The model
The delocalized phase
A first order transition
At low temperature

Charged polymers with attractive charges: a first order transition

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Fields Institute, Toronto
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The model

Consider $q = (q_k)_{k \geqslant 0}$ an i.i.d. sequence in $\mathbb{R}$ and $S = (S_k)_{k \geqslant 0}$ the simple symmetric random walk in $\mathbb{Z}^d$, independent of q. We denote their joint law by P.

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The model

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The charge at $x \in \mathbb{Z}^d$ induced by the first N monomers is

$$Q_N^x = \sum_{0 \leqslant k < N} q_k \mathbf{1}_{\{S_k = x\}}$$

and we call

$$H_N = \sum_{x \in \mathbb{Z}^d} (Q_N^x)^2 = \sum_{0 \leqslant j,k < N} q_j q_k \mathbf{1}_{\{S_j = S_k\}}.$$

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We focus on the quenched polymer model with Hamiltonian $-H_N/N$:

$$
\begin{aligned}
H_N &= \sum_{x \in \mathbb{Z}^d} (Q_N^x)^2 = \sum_{0 \leqslant j,k < N} q_j q_k \mathbf{1}_{\{S_j = S_k\}} \\
Z_N(\beta) &= \mathrm{E}\left(\exp\left(\frac{\beta}{N} H_N \right) \middle| q_0, \ldots, q_{N-1} \right) \\
\mathrm{P}_N^\beta(A) &= \frac{1}{Z_N(\beta)} \mathrm{E}\left(\mathbf{1}_A \exp\left(\frac{\beta}{N} H_N \right) \middle| q_0, \ldots, q_{N-1} \right)
\end{aligned}
$$

In this model, charges with the same sign attract.

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Literature

$$H_N = \sum_{0 \leqslant j, k < N} q_j q_k \mathbf{1}_{\{S_j = S_k\}}$$

- Garel and Orland. Mean-field model for protein folding, EPL 1988.

  Quenched polymer with Hamiltonian $-H_N/N$ on the complete graph
  has a phase transition between a swollen phase at high temperature
  to a collapsed phase at low temperature.

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Literature

$$H_N = \sum_{0 \leqslant j, k < N} q_j q_k \mathbf{1}_{\{S_j = S_k\}}$$

- Garel and Orland. Mean-field model for protein folding, EPL 1988.
- Garel and Orland. Chemical sequence and spatial structure in simple models of biopolymers. EPL 1988.

  Extensions of the previous work with q_k a vector instead of a scalar, chain constraints. Similar phase transition.

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$$H_N = \sum_{0 \leqslant j,k < N} q_j q_k \mathbf{1}_{\{S_j = S_k\}}$$

- Garel and Orland. Mean-field model for protein folding, EPL 1988.

- Garel and Orland. Chemical sequence and spatial structure in simple models of biopolymers. EPL 1988.

- Brydges and Slade. The diffusive phase of a model of self-interacting walks. PTRF 1995.

  Non-random $q = 1$ and Hamiltonian $-H_N/N$ has a diffusive phase $-\infty < \beta < \beta_0$, where $\beta_0 > 0$.

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Literature

$$H_N = \sum_{0 \leqslant j,k < N} q_j q_k \mathbf{1}_{\{S_j = S_k\}}$$

- Garel and Orland. Mean-field model for protein folding, EPL 1988.
- Garel and Orland. Chemical sequence and spatial structure in simple models of biopolymers. EPL 1988.
- Brydges and Slade. The diffusive phase of a model of self-interacting walks. PTRF 1995.
- Bolthausen and Schmock. On self-interacting d-dimensional random walks. Ann. Prob. 1997.

  For a continuous polymer with non-random $q = 1$ and Hamiltonian corresponding to $-H_N/N$, the end-to-end distance of the polymer has bounded exponential moments for large β, uniformly in the length of the polymer.

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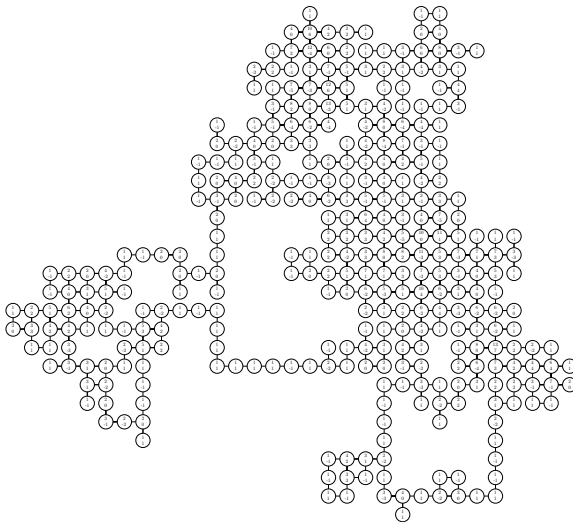A brief overview of the literature
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Polymer model with Hamiltonian H_N was considered in

- Kantor and Kardar. Polymers with random self-interactions. EPL 1991.

- Derrida, Griffiths, and Higgs. A model of directed walks with random self-interactions. EPL 1992.

- Derrida and Higgs. Low-temperature properties of directed walks with random self interactions. J. Phys. A 1994.

- Golding and Kantor. Two-dimensional polymers with random short-range interactions. Phys. Rev. E 1997.

- van der Hofstad and König. A survey of one-dimensional random polymers. J. Statist. Phys. 2001.
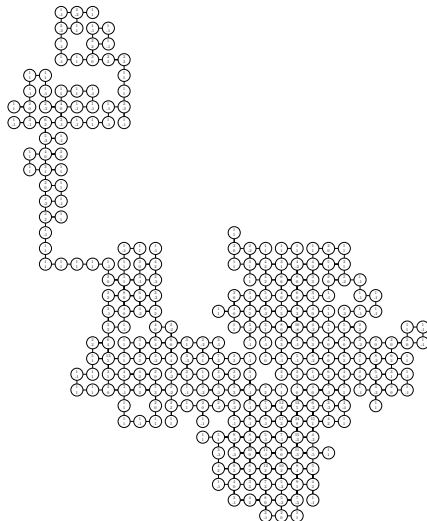
- den Hollander. Random polymers, LNM 2009.

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and H_N was studied in

- Chen. Limit laws for the energy of a charged polymer. Ann. IHP 2008.

- Chen and Khoshnevisan. From charged polymers to random walk in random scenary. IMS Lecture Notes 2009.

- Hu and Khoshnevisan. Strong approximations in a charged-polymer model. Periodica Mathematica Hungaria 2010.

- Asselah. Annealed lower tails for the energy of a polymer. JSP 2010.

- Asselah. Annealed upper tails for the energy of a polymer. Ann. IHP 2011.
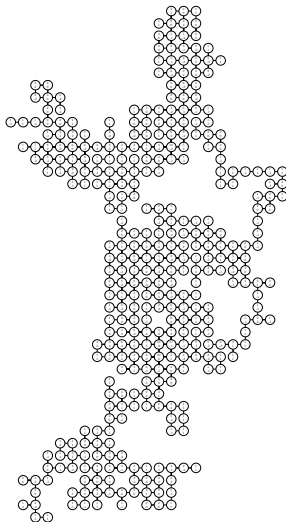
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A sample with $\beta = 3.50$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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A sample with $\beta = 4.00$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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A sample with $\beta = 4.10$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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A sample with $\beta = 4.20$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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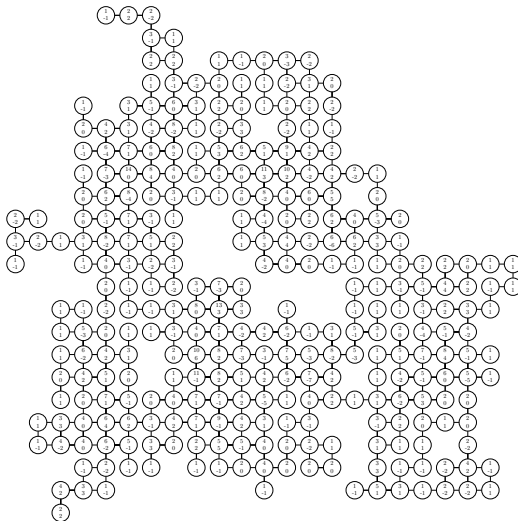
A sample with $\beta = 4.30$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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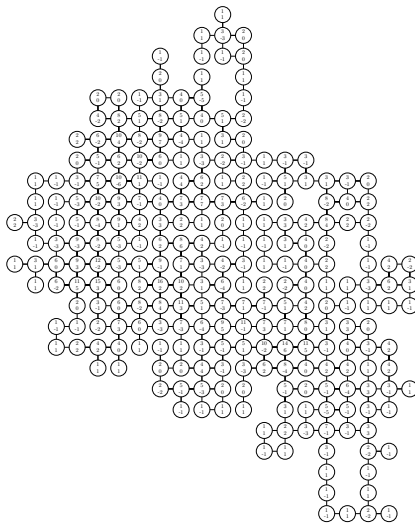
A sample with $\beta = 4.32$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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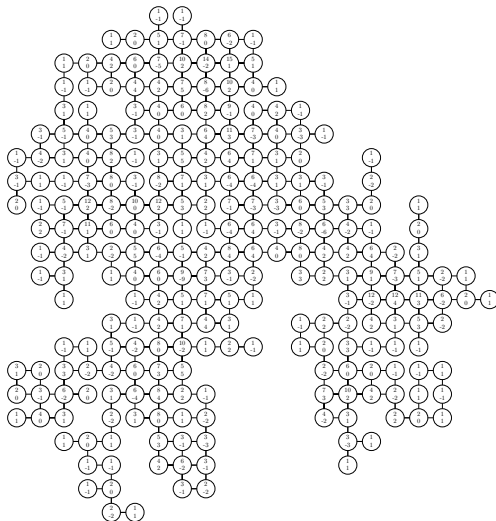
A sample with $\beta = 4.34$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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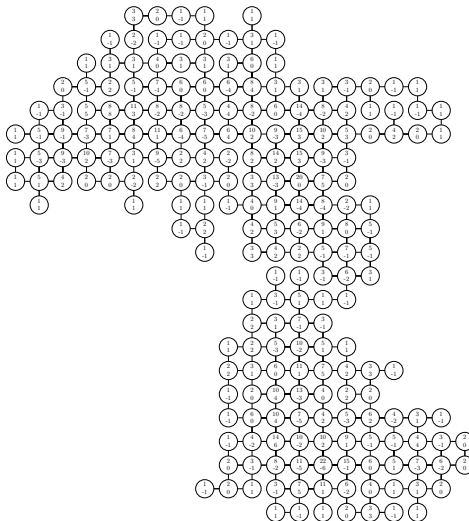
A sample with $\beta = 4.35$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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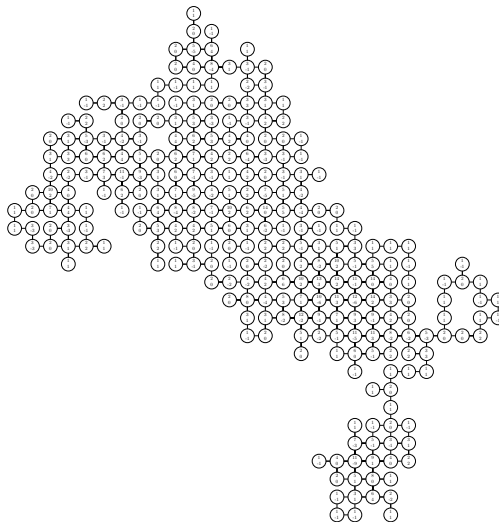
A sample with $\beta = 4.36$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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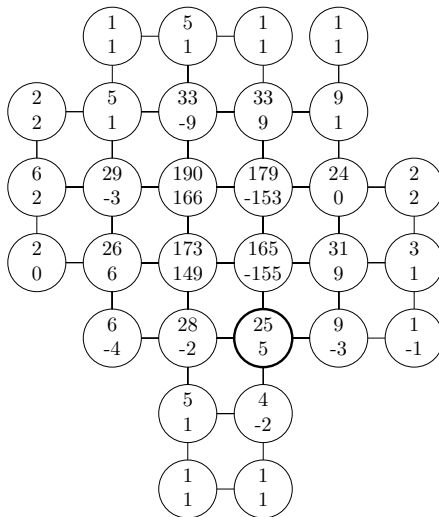
A sample with $\beta = 4.38$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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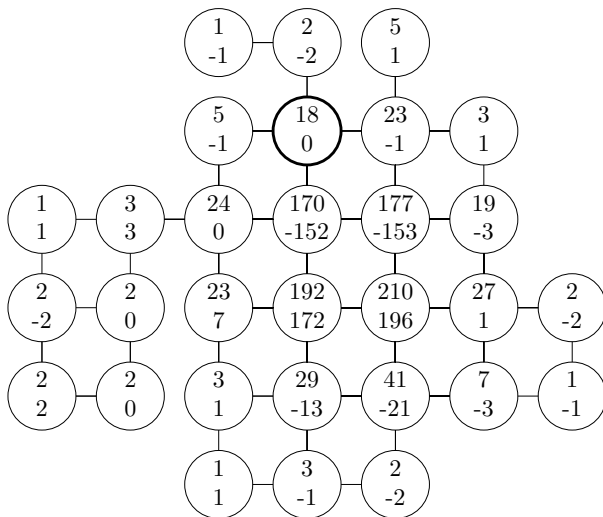
A sample with $\beta = 4.40$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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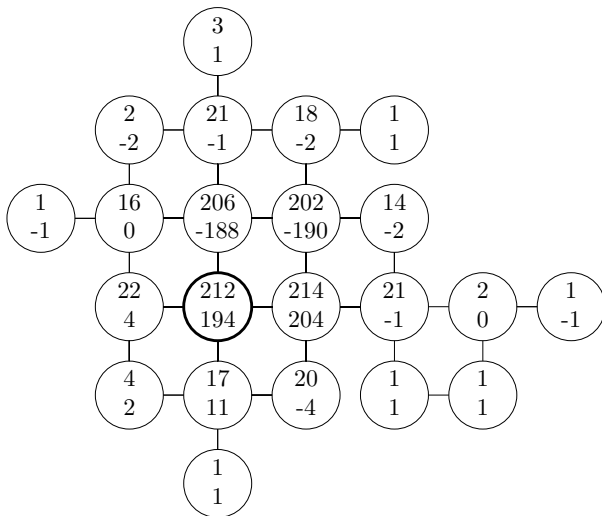
A sample with $\beta = 4.50$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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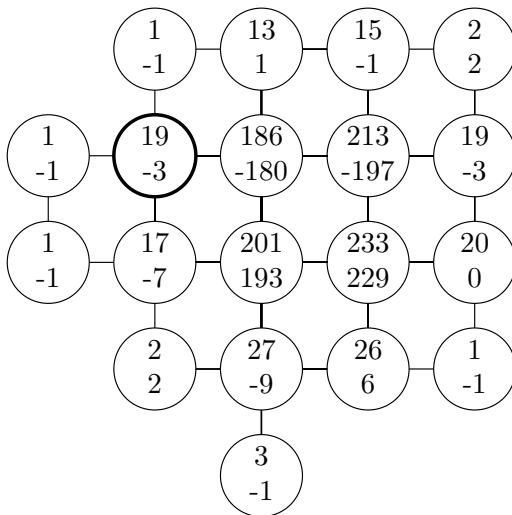
A sample with $\beta = 5.00$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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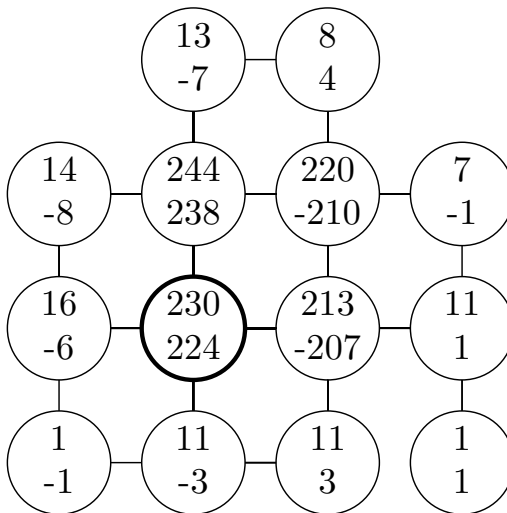
A sample with $\beta = 5.50$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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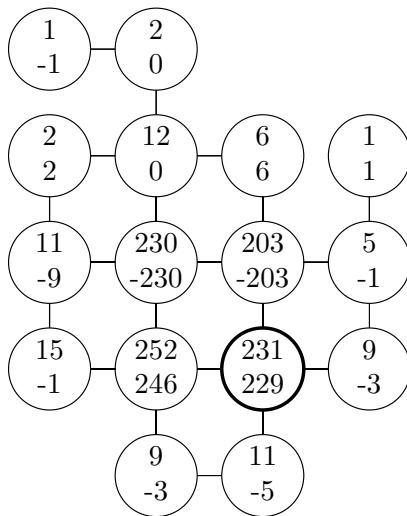
A sample with $\beta = 6.00$, $d = 2$, $N = 1000$, $q_0 = \pm 1$

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The delocalized phase

Assumption $(\mathcal{H})$

- $\mathrm{E}q_0 = 0$ and $\mathrm{Var}q_0 = 1$
- There is $\kappa < \infty$ such that $\mathrm{E}e^{tq_0} \leqslant e^{\kappa t^2/2}, \forall t \in \mathbb{R}$.

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- There is $\kappa < \infty$ such that $\mathrm{E}e^{tq_0} \leqslant e^{\kappa t^2/2}, \forall t \in \mathbb{R}$.

This holds with $\kappa = 1$ if $q_0 = \pm 1$ unbiased or $q_0 \sim \mathcal{N}(0, 1)$.

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- There is $\kappa < \infty$ such that $\mathrm{E}e^{tq_0} \leqslant e^{\kappa t^2/2}, \forall t \in \mathbb{R}$.

This holds with $\kappa = 1$ if $q_0 = \pm 1$ unbiased or $q_0 \sim \mathcal{N}(0,1)$. Let

$$
\mathcal{D} = \left\{ \beta \in \mathbb{R} : Z_N(\beta) \xrightarrow[N\to\infty]{\mathrm{P}} \exp(\beta) \right\}.
$$

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Assumption ($\mathcal{H}$)

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- There is $\kappa < \infty$ such that $\mathrm{E}e^{tq_0} \leqslant e^{\kappa t^2/2}, \forall t \in \mathbb{R}$.

This holds with $\kappa = 1$ if $q_0 = \pm 1$ unbiased or $q_0 \sim \mathcal{N}(0,1)$. Let

$$\mathcal{D} = \left\{ \beta \in \mathbb{R} : Z_N(\beta) \xrightarrow[N\to\infty]{\mathrm{P}} \exp(\beta) \right\}.$$

Theorem (Hu, Khoshnevisan, W. 2010)

Assume ($\mathcal{H}$). Then $\mathcal{D}$ is an interval that contains $(-\infty, 1/\kappa)$ and

$$\left\| \mathrm{P}_N^\beta - \mathrm{P}(\cdot|q_0, \ldots, q_{N-1}) \right\|_{\mathrm{TV}} \xrightarrow[N\to\infty]{\mathrm{P}} 0, \quad \forall \beta \in \mathcal{D}.$$

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The restricted partition function

Let $L_N^x = \sum_{0 \leqslant k < N} \mathbf{1}_{S_k = x}$ be the local time at $x \in \mathbb{Z}^d$ and $L_N^\star = \max_{x \in \mathbb{Z}^d}(L_N^x)$ the maximum local time. For any $\varepsilon > 0$, we consider

$$Z_N^\varepsilon(\beta) = \mathrm{E}\left(\exp\left(\frac{\beta}{N} H_N \right) \mathbf{1}_{\{L_N^\star \leqslant \varepsilon N\}} \,\middle|\, q_0, \ldots, q_{N-1} \right)$$

The former theorem is a consequence of:

Proposition

Assume $(\mathcal{H})$. For any $\beta \in \mathbb{R}$ and $\varepsilon > 0$ such that $2\kappa\beta\varepsilon < 1$,

$$\mathrm{E}Z_N^\varepsilon(\beta) \underset{N \to \infty}{\longrightarrow} \exp(\beta)$$

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Proof of the theorem

- $Z_N^\varepsilon(\beta) \xrightarrow{L^2(\mathrm{P})} \exp(\beta)$ when $4\kappa\beta\varepsilon < 1$.

  Indeed,

  $$
  \begin{aligned}
  \mathrm{E}\left(Z_N^\varepsilon(\beta) - e^\beta \right)^2
  &= \mathrm{E}Z_N^\varepsilon(\beta)^2 + e^{2\beta} - 2\mathrm{E}Z_N^\varepsilon(\beta)e^\beta \\
  &\leqslant \mathrm{E}Z_N^\varepsilon(2\beta) + e^{2\beta} - 2\mathrm{E}Z_N^\varepsilon(\beta)e^\beta \\
  &\longrightarrow 0
  \end{aligned}
  $$

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Proof of the theorem

- $Z_N^\varepsilon(\beta) \xrightarrow{L^2(\mathrm{P})} \exp(\beta)$ when $4\kappa\beta\varepsilon < 1$.
- $Z_N^\varepsilon(\beta) \xrightarrow{\mathrm{P}} \exp(\beta)$ when $2\kappa\beta\varepsilon < 1$.

  Indeed, $Z_N^{\varepsilon/2}(\beta) \xrightarrow{\mathrm{P}} \exp(\beta)$ while $Z_N^\varepsilon(\beta) - Z_N^{\varepsilon/2}(\beta)$ is a positive variable which expectation goes to 0.

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Proof of the theorem

- $Z_N^\varepsilon(\beta) \xrightarrow{L^2(\mathrm{P})} \exp(\beta)$ when $4\kappa\beta\varepsilon < 1$.
- $Z_N^\varepsilon(\beta) \xrightarrow{\mathrm{P}} \exp(\beta)$ when $2\kappa\beta\varepsilon < 1$.
- $(-\infty, 1/\kappa) \subset \mathcal{D}$ as $Z_N^\varepsilon(\beta) = Z_N(\beta)$ when $\varepsilon > 1/2$, N large.

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Proof of the theorem

- $Z_N^\varepsilon(\beta) \xrightarrow{L^2(\mathrm{P})} \exp(\beta)$ when $4\kappa\beta\varepsilon < 1$.
- $Z_N^\varepsilon(\beta) \xrightarrow{\mathrm{P}} \exp(\beta)$ when $2\kappa\beta\varepsilon < 1$.
- $(-\infty, 1/\kappa) \subset \mathcal{D}$ as $Z_N^\varepsilon(\beta) = Z_N(\beta)$ when $\varepsilon > 1/2$, N large.
- $\mathcal{D}$ is an interval according to Jensen's inequality

$$Z_N(\beta_1)^{\beta/\beta_1} \leqslant Z_N(\beta) \leqslant Z_N(\beta_2)^{\beta/\beta_2}$$

when $0 \leqslant \beta_1 \leqslant \beta \leqslant \beta_2$.

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Proof of the theorem

Total variation distance

$$\left\| P_N^\beta - P\left(\cdot \left| q_0, \ldots, q_{N-1} \right. \right) \right\|_{TV} = \sup_A \left| P_N^\beta\left(A \right) - P\left(A \left| q_0, \ldots, q_{N-1} \right. \right) \right|$$

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Proof of the theorem

Total variation distance

$$\left\| P_N^\beta - P\left(\cdot \,|\, q_0, \ldots, q_{N-1} \right) \right\|_{\mathrm{TV}} = \sup_A \left| P_N^\beta(A) - P\left(A \,|\, q_0, \ldots, q_{N-1} \right) \right|$$

does not exceed $\sup_A d_1(A) + d_2$ where

$$d_1(A) = \left| P_N^\beta \left(A \cap \{ L_N^\star \leqslant \varepsilon N \} \right) - P\left(A \cap \{ L_N^\star \leqslant \varepsilon N \} \,|\, q_0, \ldots, q_{N-1} \right) \right|$$

$$d_2 = P_N^\beta \left(\{ L_N^\star > \varepsilon N \} \right) + P\left(\{ L_N^\star > \varepsilon N \} \right).$$

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does not exceed $\sup_A d_1(A) + d_2$ where

$$d_1(A) = \left| P_N^\beta\left(A \cap \{L_N^\star \leqslant \varepsilon N\}\right) - P\left(A \cap \{L_N^\star \leqslant \varepsilon N\} \,\middle|\, q_0, \ldots, q_{N-1}\right) \right|$$

$$d_2 = P_N^\beta\left(\{L_N^\star > \varepsilon N\}\right) + P\left(\{L_N^\star > \varepsilon N\}\right).$$

When $\beta \in \mathcal{D}$, $d_2 \xrightarrow{\ P\ } 0$.

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Total variation distance

$$\left\| P_N^\beta - P\left(\cdot \,|\, q_0, \ldots, q_{N-1}\right) \right\|_{\mathrm{TV}} = \sup_A \left| P_N^\beta(A) - P\left(A \,|\, q_0, \ldots, q_{N-1}\right) \right|$$

does not exceed $\sup_A d_1(A) + d_2$ where

$$d_1(A) = \left| P_N^\beta\left(A \cap \{L_N^\star \leqslant \varepsilon N\}\right) - P\left(A \cap \{L_N^\star \leqslant \varepsilon N\} \,|\, q_0, \ldots, q_{N-1}\right) \right|$$

$$d_2 = P_N^\beta\left(\{L_N^\star > \varepsilon N\}\right) + P\left(\{L_N^\star > \varepsilon N\}\right).$$

When $\beta \in \mathcal{D}$, $d_2 \xrightarrow{\mathrm{P}} 0$. Furthermore

$$d_1(A) \leqslant \mathrm{E}\left[\left| \frac{\exp\left(\beta H_N / N\right)}{Z_N(\beta)} - 1 \right|^2 \mathbf{1}_{\{L_N^\star \leqslant \varepsilon N\}} \,\middle|\, q_0, q_1, \ldots, q_{N-1} \right]^{1/2}$$

$$= \left[\frac{Z_N^\varepsilon(2\beta)}{Z_N(\beta)^2} - 2\frac{Z_N^\varepsilon(\beta)}{Z_N(\beta)} + P\left(\{L_N^\star \leqslant \varepsilon N\}\right) \right]^{1/2} \xrightarrow{\mathrm{P}} 0.$$

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Lower bound on $\mathrm{E}Z_N^\varepsilon(\beta)$

As $H_N = \sum_{0 \leqslant j, k < N} q_j q_k \mathbf{1}_{\{S_j = S_k\}}$, $(\mathcal{H})$ implies that

$$\mathrm{E}(H_N | S) = \mathrm{E}\left(\sum_{0 \leqslant j, k < N} \mathbf{1}_{\{j=k, S_j = S_k\}} \,\middle|\, S \right) = N.$$

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Lower bound on $\mathrm{E}Z_N^\varepsilon(\beta)$

As $H_N = \sum_{0 \leqslant j,k < N} q_j q_k \mathbf{1}_{\{S_j = S_k\}}$, $(\mathcal{H})$ implies that

$$\mathrm{E}(H_N | S) = \mathrm{E}\left(\sum_{0 \leqslant j,k < N} \mathbf{1}_{\{j=k, S_j = S_k\}} \middle| S \right) = N.$$

By Jensen's conditional inequality,

$$
\begin{aligned}
\mathrm{E}Z_N^\varepsilon(\beta) &= \mathrm{E}\left(\mathrm{E}\left(\exp\left(\frac{\beta}{N} H_N \right) \middle| S \right) \mathbf{1}_{\{L_N^\star \leqslant \varepsilon N\}} \right) \\
&\geqslant \exp(\beta) \mathrm{P}(L_N^\star \leqslant \varepsilon N) \\
&\xrightarrow[N \to \infty]{} \exp(\beta).
\end{aligned}
$$

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Upper bound on $\mathrm{E}Z_N^\varepsilon(\beta)$

Lemma

Assume $(\mathcal{H})$. Let $\varepsilon > 0$ and $\beta \in \mathbb{R}$ such that $2\kappa\beta\varepsilon < 1$. Let $\delta > 0$ small enough. Then, there is $C < \infty$ such that, for every N sufficiently large,

$$\mathrm{E}\exp\left(\frac{\beta}{N}(q_0 + \cdots + q_{L-1})^2\right) \leqslant \exp\left(\beta\frac{L}{N} + \delta|\beta|\frac{L}{N} + C\frac{L^2}{N^2}\right)$$

uniformly in $L \in \{0, \ldots [\varepsilon N]\}$.

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Upper bound on $\mathrm{E} Z_N^\varepsilon(\beta)$

Assume $\beta > 0$. Introduce ξ a centered unitary gaussian variable independent of q and the Laplace transform $\Psi(t) = \mathrm{E}\exp(tq_0)$. Then

$$
\begin{aligned}
\mathrm{E}\exp\left(\frac{\beta}{N}(q_0 + \cdots + q_{L-1})^2\right) &= \mathrm{E}\exp\left(\sqrt{\frac{2\beta}{N}}\xi(q_0 + \cdots + q_{L-1})\right) \\
&= \mathrm{E}\left[\Psi\left(\sqrt{\frac{2\beta}{N}}\xi\right)^L\right].
\end{aligned}
$$

As $\Psi(t) \leqslant \exp(\kappa t^2/2)$ and $L \leqslant \varepsilon N$, the contribution of ξ with $|\sqrt{2\beta/N}\xi| \geqslant \delta$ is negligible. For the remaining part, use

$$
\Psi(t) = \exp\left(\frac{t^2}{2} + \underset{t\to 0}{o}(t^2)\right).
$$

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Our main result
The restricted partition function
An insight at the proof

Upper bound on $\mathrm{E}Z_N^\varepsilon(\beta)$

Consequence of the lemma: when $2\kappa\beta\varepsilon < 1$,

$$
\begin{aligned}
\mathrm{E}Z_N^\varepsilon(\beta) &= \mathrm{E}\left(\mathrm{E}\left(\left.\exp\left(\frac{\beta}{N}H_N\right)\right| S\right)\mathbf{1}_{\{L_N^\star \leqslant \varepsilon\}}\right) \\
&= \mathrm{E}\left(\prod_{x\in\mathbb{Z}^d}\mathrm{E}\left(\left.\exp\left(\frac{\beta}{N}(Q_N^x)^2\right)\right| S\right)\mathbf{1}_{\{L_N^\star \leqslant \varepsilon\}}\right) \\
&\leqslant \mathrm{E}\left(\exp\left(\beta\sum_{x\in\mathbb{Z}^d}\frac{L_N^x}{N} + \delta|\beta|\sum_{x\in\mathbb{Z}^d}\frac{L_N^x}{N} + C\sum_{x\in\mathbb{Z}^d}\frac{(L_N^x)^2}{N^2}\right)\right) \\
&\xrightarrow[N\to\infty]{} \exp(\beta + \delta|\beta|).
\end{aligned}
$$

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Our result
An excluded range for $L_N^\star / N$

A first order transition

As H_N/N is sub-additive, the free energy

$$F(\beta) = \lim_N \frac{1}{N} \log Z_N(\beta)$$

exists a.s. and in L^1 when $\mathrm{Var} q_0 < \infty$. Let $\beta_c := \sup \mathcal{D}$.

Theorem (Hu, Khoshnevisan, W. 2010)

Assume $(\mathcal{H})$. For any $\beta \leqslant \beta_c$, $F(\beta) = 0$. There is $c > 0$ such that,

$$F(\beta) \geqslant c(\beta - \beta_c), \quad \forall \beta > \beta_c.$$

Furthermore, for all $\beta > \beta_c$, for all $\varepsilon > 0$,

$$\mathrm{P}_N^\beta \left(\frac{L_N^\star}{N} \geqslant (1 - \varepsilon) \max \left(\frac{F(\beta)}{\beta}, \frac{1}{2\kappa\beta} \right) \right) \xrightarrow[N \to \infty]{\mathrm{P}} 1.$$

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A signal of the first order transition

Assume $(\mathcal{H})$ and let $\beta, \varepsilon, \eta > 0$ such that $\varepsilon < (1-\eta)/(2\kappa\beta)$. Then

$$
\begin{aligned}
\mathrm{EP}_N^\beta \left(\varepsilon < \frac{L_N^\star}{N} \leqslant \frac{1-\eta}{2\kappa\beta} \right) \quad &= \quad \mathrm{E}\frac{Z_N^{(1-\eta)/(2\kappa\beta)}(\beta) - Z_N^\varepsilon(\beta)}{Z_N(\beta)} \\
&\leqslant \quad \mathrm{E}\left(Z_N^{(1-\eta)/(2\kappa\beta)}(\beta) - Z_N^\varepsilon(\beta) \right) \\
&\underset{N \to \infty}{\longrightarrow} \quad 0
\end{aligned}
$$

according to the proposition.

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The four points
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Let $\varepsilon \in \{\pm\}$ and $p \in \{\mathrm{odd}, \mathrm{even}\}$. Then

$$Q_\varepsilon^p = \sum_{0 \leqslant k < N : k \equiv p} (q_k)^\varepsilon$$

is the total charge of sign ε available at the sites $x \in \mathbb{Z}^d$ with parity p (i.e. $x_1 + \ldots + x_d \equiv p$).

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Claim

Assume $d \geqslant 2$. Then, for any q,

$$\max_S H_N = \sum_{\varepsilon \in \{\pm\}, p \in \{\mathrm{odd, even}\}} (Q_\varepsilon^p)^2.$$

In particular, $\max_S H_N$ is typically of order N^2 under P.

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The four points

Let $0 < \alpha < 1$. Denote

$$\mathcal{S}_N(\alpha) = \left\{ \begin{array}{l} \text{There exists a square with vertices } x_\varepsilon^p \\ \text{such that } (Q_N^{x_\varepsilon^p})^\varepsilon \geqslant \frac{1+\alpha}{2} Q_\varepsilon^p \end{array} \right\}.$$

Theorem (Hu, Khoshnevisan, W. 2010)

Let $d \geqslant 2$. Assume that q_0 takes both positive and negative values. Let $0 < \alpha < 1$. For β large enough, there is $c > 0$ such that

$$\mathrm{EP}_N^\beta (\mathcal{S}_N(\alpha)^c) < \exp(-cN)$$

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Excursions have exponential tail

When $\mathcal{S}_N(\alpha)$ occurs, folding excursions onto the square increases significantly the energy. As a consequence, excursions from the square have exponential tail when β is large.

Proposition

Let $d \geqslant 2$. Assume that q_0 takes both positive and negative values. For β large enough, there is $C < \infty$ such that

$$\mathrm{EP}_N^\beta \left(\mathrm{Diam}(S_0, \ldots, S_{N-1}) < C \log N \right) \quad \underset{N \to \infty}{\longrightarrow} \quad 1$$

$$\sup_N \mathrm{EE}_N^\beta \left(|S_{N-1}| \right) \quad < \quad C.$$

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Open questions

- What happens at β_c ?

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Open questions

- What happens at β_c ?
- Is it true that $\sup_N \mathrm{EE}_N^{\beta}|S_{N-1}| < \infty$ for all $\beta > \beta_c$? Do we still have logarithmic diameter ?

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Open questions

- What happens at β_c ?
- Is it true that $\sup_N \mathrm{EE}_N^\beta |S_{N-1}| < \infty$ for all $\beta > \beta_c$? Do we still have logarithmic diameter ?
- We observe no phase transition for $\beta < 0$, instead the polymer is always delocalized. What is the correct scaling for observing the transition to a folded state ? What is that folded state ?

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Thanks