# Interacting partially directed self-avoiding walk (polymer collapse)

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1. A directed model : the IPDSAW
2. Geometric description of the path in each regime
3. Open problems
4. A non-directed model : the IPRSAW

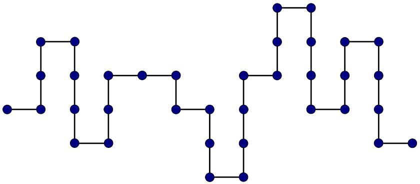
1 A directed model : the IPDSAW

Introduced by Zwanzig and Lauritzen (1968)

## 1.1) Trajectories.

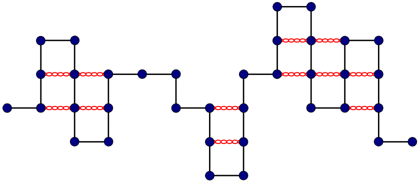
For a polymer of length $L \in \mathbb{N}$ the set of allowed configurations is

$$\Omega_L = \Big\{ L - \text{step directed self-avoiding paths starting at the origin and taking steps in } \{\uparrow, \rightarrow, \downarrow\} \Big\}.$$



## 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

$$H_{L,\beta}(\pi) := \beta \sum_{\substack{i,j=0 \\ i<j-1}}^{L} \mathbf{1}_{\{\|\pi_i - \pi_j\|=1\}}$$

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

## 1.4) Polymer measure.

For every $\pi \in \Omega_L$ ;

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

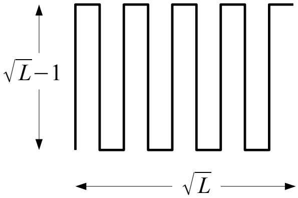
with the partition function

$$Z_{L,\beta} = \sum_{\pi \in \Omega_L} e^{H_{L,\beta}(\pi)}$$

## 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 $L \in \mathbb{N}^2$)

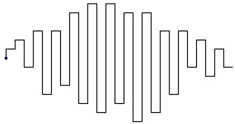



$$H_{L,\beta}(\tilde{\pi}) = \beta(\sqrt{L} - 1)^2$$

$$\beta_c := \inf\{\beta \geq 0 : f(\beta) = \beta\}$$

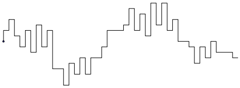
Partition $[0, \infty)$ into a collapsed $(\mathcal{C})$ and an extended $(\mathcal{E})$ phase

$$\mathcal{C} := \{\beta : f(\beta) = \beta\} = \{\beta : \beta \geq \beta_c\}$$



and

$$\mathcal{E} := \{\beta : f(\beta) > \beta\} = \{\beta : \beta < \beta_c\}.$$



## 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.

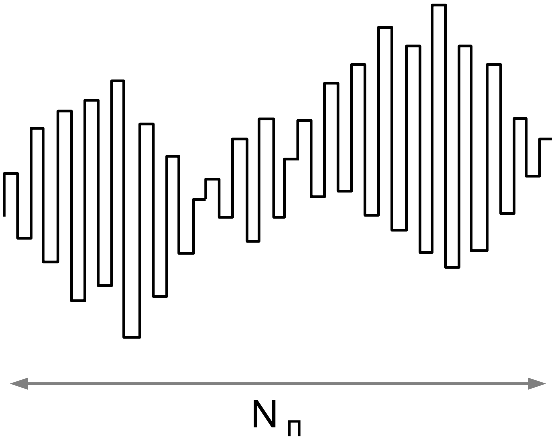
$$\tilde{f}(\beta_c - \epsilon) - \tilde{f}(\beta_c) = \gamma \epsilon^{\alpha}$$

- **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 $L$.

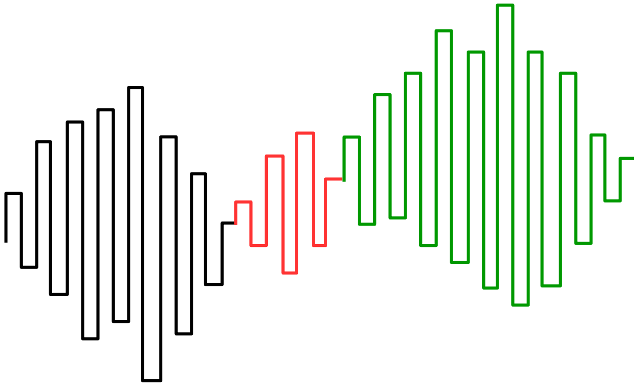
2. Geometric description of the path in each regime

## 2.1) Three features of interest

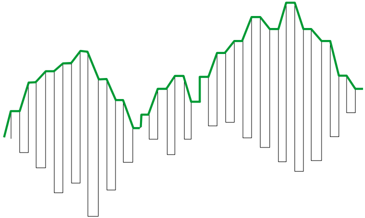
- The horizontal expansion $N_\pi$ of $\pi \in \Omega_L$



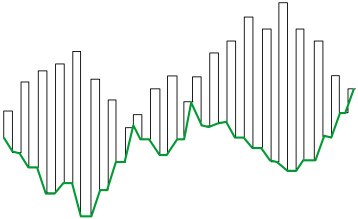
- The decomposition into beads

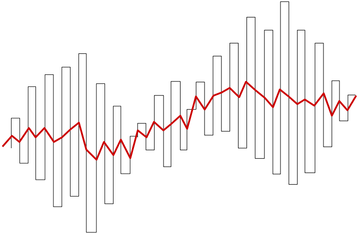


Upper envelope : $\mathcal{E}_\pi^+ = (\mathcal{E}_{\pi,i}^+)_{i=0}^{N_\pi}$

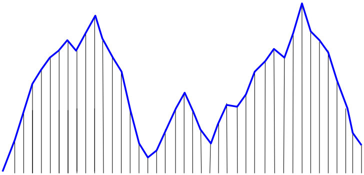


Lower envelope : $\mathcal{E}_\pi^-$





Center of mass walk : $\mathcal{M}_\pi$



Profile : $\mathcal{T}_\pi$

## 3.2) Horizontal expansion

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

**Theorem (PC GN NP (2013-2016))**

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

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

(2) *Critical :*

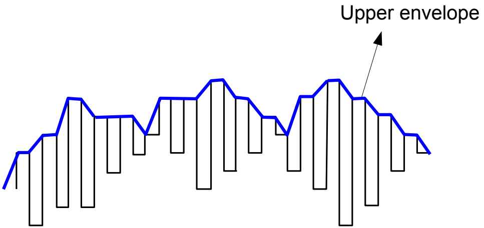
$$\lim_{L\to\infty} \frac{N_\pi}{L^{2/3}} =_{law} \inf\{s \geq 0 \colon\ \textstyle\int_0^s |B_s| ds = 1\}.$$

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

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

## 3.3) Vertical expansion

For $\pi \in \Omega_L$ let $\mathcal{E}_\pi^+ = (\mathcal{E}_{\pi,i}^+)_{i=0}^{N_\pi}$ and $\mathcal{E}_\pi^- = (\mathcal{E}_{\pi,i}^-)_{i=0}^{N_\pi}$ be the upper and lower envelops of the path $\pi$.




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

$$\tilde{\mathcal{E}}_\pi^a(t) = \mathcal{E}^a_{\pi,\lfloor t\,(N_\pi+1)\rfloor}, \quad a \in \{\pm\},\ t \in [0,1].$$

### 3.3.1) Inside the extended phase $(\beta < \beta_c)$

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

**Theorem (PC NP (2016))**

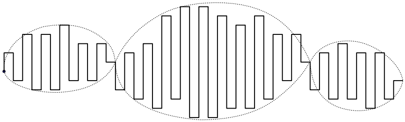
*For $\beta < \beta_c$, and with $\pi$ sampled from $P_{L,\beta}$, there exists a $\sigma_\beta > 0$ such that*

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

*and $\sigma_\beta$ is explicit.*

## 3.3.2) Inside the collapsed phase ($\beta > \beta_c$)

Divide the path into beads :



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

**Theorem (One bead Theorem, PC GN NP (2015))**

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

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

**Theorem (Convergence to Wulff shapes, PC NP GB (2015))**

*For $\beta > \beta_c$ and $\epsilon > 0$,*

$$\lim_{L\to\infty} P_{L,\beta}\left(\left\|\frac{\widetilde{\mathcal{E}}_\pi^+}{N_\pi} - \frac{\gamma_\beta^*}{2}\right\|_\infty > \epsilon\right) = 0,$$

$$\lim_{L\to\infty} P_{L,\beta}\left(\left\|\frac{\widetilde{\mathcal{E}}_\pi^-}{N_\pi} + \frac{\gamma_\beta^*}{2}\right\|_\infty > \epsilon\right) = 0.$$

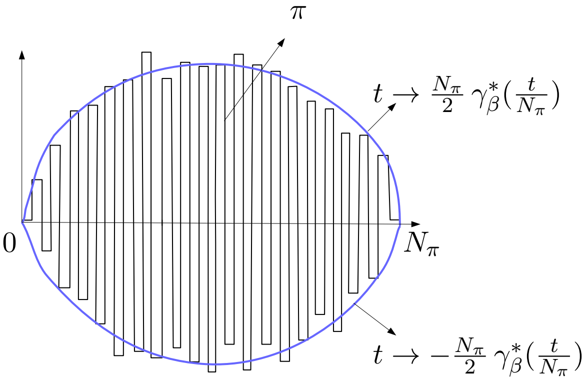
where $\gamma_\beta^*$ is the Wulff shape given by

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

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 $\quad h\int_0^1 L'(h(x-\frac{1}{2}))dx = \frac{1}{a_\beta^2}$.

Thus, for $\pi \in \mathcal{W}_L$ sampled from $P_{L,\beta}$, we observe



## Theorem (Fluctuation around Wulff Shape, PC NP (2016))

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

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

*with*

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

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

- $\xi_\beta^c$ *independent of* $\xi_\beta$ *with the same law but conditioned on* $\xi_\beta^c(1) = \int_0^1 \xi_\beta^c(s)ds = 0$

The last result is not obtained under $P_{L,\beta}$ but under $\widetilde{P}_{L,\beta}$ that is

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

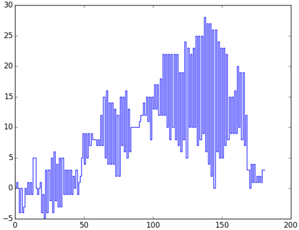
with

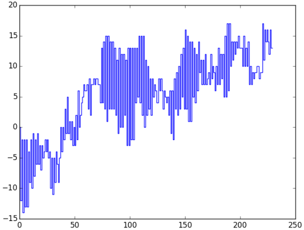
- $K_L = \{-(\log L)^5, \dots, (\log L)^5\}$
- $\Omega'_L = \cup_{L' \in K_L} \Omega'_L$

### 3.3.3) At criticality ($\beta = \beta_c$)

Let $\widehat{\mathcal{E}}^{+}_{L,\pi}$ and $\widehat{\mathcal{E}}^{-}_{L,\pi} : [0,\infty) \to \mathbb{R}$ be the time-space rescaled cadlag process defined as

$$\hat{\mathcal{E}}^{a}_{L,\pi}(s) = \frac{1}{L^{1/3}}\,\mathcal{E}^{a}_{\pi,\lfloor sL^{2/3}\rfloor \wedge N_\pi}, \quad a \in \{\pm\},\ s \in [0,\infty).$$



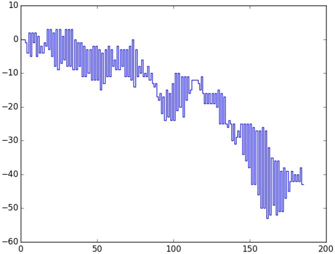
**Theorem (Convergence at criticality, PC NP (2016))**

*For* $\beta = \beta_c$ *and* $\pi$ *sampled from* $P_{L,\beta}$*,*

$$\lim_{L\to\infty} \left(\hat{\mathcal{E}}^{+}_{L,\pi}, \hat{\mathcal{E}}^{-}_{L,\pi}\right) =_{Law} \sigma_\beta \left[D_{s\wedge g(1)} + \frac{1}{2}\left(|B_{s\wedge g(1)}|, -|B_{s\wedge g(1)}|\right)\right]_{s\geq 0},$$

*with*

- $D$ *and* $B$ *two independent standard BM,*
- $g(1)$ *satisfies* $\int_0^{g(1)} |B_s| ds = 1$
- $B$ *is conditioned by* $B_{g(1)} = 0$.


10
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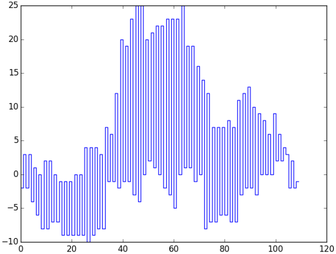
100
150
200


25
20
15
10
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20
40
60
80
100
120

3. Open problems

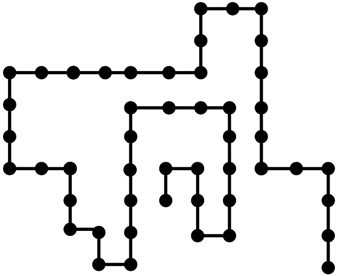
## Three directions for further investigations

- **Disordered IPDSAW :** introduce a random component in the intensity of the interactions ($\beta$ becomes $\beta + s\xi_{i,j}$).
- **Higher dimension :** Investigate a partially directed version of the model in dimension $d \geq 3$.
- **A non directed model :** in dimension 2, investigate a new model built with the prudent walk.

4. A non-directed model : the IPRSAW

## 4.1) Definition of the model

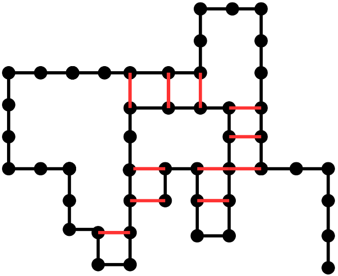
The prudent walk can not take a step in the direction of a site that has already been visited :



- **Detheridge and Guttman** (2008), **Bousquet-Melou** (2009), **Beaton and Iliev** (2015) (Combinatorics)
- **Beffara, Friedli and Velenik** (2009) (Scaling limit)

IPRSAW : the model is defined exactly like the IPDSAW except that the set of trajectories is enlarged to contain all $L$-steps prudent walks in 2 dimension, i.e.,

$$\Omega_L = \{L\text{-steps self-avoiding paths satisfying the prudent condition}\}$$



The free energy of IPRSAW is defined as

$$f^{\mathrm{pr}}(\beta) = \lim_{L\to\infty} \frac{1}{L} \log Z^{\mathrm{pr}}_{L,\beta}$$

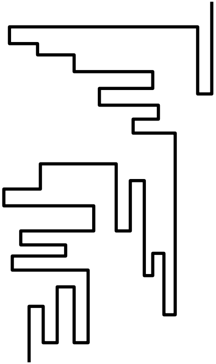
**Theorem (Collapse transition of IPRSAW, NP NT (2016))**

*There exists* $\beta_c^{pr} \in [\beta_c, \infty)$ *such that*

- $f^{pr}(\beta) > \beta \quad for \quad \beta \geq \beta_c^{pr}$
- $f^{pr}(\beta) = \beta \quad for \quad \beta < \beta_c^{pr}$

## 4.2) A 2-sided version of IPRSAW

A subclass of the prudent path of length $L$ is the 2-sided $L$ step prudent path, i.e.,



We can therefore define the 2-sided PRSAW, with a free energy

$$f^{\text{pr,2-sided}}(\beta) = \lim_{L\to\infty} \frac{1}{L} \log Z_{L,\beta}^{\text{pr,2-sided}}$$

**Theorem (2-sided IPRSAW NP NT (2016))**

*For every $\beta \geq 0$*

$$f^{pr}(\beta) = f^{pr,\textit{2-sided}}(\beta)$$

At $\beta = 0$, this answers a conjectures raised in **Detheridge and Guttman** (2008) or **Bousquet-Melou** (2009), i.e., the exponential growth rate of 2-sided prudent path equals that of general prudent path in dimension 2.