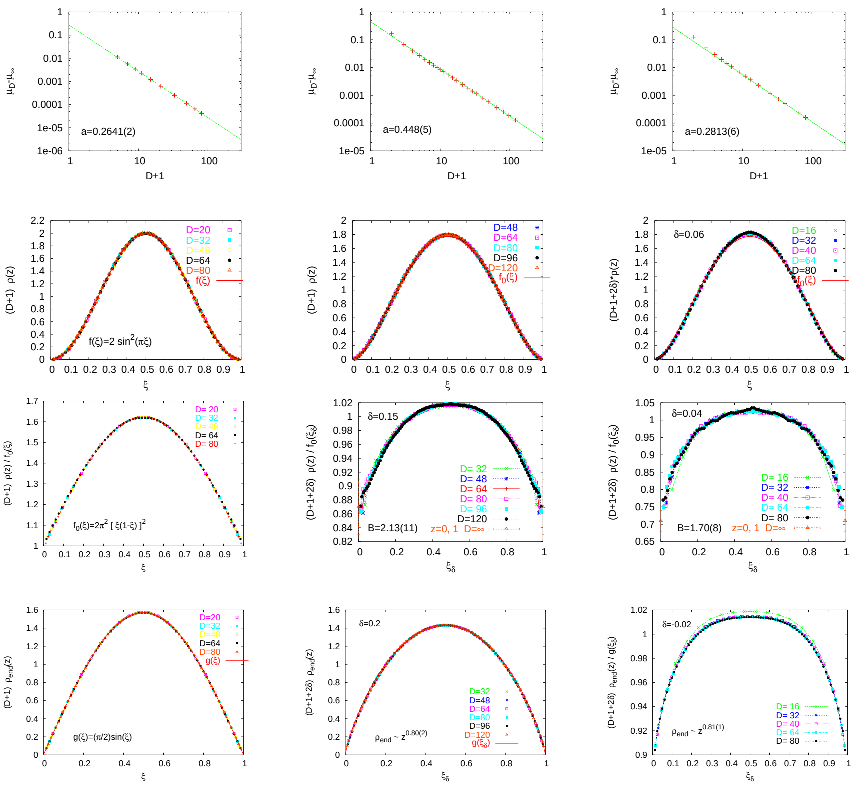
- Ansatz: $\rho(z) \approx \frac{1}{(D+1)} f_0(\frac{z}{D+1})$ (SAW)
  with $f_0(\xi) = A[\xi(1-\xi)]^{1/\nu_3}$
- Modification: $\xi \rightarrow \xi_\delta$, $\xi_\delta = \frac{z+\delta}{D+1+2\delta}$
  δ: extrapolation length

III. End point density $\rho_{\text{end}}(z)$:

- Partition sum of a SAW, one end of which is glued to an impenetrable wall,
  $$Z_N^{(1)} \sim \mu_\infty^{-N} N^{\gamma_d^{(1)}-1}$$
  with $\gamma_3^{(1)} = 0.679(2)$
- $\rho_{\text{end}} \approx z^{(\gamma-\gamma_3^{(1)})/\nu_3} \approx z^{0.814(6)}$

Eisenriegler et. al., J. Chem. Phys. 77, 6296 (1982)

Results



Random Walks | Self-Avoiding Walks | Domb-Joyce Model