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A first order localization/delocalization transition in charged polymers

Marc Wouts

Abstract

We study a quenched charged-polymer model, introduced by Garel and Orland in 1988, that reproduces the folding/unfolding transition of biopolymers. We prove that, below the critical inverse temperature, the polymer is delocalized in the sense that: (1) The rescaled trajectory of the polymer converges to the Brownian path; and (2) The partition function remains bounded.

At the critical inverse temperature, we show that the maximum time spent at points jumps discontinuously from 0 to a positive fraction of the number of monomers, in the limit as the number of monomers tends to infinity.

Finally, when the critical inverse temperature is large, we prove that the polymer collapses in the sense that a large fraction of its monomers live on four adjacent positions, and its diameter grows only logarithmically with the number of the monomers.

Our methods also provide some insight into the annealed phase transition and at the transition due to a pulling force; both phase transitions are shown to be discontinuous.

We consider a polymer model introduced by Garel and Orland [EPL 1988] for modeling the trajectory of biological proteins made of hydrophobic monomers. Let $\{q_i\}_{i=0}^{\infty}$ be i.i.d. real variables and $\{S_i\}_{i=0}^{\infty}$ an independent simple random walk on $\mathbf{Z}^d$ with $S_0 = 0$. Both stochastic processes exist on a common probability space $(\Omega\,, \mathcal{F}, \mathrm{P})$. Given a realization of q and S, we consider

$$Q_N^x := \sum_{0 \leqslant i < N} q_i \mathbf{1}_{\{S_i = x\}}, \quad \text{and} \tag{0.1}$$

$$H_N := \sum_{x \in \mathbf{Z}^d} \left(Q_N^x\right)^2. \tag{0.2}$$

We think of the q_i's as *charges*, Q_N^x as the *total charge* at position $x \in \mathbf{Z}^d$, and H_N as the *energy* of the polymer.

For all $\beta \in \mathbf{R}$ and $N \geqslant 1$ consider the quenched probability measure P_N^β,

$$\mathrm{P}_N^\beta(A) := \frac{1}{Z_N(\beta)} \mathrm{E}\left[\mathbf{1}_A \exp\left(\frac{\beta}{N} H_N\right) \middle| q_0, q_1, \ldots, q_{N-1}\right], \tag{0.3}$$

where $Z_N(\beta)$ is defined so that P_N^β is indeed a probability measure; that is,

$$Z_N(\beta) := \mathrm{E}\left[\exp\left(\frac{\beta}{N} H_N\right) \middle| q_0, q_1, \ldots, q_{N-1}\right]. \tag{0.4}$$

In our model, like charges attract when $\beta > 0$. This accounts for the hydrophobic properties of monomers immersed in water. And the scaling H_N/N makes the energy subadditive.

Unless it is stated to the contrary, we assume that $\mathrm{E}q_0 = 0$, $\operatorname{Var} q_0 = 1$, and that the charges are *subgaussian*; that is, $\kappa < \infty$, where

$$\kappa := \inf\left\{c \in (-\infty\,, \infty] : \ \mathrm{E}\mathrm{e}^{tq_0} \leqslant \mathrm{e}^{ct^2/2} \quad \text{for all} \quad t \in \mathbf{R}\right\}. \tag{0.5}$$

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Joint work with Yueyun Hu (Paris 13) and Davar Khoshnevisan (Utah), see arxiv:1011.1452.

We have $\kappa \geqslant 1$ as long as q_0 has a finite moment generating function near zero and $\mathrm{E}q_0 = 0$. And $\kappa = 1$ both when the q_i's have the Rademacher distribution $[\mathrm{P}\{q_0 = \pm 1\} = 1/2]$ and when they have a standard normal distribution.

Now we introduce

$$\mathscr{D} := \left\{\beta \in \mathbf{R} : \ Z_N(\beta) \xrightarrow{\mathrm{P}} \mathrm{e}^{\beta} \quad \text{as } N \to \infty\right\}, \tag{0.6}$$

where "$\xrightarrow{\mathrm{P}}$" denotes convergence in probability. As is customary, we call

$$L_N^x := \sum_{i=0}^{N-1} \mathbf{1}_{\{S_i = x\}} \quad \text{and} \quad L_N^\star := \max_{x \in \mathbf{Z}^d} L_N^x, \tag{0.7}$$

respectively, the *local time* of $\{S_i\}_{i=0}^{N-1}$ at x and the maximum local time.

The next theorem tells us that the set $\mathscr{D}$ characterizes the region of β for which the trajectory of the polymer is [asymptotically] indistinguishable from that of a random walk. In other words, the polymer is *delocalized* when $\beta \in \mathscr{D}$ and N is large.

Theorem 1. *If* $\mathrm{E}q_0 = 0$, $\operatorname{Var} q_0 = 1$, *and* $\kappa < \infty$, *then:*

(1) $\mathscr{D}$ *is an interval that contains* $(-\infty\,, 1/\kappa)$.

(2) $\beta \in \mathscr{D}$ *if and only if for all* $\varepsilon > 0$,

$$\mathrm{P}_N^\beta\{L_N^\star \leqslant \varepsilon N\} \xrightarrow{\mathrm{P}} 1 \qquad \text{as } N \to \infty. \tag{0.8}$$

(3) $\beta \in \mathscr{D}$ *if and only if:*

$$\left\| \mathrm{P}_N^\beta - \mathrm{P}\left[\,\cdot\,|q_0\,, \ldots, q_{N-1}\right] \right\|_{\mathrm{TV}} \xrightarrow{\mathrm{P}} 0 \qquad \text{as } N \to \infty, \tag{0.9}$$

where $\|\mu - \nu\|_{\mathrm{TV}} := \sup_A |\mu(A) - \nu(A)|$ *is the total variation distance.*

A consequence of Theorem 1 is the following: if $\mathscr{S}_N$ is defined uniquely as the piecewise-linear function that takes the values $S_k/\sqrt{N}$ at $t = k/N$ for all integers $k = 0, \ldots, N$, then:

Corollary 2. *If* $\mathrm{E}q_0 = 0$, $\operatorname{Var} q_0 = 1$, *and* $\kappa < \infty$, *then for all* $\beta \in \mathscr{D}$ *and* $\Phi : C([0\,,1]) \to \mathbf{R}$ *bounded and continuous,*

$$\mathrm{E}_N^\beta\left[\Phi\left(\mathscr{S}_N\right)\right] \quad \xrightarrow[N\to\infty]{\mathrm{P}} \quad \mathrm{E}\left[\Phi\left(\mathscr{B}\right)\right], \tag{0.10}$$

where $\mathscr{B}$ *denotes d-dimensional Brownian motion.*

As we said earlier, the normalized energy H_N/N is subadditive. It follows from that fact that the *free energy* $\digamma$ exists:

Proposition 3. *If* $\mathrm{E}(q_0^2) < \infty$, *then for all* $\beta \in \mathbf{R}$,

$$\digamma(\beta) := \lim_{N\to\infty} \frac{1}{N} \ln Z_N\left(\beta\right) \tag{0.11}$$

exists a.s. and in $L^1(\mathrm{P})$, *and* $\digamma(\beta)$ *is nonrandom. The function* $\mathbf{R} \ni \beta \to \digamma(\beta)$ *is nonnegative, nondecreasing, and convex with* $\digamma(0) = 0$.

Define the *critical inverse temperature*,

$$\beta_c := \sup \mathscr{D}. \tag{0.12}$$

Clearly, $\digamma(\beta) = 0$ whenever $\beta \leqslant \beta_c$. Our next theorem shows the converse is true and that a first-order phase transition occurs at β_c.

Theorem 4. *If* $\mathrm{E}q_0 = 0$, $\operatorname{Var} q_0 = 1$, *and* $\kappa < \infty$, *then* $\digamma(\beta_c) = 0$, *whereas* $\digamma(\beta) > 0$ *for all* $\beta > \beta_c$. *Moreover, there is a first-order phase transition at* β_c; *i.e.,*

$$\lim_{\beta \downarrow \beta_c} \frac{\digamma(\beta)}{\beta - \beta_c} \in (0\,, \infty). \tag{0.13}$$

Furthermore, if $\beta > \beta_c$, *then for all* $\varepsilon > 0$,

$$\mathrm{P}_N^\beta\left\{\frac{L_N^\star}{N} \geqslant \frac{1-\varepsilon}{\beta} \max\left(\digamma(\beta)\,, \frac{1}{2\kappa}\right)\right\} \xrightarrow{\mathrm{P}} 1 \quad \text{as } N \to \infty. \tag{0.14}$$

Our work also addresses the behavior of the polymer at low temperatures. We show that, when $d \geqslant 2$ and when β is large, most of the charges of the polymer are concentrated on the vertices of a unit square, that the expectation of S_N remains bounded while the diameter of the polymer is of order $\log N$. Most of our results hold as well for the corresponding annealed model ; and we discuss the influence of a pulling force, that again is able to trigger a first-order phase transition.