# Confined Polymers in a Strip

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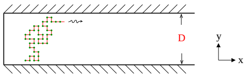
## Model

Single polymers confined inside a strip in 2D

= Self-avoiding random walks (SAW) on a square lattice between two parallel hard walls with width $D$




## Algorithm: PERM

- PERM = Pruned-enriched Rosenbluth method *(P. Grassberger, Phys. Rev. E56, (1997) 3682.)*
- Chain growth algorithm: polymer chains are built like random walks by adding one monomer at each step
- Depth-first implementation
- Rosenbluth like bias for self-avoidance with $k$-step Markovian anticipation $\Rightarrow$weighted sample
- Partition sum estimate: $\hat{Z}_n = M_n^{-1} \sum_{\alpha=1}^{M_n} W_n(\alpha)$

  $W_n = \prod_{n' \leq n} w_{i_{n'}}$ is the total weight of a chain of length $n$ and $w_i = 1/p_i$ is the weight factor
- Population control: compare the current weight $W_n$ with the thresholds $W_n^+$ and $W_n^-$
  IF $W_n > W_n^+$ clone !
  IF $W_n < W_n^-$ prune ! (with 50% probability)

## $k$-step Markovian anticipation

- An additional bias based on the statistics of sequences of $k+1$ successsive steps.
- A sequence of $k+1$ steps:
  $\mathbf{S} = (s_{-k}, \ldots s_0) = (\mathbf{s}, s_0),\ s = 0, \ldots 2d-1$
  ($d$-dimensional hypercubic lattice)
- Ideal bias in $k$-step Markovian anticipation

$$p(s_0 \mid \mathbf{s}) = P_{N,m}(\mathbf{s}, s_0) / \sum_{s_0'=0}^{2d-1} P_{N,m}(\mathbf{s}, s_0')$$

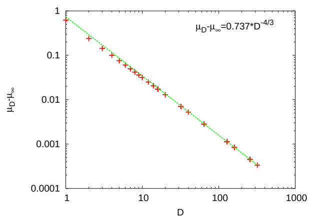
  with $N >> m >> 1$ and $P_{N,m}(\mathbf{s}, s_0')$ is the statistical weight of all $N$-step chains in an unbiased sample that had followed the sequence $\mathbf{S}$ during steps $N-m-k, \ldots, N-m$

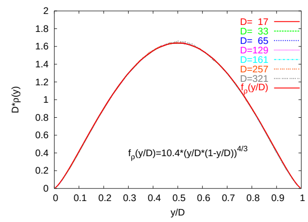
## Results

- Finite $D$: $Z_N \approx (\mu_D)^{-N}$
- Scaling law of fugacity $\mu$: $(\mu_D - \mu_\infty) \sim aD^{-1/\nu}$, $\mu_\infty \approx 0.37905228$ and $a \approx 0.737$
- Relationship between density $\rho(y)$ (normalized to $\sum_y \rho(y) = 1$) and force $f = \frac{k_B T}{N} \frac{\partial \ln Z_N}{\partial D}$ (per monomer)

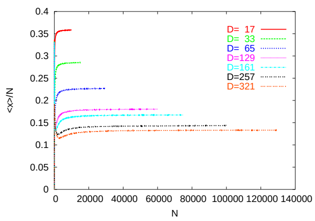
$$lim_{y\to 0}\, k\rho(y)/y^{1/\nu} = Bf/k_B T = \frac{4}{3} B \frac{a}{\mu_\infty} D^{-1-1/\nu}.$$

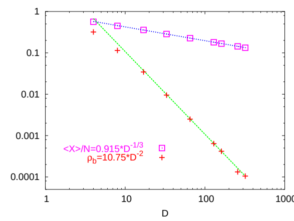
  Here $k = R_x^{1/\nu}/N \approx 0.5299$ (SAW on square lattice) and $B$ is a universal number, $B = 2$ (ideal chains) and $B \approx 2(1 - b_1\epsilon)$ (chains with excluded volume, $\epsilon = 4 - d$, $b_1 = 0.075$)
  *(E. Eisenriegler, Phys. Rev. E 55, (1996) 3116)*
- Simulations: $B \approx 2.12(1)$

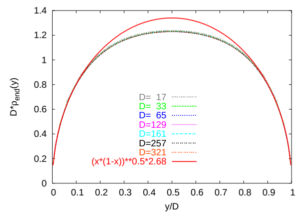



- As $N \to \infty$, curve of $< x > /N$ becomes horizontal
- Scaling law of $< x > /N$: $< x > /N \sim D^{-1/3}$
- Scaling law of # of wall contacts / unit length: $\rho_b \sim D^{-2}$




- Probability density that chain end is at the distance $y$ from wall:

$$D\rho_{end} \propto \sqrt{y/D(1-y/D)}$$

  near the wall