Interacting partially directed self-avoiding walk (polymer collapse)

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1 A directed model: the IPDSAW
Introduced by Zwanzig and Lauritzen (1968)

1.1) Trajectories.

For a polymer of length $L \in \mathbb{N}$ the set of allowed configurations is

$$\Omega_L = \{ L \text{ - step directed self-avoiding paths starting at the origin and taking steps in } \{\uparrow, \to, \downarrow\} \}.$$
1.2) Self-interactions.

An energetic reward $\beta \in (0, \infty)$ is associated with each self touching made by the polymer.

Self-touching: two non-consecutive sites along the path at distance 1 from each other.
1.3) Hamiltonian.

With each \( \pi \in \Omega_L \) we associate an energy given by the Hamiltonian

\[
H_{L,\beta}(\pi) := \beta \sum_{i,j=0 \atop i<j}^{L} 1\{|\pi_i - \pi_j| = 1\}
\]

\( \beta \in (0, \infty) \) : intensité de l’attraction (self-touching).

1.4) Polymer measure.

For every \( \pi \in \Omega_L \); 

\[
P_{L,\beta}(\pi) = \frac{e^{H_{L,\beta}(\pi)}}{Z_{L,\beta}}
\]

with the partition function

\[
Z_{L,\beta} = \sum_{\pi \in \Omega_L} e^{H_{L,\beta}(\pi)}
\]
1.5) Phase transition.

Free energy: for $\beta \in (0, \infty)$, set $f(\beta) := \lim_{L \to \infty} \frac{1}{L} \log Z_{L,\beta}$.

For all $\beta \in (0, \infty)$, $f(\beta) \geq \beta$ because (for $L \in \mathbb{N}^2$)

$$H_{L,\beta}(\tilde{\pi}) = \beta(\sqrt{L} - 1)^2$$
\[ \beta_c := \inf\{\beta \geq 0 : f(\beta) = \beta\} \]

Partition \([0, \infty)\) into a collapsed (\(C\)) and an extended (\(E\)) phase

\[ C := \{\beta : f(\beta) = \beta\} = \{\beta : \beta \geq \beta_c\} \]

and

\[ E := \{\beta : f(\beta) > \beta\} = \{\beta : \beta < \beta_c\}. \]
1.6) What do we want to show?

- **Assymptotics of the free energy close to $\beta_c$**:
  - spot $\beta_c$
  - and find $\gamma > 0$ and $\alpha > 0$ s.t.
    \[
    \tilde{f}(\beta_c - \epsilon) - \tilde{f}(\beta_c) = \gamma \epsilon^\alpha
    \]

- **Path results**:
  - in each regimes (i.e., extended, critical and collapsed), describe the geometric conformation adopted by the path $\pi$ under $P_{L,\beta}$, when $L$ is large but finite. Give the infinite volume limit.

- **Simulate long polymers**:
  - sample path $\pi$ under $P_{L,\beta}$ with large $L$. 
Physical motivation
1.1) homopolymer. A long chain of monomers of the same type (ex: polystyrene).

1.2) Medium. A pure phase of a particular solvent (ex: cyclohexane).

1.3) Interactions.
Weak chemical affinity between the monomers and the solvent: repulsion.
Collapse transition:

Random coil $\leftrightarrow$ Compact ball
Background and new approach
3.1) Combinatoric techniques.

\[ G(\beta, z) = \sum_{L=1}^{\infty} Z_{L,\beta} z^L \]

Use some smart concatenations of path to provide an explicit formula for \( G(\beta, z) \). Study \( G(\beta, z) \) and obtain:

- results on the free energy
- weak results on the path
- no results on the disordered version of the model
3.2) New probabilistic approach.

Let $P_\beta$ be the law of the random walk $V$ with geometric increment, i.e., $V_0 = 0$ and $(V_{i+1} - V_i)_{i \in \mathbb{N}}$ is i.i.d. and

$$
P_\beta(V_1 = k) = \frac{e^{-\frac{\beta}{2}|k|}}{c_\beta}, \quad k \in \mathbb{N}.
$$

We get

$$
Z_{L,\beta} = e^{\beta L} \sum_{N=1}^{L} (\Gamma_\beta)^N P_\beta(V_{N+1,L-N}).
$$

with $\Gamma_\beta = \frac{c_\beta}{e^\beta}$, and also for $N \in \{1, \ldots, L\}$:

$$
P_{L,\beta}(\pi \in \cdot \mid N\pi = N) = P_\beta(T_N(V) \in \cdot \mid V \in \mathcal{V}_{N+1,L-N}).
$$
4 Phase transition asymptotics
Theorem (Phase transition asymptotics)

The phase transition occurs at $\beta_c$ the unique solution of $e^{\beta} = c_\beta$. It is second order with critical exponent $3/2$, i.e.,

$$\lim_{\epsilon \to 0^+} \frac{\tilde{f}(\beta_c - \epsilon)}{\epsilon^{3/2}} = \left( \frac{b}{d} \right)^{3/2}$$

where

- $b = 1 + \frac{e^{-\beta_c/2}}{1 - e^{-\beta_c}}$
- $d = -\lim_{T \to \infty} \frac{1}{T} \log \mathbb{E}(e^{-\sigma_{\beta_c} \int_0^T |B(t)|dt}) = 2^{-1/3} |a'_1| \sigma_{\beta_c}^{2/3}$
- $\sigma_{\beta}^2 = \mathbb{E}_\beta(V_1^2)$
- $a'_1 :$ smallest zero (in modulus) of the first derivative of the Airy function.
Geometry of the path
5.1) Three features of interest

- The horizontal expansion $N_\pi$ of $\pi \in \Omega_L$
The decomposition into beads
Upper envelope: $\mathcal{E}_\pi^+ = (\mathcal{E}_{\pi,i}^+)^{N_\pi}_{i=0}$

Lower envelope: $\mathcal{E}_\pi^-$

Center of mass walk: $M_\pi$

Profile: $T_\pi$
5.2) Horizontal expansion

$N_{\pi}$ : number of horizontal step of $\pi$ (sampled from $P_{L,\beta}$).

Theorem

(1) *Extended:* there exists $e_\beta \in (0, 1)$ so that

$$\lim_{L \to \infty} P_{L,\beta} \left( \left| \frac{N_{\pi}}{L} - e_\beta \right| \geq \epsilon \right) = 0.$$

(2) *Critical:*

$$\lim_{L \to \infty} \frac{N_{\pi}}{L^{2/3}} = \text{law} \sum_{i=1}^{\infty} Y_i U_i^{2/3}$$

(3) *Collapsed:* there exists $a_\beta \in (0, \infty)$ so that

$$\lim_{L \to \infty} P_{L,\beta} \left( \left| \frac{N_{\pi}}{\sqrt{L}} - a_\beta \right| \geq \epsilon \right) = 0.$$
5.3) Vertical expansion

For $\pi \in \Omega_L$ let $\mathcal{E}_\pi^+ = (\mathcal{E}_{\pi,i}^+)_i^{N_\pi}$ and $\mathcal{E}_\pi^- = (\mathcal{E}_{\pi,i}^-)_i^{N_\pi}$ be the upper and lower envelops of the path $\pi$.

Let $\tilde{\mathcal{E}}_\pi^+$ and $\tilde{\mathcal{E}}_\pi^-$ : $[0, 1] \rightarrow \mathbb{R}$ be the time-space rescaled cadlag process defined as

$$\tilde{\mathcal{E}}_\pi^a(t) = \frac{1}{N_\pi + 1} \mathcal{E}_\pi^a, [t(N_\pi+1)], \quad a \in \{\pm\}, \; t \in [0, 1].$$
5.3.1) Extended phase

When $\beta < \beta_c$ and under $P_{L,\beta}$, we let also $(B_s)_{s\in[0,1]}$ be a standard Brownian motion.

**Theorem**

*For $\beta < \beta_c$, and with $\pi$ sampled from $P_{L,\beta}$, there exists a $\sigma_\beta > 0$ such that*

$$\lim_{L \to \infty} \sqrt{N_\pi}(\tilde{E}_\pi^+, \tilde{E}_\pi^-) = \text{Law } \sigma_\beta (B_s, B_s)_{s\in[0,1]},$$

*and $\sigma_\beta$ is explicit.*
5.3.2) Path results: inside the collapsed phase ($\beta > \beta_c$)

Divide the path into beads:

Let $I_{\text{max}}(\pi)$ be the number of steps made by the path $\pi \in \mathcal{W}_L$ inside its largest bead.

**Theorem (One bead Theorem)**

For $\beta > \beta_c$ there exists $c > 0$ such that

$$\lim_{L \to \infty} P_{L,\beta}(I_{\text{max}}(\pi) \geq L - c (\log L)^4) = 1.$$
Theorem (Convergence to Wulff shapes)

For \( \beta > \beta_c \) and \( \epsilon > 0 \),

\[
\lim_{L \to \infty} P_{L,\beta} \left( \| \tilde{E}^+ - \frac{\gamma^*_\beta}{2} \|_\infty > \epsilon \right) = 0,
\]

\[
\lim_{L \to \infty} P_{L,\beta} \left( \| \tilde{E}^- + \frac{\gamma^*_\beta}{2} \|_\infty > \epsilon \right) = 0.
\]

where \( \gamma^*_\beta \) is the Wulff shape given by

\[
\gamma^*_\beta(s) = \int_0^s L' \left[ \left( \frac{1}{2} - x \right) \tilde{h}_\beta \right] dx, \quad s \in [0, 1]
\]

and

- \( L(x) = \log \mathbf{E}_\beta[\exp(xV_1)] \) for \( x \in (-\frac{\beta}{2}, \frac{\beta}{2}) \)

- \( \tilde{h}_\beta \) is the unique sol. of \( h \int_0^1 L'(h(x - \frac{1}{2}))dx = \frac{1}{2a^2_\beta} \).
Theorem (Fluctuation around Wulff Shape)

For $\beta > \beta_c$ and $\pi$ sampled from $\tilde{P}_{L,\beta}$,

$$\lim_{L \to \infty} \sqrt{N_\pi} \left( \tilde{E}_\pi^+ - \frac{\gamma_\beta^*}{2}, \tilde{E}_\pi^- + \frac{\gamma_\beta^*}{2} \right) = \text{Law} \left( \xi_\beta - \xi_c^\beta, \xi_\beta + \xi_c^\beta \right),$$

with

- $W$ a standard BM,
- $\xi_\beta$ defined as

$$\xi_\beta(t) := \int_0^t \sqrt{L''((\frac{1}{2} - x)\tilde{h}_\beta)} \, dW_x, \quad t \in [0, 1]$$

- $\xi_c^\beta$ independent of $\xi_\beta$ with the same law but conditioned on $\xi_c^\beta(1) = \int_0^1 \xi_c^\beta(s) \, ds = 0$.
The last result is not obtained under $P_{L,\beta}$ but under $\tilde{P}_{L,\beta}$ that is

$$\tilde{P}_{L,\beta}(\pi) = \sum_{L' \in K_L} \frac{\tilde{Z}_{L',\beta}}{\sum_{k \in K_L} \tilde{Z}_{k,\beta}} P_{L',\beta}(\pi) 1\{\pi \in \tilde{\Omega}_{L'}\}, \quad \text{for } \pi \in \tilde{\Omega}_L.$$ 

with

- $K_L = \{-(\log L)^5, \ldots, (\log L)^5\}$
- $\Omega'_L = \bigcup_{L' \in K_L} \Omega'_{L'}$
6 Exact simulation
random walk representation
7.1) New probabilistic approach.

Let \((V_i)_{i \in \mathbb{N}}\) be an auxiliary random walk on \(\mathbb{Z}\) with geometric increments, i.e., \(V_0 = 0\), \((V_{i+1} - V_i)_{i \in \mathbb{N}}\) is i.i.d. and

\[
P_\beta(V_1 = k) = \frac{e^{-\frac{\beta}{2}|k|}}{c_\beta}, \quad k \in \mathbb{N}.
\]

Build \(T_N\) a bijection between \(\mathcal{L}_{N,L}\) and

\[
\mathcal{V}_{N+1,L-N} = \{ V \in \{0\} \times \mathbb{Z}^N : G_N(V) = L - N, \ V_{N+1} = 0 \}
\]

with \(G_N(V) = \sum_{i=1}^{N} |V_i|\) so that \(T_N\) transforms the self-touching interaction on \(\pi \in \mathcal{L}_{N,L}\) into a probability law on \(V\).
Let $P_\beta$ be the law of the random walk $V$ with geometric increment, i.e., $V_0 = 0$ and $(V_{i+1} - V_i)_{i \in \mathbb{N}}$ is i.i.d. and

$$P_\beta(V_1 = k) = \frac{e^{-\frac{\beta}{2}|k|}}{c_\beta}, \quad k \in \mathbb{N}.$$ 

We obtain (with $\Gamma_\beta = \frac{c_\beta}{e^\beta}$),

$$Z_{L,\beta} = e^{\beta L} \sum_{N=1}^{L} (\Gamma_\beta)^N P_\beta(V_{N+1,L-N}).$$

and

$$P_{L,\beta}(l \in \cdot \mid N_L(l) = N) = P_\beta(T_N(V) \in \cdot \mid V_N = 0, = L - N).$$
7.2) Analysis of the phase transition.

Theorem (Variational characterizations of $\tilde{f}$)

The excess free energy $\tilde{f}(\beta)$ is given by

$$\tilde{f}(\beta) = \sup_{\alpha \in [0,1]} \left[ \alpha \log \Gamma(\beta) + \alpha g_\beta \left( \frac{1-\alpha}{\alpha} \right) \right],$$

where

$$g_\beta(\alpha) := \lim_{N \to \infty} \frac{1}{N} \log P_\beta(G_N \leq \alpha N, V_N = 0), \quad \alpha \in [0, \infty).$$

A straightforward consequence is that $\beta_c$ is the unique positive solution of $\Gamma_{\beta} = 1$. 