Statistical Physics of Stretched Polymers

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based on joint works with D. Ioffe

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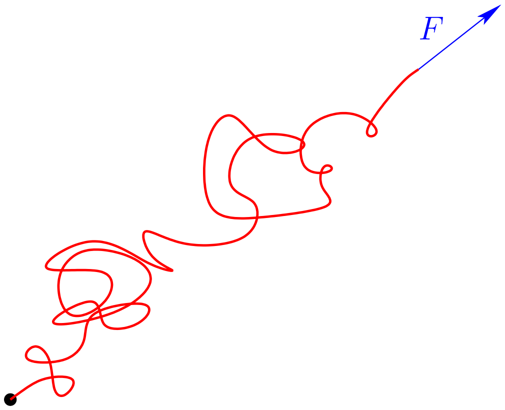
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Polymer models

Polymer configuration:

$\gamma = (\gamma(0), \ldots, \gamma(n))$: n.-n. path on $\mathbb{Z}^d$ with $\gamma(0) = 0$

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Internal energy:

$$\Phi(\gamma) = \sum_{x \in \mathbb{Z}^d} \phi(\ell_x(\gamma))$$

$\phi : \mathbb{N} \to \overline{\mathbb{R}}$: nonnegative, nondecreasing, $\phi(0) = 0$

$\ell_x(\gamma) = \sum_{k=0}^{n} \mathbf{1}_{\{\gamma(k)=x\}}$ (local times)

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Probability:

$$\mathbb{P}_n(\gamma) \propto e^{-\Phi(\gamma)}$$

Classes of interactions

Two main classes of interactions:

Repulsive interactions

$$\phi(n+m) \geq \phi(n) + \phi(m)$$

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Repulsive interactions

$$\phi(n+m) \geq \phi(n) + \phi(m)$$

Attractive interactions

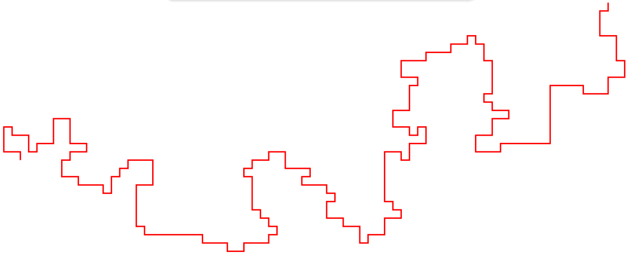
$$\phi(n+m) \leq \phi(n) + \phi(m)$$

(and, w.l.o.g., $\lim_{n\to\infty} \phi(n)/n = 0$)

Examples: repulsive interactions

Self-Avoiding walk (SAW)

$$\phi(\ell) = \begin{cases} \infty & \text{if } \ell > 1 \\ 0 & \text{otherwise} \end{cases}$$



Examples: repulsive interactions

Domb-Joyce model

Defined by

$$\Phi(\gamma) = \beta \sum_{0\le i<j\le n} \mathbf{1}_{\{\gamma(i)=\gamma(j)\}} \qquad\qquad (\beta \ge 0)$$

This corresponds to the choice

$$\phi(\ell) = \tfrac{1}{2}\beta\ell(\ell - 1)$$

Examples: attractive interactions

Discrete sausage

$$\mathbb{P}_n(\gamma) \propto e^{-\beta \cdot \#\text{ of sites visited by }\gamma} \qquad (\beta \geq 0)$$

corresponds to the choice

$$\phi(\ell) = \begin{cases} \beta & \text{if } \ell \geq 1 \\ 0 & \text{if } \ell = 0 \end{cases}$$

Examples: attractive interactions

Reinforced Polymer

$(\beta_k)_{k\geq 1}$: non-negative, non-increasing sequence.

β_k = energetic cost associated to k^{th} visit at a site.

$$\phi(\ell) = \sum_{k=1}^{\ell} \beta_k$$

Examples: attractive interactions

Polymer in Annealed Random Environment

Environment: $(V_x)_{x\in\mathbb{Z}^d}$, i.i.d. non-negative random variables

Quenched weight: $\mathsf{w}^{\omega}(\gamma) = e^{-\sum_{i=0}^{n} V_{\gamma(i)}(\omega)}$

Annealed weight: $\mathsf{w}_{\rm an}(\gamma) = \mathbb{E}\mathsf{w}^{\cdot}(\gamma)$

Examples: attractive interactions

Polymer in Annealed Random Environment

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Annealed weight: $\mathrm{w}_{\mathrm{an}}(\gamma) = \mathbb{E}\mathrm{w}^{\cdot}(\gamma) \equiv e^{-\Phi(\gamma)}$

$$\phi(\ell) = -\log \mathbb{E} e^{-\ell V}$$

2-point function

Let $|\gamma|$ denote the length of γ.
For all $x \in \mathbb{Z}^d$, the 2-point function

$$\mathbf{G}_\lambda(x) = \sum_{\gamma:0\to x} e^{-\Phi(\gamma)-\lambda|\gamma|}$$

is well-defined for all $\lambda > \lambda_0$, where

$$\lambda_0 = \lim_{n\to\infty} \frac{1}{n} \log \sum_{\gamma(0)=0,\, |\gamma|=n} e^{-\Phi(\gamma)}$$

is well-defined and finite (attractive case: $\lambda_0 = \log(2d)$).

Inverse correlation length

Exponential decay of 2-point function

For all $\lambda > \lambda_0$ and all $x \in \mathbb{R}^d$:

$$\xi_\lambda(x) = \lim_{k\to\infty} -\frac{1}{k} \log \mathbf{G}_\lambda([kx])$$

is a well-defined, equivalent norm on $\mathbb{R}^d$.

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This means that, for any $x \in \mathbb{Z}^d$,

$$\mathbf{G}_\lambda(x) = e^{-\xi_\lambda(n_x)\|x\|\,(1+o(1))},$$

where $n_x = x/\|x\|$.

$\xi_\lambda(n_x)$ is the **inverse correlation length** in direction n_x.

Inverse correlation length

Exponential decay of 2-point function

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is a well-defined, equivalent norm on $\mathbb{R}^d$.

Behaviour as $\lambda \downarrow \lambda_0$

$$\xi_{\lambda_0} \equiv \lim_{\lambda\downarrow\lambda_0} \xi_\lambda$$

Repulsive: $\xi_{\lambda_0} \equiv 0$ **Attractive:** $\xi_{\lambda_0} > 0$

Stretched polymer

We are interested in the following probability measure on paths $\gamma = (\gamma(0), \dots, \gamma(n))$, $\gamma(0) = 0$:

$$\mathbb{P}_n^F(\gamma) \propto e^{-\Phi(\gamma)+\langle F,\gamma(n)\rangle}$$

where

$$-\langle F, \gamma(n)\rangle$$

is the contribution to the polymer energy due to the force $F \in \mathbb{R}^d$ acting on its free end.

Main problems

- Determine whether the polymer is collapsed or stretched.
- When stretched, determine the distribution of its free end.
- When stretched, describe the fluctuations of the polymer.
- When stretched, describe the micro structure of the polymer.

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Wulff shape

For all $\lambda \geq \lambda_0$:

$$\mathbf{K}_\lambda = \left\{ F \in \mathbb{R}^d \,:\, \langle F, x \rangle \leq \xi_\lambda(x),\ \forall x \in \mathbb{R}^d \right\}$$

(Alternatively, $\mathbf{K}_\lambda$ is the unit-ball in polar norm.)

Increasing family of convex bodies

Wulff shape

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$$\mathbf{K}_\lambda = \left\{ F \in \mathbb{R}^d \, : \, \langle F, x \rangle \leq \xi_\lambda(x), \; \forall x \in \mathbb{R}^d \right\}$$

(Alternatively, $\mathbf{K}_\lambda$ is the unit-ball in polar norm.)

Increasing family of convex bodies

Behaviour as $\lambda \downarrow \lambda_0$

Repulsive: $\mathbf{K}_{\lambda_0} = \{0\}$ **Attractive:** $\mathring{\mathbf{K}}_{\lambda_0} \neq \varnothing$

Phase transition

Attractive case: Transition between a collapsed phase and a stretched phase.

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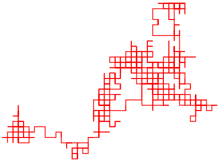
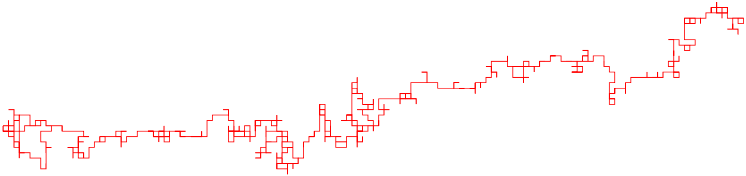


$$F \in \mathring{\mathbf{K}}_{\lambda_0}$$

Phase transition

Attractive case: Transition between a collapsed phase and a stretched phase.



$$F \notin \mathbf{K}_{\lambda_0}$$

Phase transition

Attractive case: Transition between a collapsed phase and a stretched phase.

Attractive case – Collapsed phase

For all $F \in \mathring{\mathbf{K}}_{\lambda_0}, \exists c > 0$ such that

$$\mathbb{P}_n^F\left(\tfrac{1}{n}\gamma(n) \notin B_\epsilon(0)\right) \leq e^{-c\epsilon n}$$

for all $\epsilon > 0$ and $n > n_0(\epsilon)$.

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Stretched phase

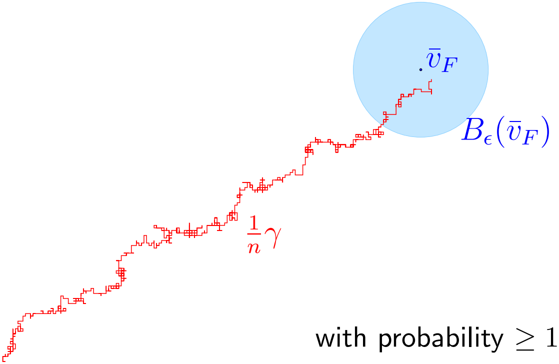
We turn to the description of the **stretched phase**, $F \notin \mathbf{K}_{\lambda_0}$.

The results hold for both **attractive** and **repulsive** interactions.

(Remember that $\mathbf{K}_{\lambda_0} = \{0\}$ in the repulsive case, so an arbitrary force $F \neq 0$ results in a stretched polymer.)

Stretched phase – position of endpoint

There exists $\bar{v}_F \in \mathbb{R}^d$, $\bar{v}_F \neq 0$, such that



with probability $\geq 1 - e^{-\kappa n}$

Stretched phase – position of endpoint

For all $x \in B_\epsilon(\bar{v}_F) \cap \frac{1}{n}\mathbb{Z}^d$,

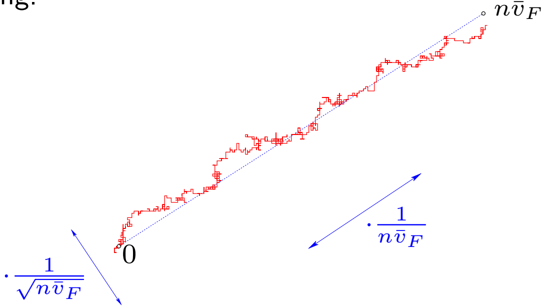
$$\mathbb{P}_n^F\left(\frac{\gamma(n)}{n} = x\right) = \frac{G(x)}{\sqrt{n^d}}\, \mathrm{e}^{-nJ_F(x)}\,(1 + o(1)).$$

G: positive and analytic on $B_\epsilon(\bar{v}_F)$

J_F: positive, analytic on $B_\epsilon(\bar{v}_F)$, and strictly convex with a non-degenerate quadratic minimum at $\bar{v}_F$

Stretched phase – Path fluctuations

This can be complemented by an **invariance principle** under diffusive scaling.



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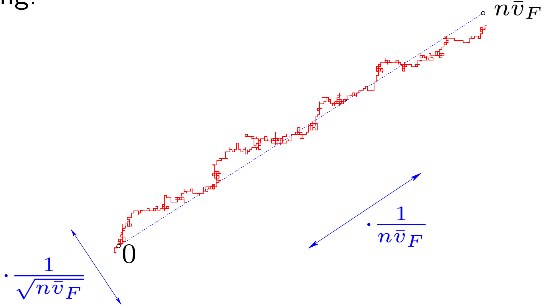
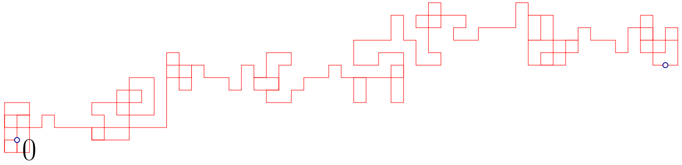
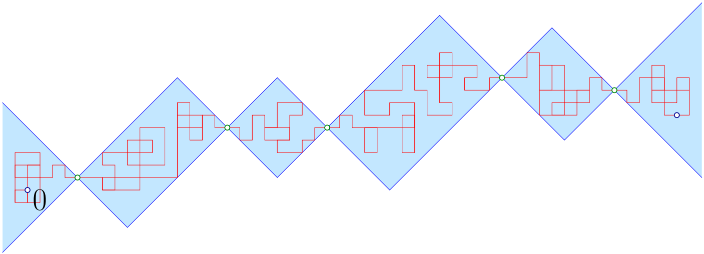


The covariance of the limiting $(d-1)$-dim. Brownian motion on $[0,1]$ is related to the geometry of $\mathbf{K}_\lambda$, where λ is uniquely determined by $F \in \partial\mathbf{K}_\lambda$.

Stretched phase – Microscopic structure



Stretched phase – Microscopic structure



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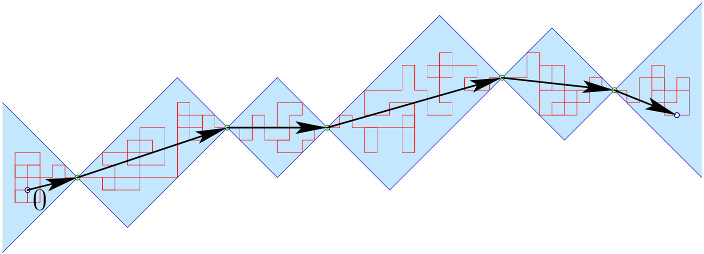
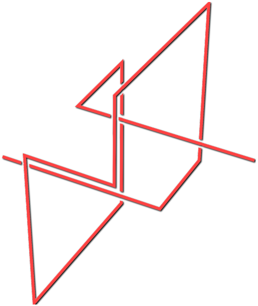


Stretched phase – Local observables

One can also obtain local limit theorems for **local observables**.

As an example, let us consider a **pattern** η, *e.g.*,



How many times does this pattern appear along the polymer?

Stretched phase – Local observables

Let $N_\eta(\gamma)$ be the number of apparitions of η along γ.

$\exists x_\eta \in (0,1)$, $\epsilon > 0$, $\nu > 0$ and a rate function J_F^η on $(x_\eta - \epsilon, x_\eta + \epsilon)$ with quadratic minimum at x_η, such that

$$\mathbb{P}_n^F \left(\left| \frac{N_\eta(\gamma)}{n} - x_\eta \right| \geq \epsilon \right) \leq \mathrm{e}^{-\nu n},$$

and, for $x \in (x_\eta - \epsilon, x_\eta + \epsilon)$,

$$\mathbb{P}_n^F \left(N_\eta(\gamma) = \lfloor nx \rfloor \right) = \frac{G_\eta(x)}{\sqrt{n}} \, e^{-n J_F^\eta(x)} \left(1 + o(1)\right),$$

where G_η is a positive real analytic function on $[x_\eta - \epsilon, x_\eta + \epsilon]$.

Stretched phase – Perturbations

The previous results are **stable under small, smooth, local perturbations** of the internal energy Φ. For example, if one considers the internal energy

$$\widetilde{\Phi}(\gamma) = \Phi(\gamma) + R(\gamma, F),$$

with

- $f \mapsto R(\gamma, f)$ analytic in a neighbourhood of F, for each γ.
- $|R(\gamma, f)| \leq \epsilon|\gamma|$ for f in a neighbourhood of F, for all γ.
- Some locality assumption, *e.g.*, $R(\gamma_1 \cup \cdots \cup \gamma_m, f) = \sum_{i=1}^m R(\gamma_i, f)$, whenever the subpaths are edge-disjoint, for all f in a neighbourhood of F.

Stretched phase – Perturbations

Two main applications of this stability are

- Models with mixed attractive/repulsive interactions (*e.g.*, strong repulsion, weak attraction).
- Dynamical processes (*e.g.*, *random walk* with drift, with small edge reinforcement).

Ideas of proof

Clearly,

$$\mathbb{P}_n^F(\gamma(n) = x) = \frac{e^{\langle F,x\rangle}\mathbf{G}(x;n)}{\sum_{y\in\mathbb{Z}^d} e^{\langle F,y\rangle}\mathbf{G}(y;n)},$$

where

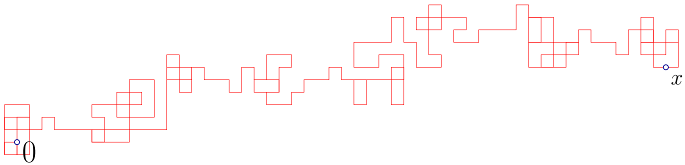
$$\mathbf{G}(x;n) = \sum_{\substack{\gamma:\,0\to x\\ |\gamma|=n}} e^{-\Phi(\gamma)}$$

We need to control this quantity!

Irreducible decomposition of $\mathbf{G}_\lambda(x)$

For any $\lambda > \lambda_0$,

$$e^{\xi_\lambda(x)}\mathbf{G}_\lambda(x) = O(e^{-\nu\|x\|}) + \sum_{m\geq c\|x\|} \mathbb{Q}_\lambda^m\Big(D(\gamma_{\mathrm{L}}) + \sum_{i=1}^m D(\gamma_i) + D(\gamma_{\mathrm{R}}) = x\Big)$$



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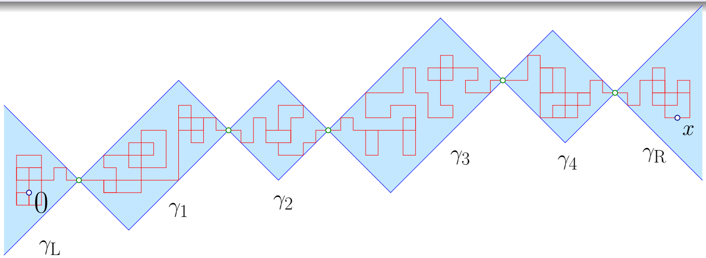

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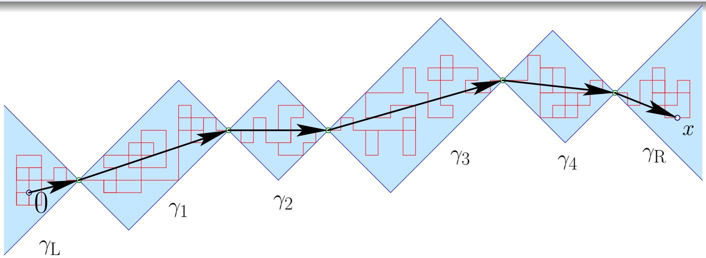

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Irreducible decomposition of $\mathbf{G}_\lambda(x)$

For any $\lambda > \lambda_0$,

$$e^{\xi_\lambda(x)}\mathbf{G}_\lambda(x) = O(e^{-\nu\|x\|}) + \sum_{m\geq c\|x\|} \mathbb{Q}_\lambda^m\Big(D(\gamma_{\mathrm{L}}) + \sum_{i=1}^m D(\gamma_i) + D(\gamma_{\mathrm{R}}) = x\Big)$$

- $\mathbb{Q}_\lambda^m = \mathbb{Q}_{\mathrm{L}} \otimes \mathbb{Q}_{\mathrm{R}} \otimes \bigotimes_{i=1}^m \mathbb{Q}$.
- $\mathbb{Q}$ is a probability measure on irreducible pieces.
- D has exp. moments under $\mathbb{Q}$, $\mathbb{Q}_{\mathrm{L}}$ and $\mathbb{Q}_{\mathrm{R}}$.

Irreducible decomposition of $\mathbf{G}_\lambda(x)$

For any $\lambda > \lambda_0$,

$$e^{\xi_\lambda(x)}\mathbf{G}_\lambda(x) = O(e^{-\nu\|x\|}) + \sum_{m\geq c\|x\|} \mathbb{Q}_\lambda^m\Big(D(\gamma_{\mathrm{L}}) + \sum_{i=1}^m D(\gamma_i) + D(\gamma_{\mathrm{R}}) = x\Big)$$

- $D(\gamma_L)$ and $D(\gamma_R)$ are typically small.
- $D(\gamma_i)$, $i = 1, \ldots, m$, are i.i.d. with exp. tails.
- $m > c\|x\|$.
- $\implies$ Asymptotics of $\mathbf{G}_\lambda$ using local limit theorem!

Asymptotics of $\mathbf{G}_\lambda(x)$

Let $n_x = x/\|x\|$.

Asymptotics of $\mathbf{G}_\lambda(x)$

For all $\lambda > \lambda_0$,

$$\mathbf{G}_\lambda(x) = \frac{\Psi(n_x)}{\|x\|^{(d-1)/2}}\, e^{-\xi_\lambda(x)}\,(1+o(1))$$

uniformly as $\|x\| \to \infty$.

Irreducible decomposition for general observables

The same remains true for any observable defined on paths: if S is such an observable, then, for any $\lambda > \lambda_0$,

$$e^{\xi_\lambda(x)} \sum_{\substack{\gamma:0\to x \\ S(\gamma)=s}} e^{-\Phi(\gamma)-\lambda|\gamma|} = O(e^{-\nu\|x\|}) + \sum_{m\geq c\|x\|} \mathbb{Q}_\lambda^m\big(D(\gamma)=x, S(\gamma)=s\big)$$

Irreducible decomposition for $\mathbf{G}(x;n)$

In particular, if

$$S(\gamma) = S(\gamma_{\rm L}) + \sum_{i=1}^{m} S(\gamma_i) + S(\gamma_{\rm R}),$$

then

$$e^{\xi_\lambda(x)} \sum_{\substack{\gamma:\,0\to x\\ S(\gamma)=s}} e^{-\Phi(\gamma)-\lambda|\gamma|} = O(e^{-\nu\|x\|}) + \sum_{m\geq c\|x\|} \mathbb{Q}_\lambda^m\Big(F(\gamma_{\rm L}) + \sum_{i=1}^{m} F(\gamma_i) + F(\gamma_{\rm R}) = (x,s)\Big)$$

where $F(\gamma) = (D(\gamma), S(\gamma))$.

Irreducible decomposition for $\mathbf{G}(x;n)$

Now, let $\lambda > \lambda_0$ be s.t. $F \in \partial \mathbf{K}_\lambda$, and let x be s.t.

$$\langle F, x\rangle = \xi_\lambda(x)$$

We then have

$$e^{\langle F,x\rangle}\mathbf{G}(x;n) = e^{\xi_\lambda(x)}\mathbf{G}(x;n)$$

and the previous result applies with $S(\gamma) = |\gamma|$, yielding the desired asymptotics. In particular,

$$\bar{v}_F = \frac{\mathbb{Q}(D(\gamma))}{\mathbb{Q}(|\gamma|)}.$$

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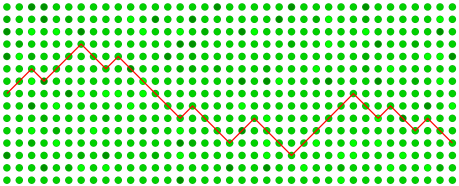
Quenched disorder

As explained before: precise results about the stretched phase for polymers in an **annealed** random potential. What happens in the **quenched** case?

Lot of progress recently, for a fully **directed** version of this model.



Most works rely heavily on **specific martingale structures** present in this version of the model.

Quenched disorder

For $x \in \mathbb{Z}^d$, we write $x = (x^\perp, x^\parallel)$, with $x^\perp \in \mathbb{Z}^{d-1}$ and $x^\parallel \in \mathbb{Z}$.

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Quenched disorder

For $x \in \mathbb{Z}^d$, we write $x = (x^\perp, x^\parallel)$, with $x^\perp \in \mathbb{Z}^{d-1}$ and $x^\parallel \in \mathbb{Z}$.

For $N \in \mathbb{N}$, Let $\mathcal{D}_N$ be the set of n.n. paths $\gamma = (\gamma(0), \dots, \gamma(n))$ on $\mathbb{Z}^d$, $n \in \mathbb{N}$, such that

- $\gamma(0) = 0$,
- $\gamma(n) \in \mathcal{L}_N = \{x \in \mathbb{Z}^d \,:\, x^\parallel = N\}$.

Quenched disorder

We associate to $\gamma \in \mathcal{D}_N$ the weight

$$W^{\omega}_{\lambda,\beta}(\gamma) = \exp\{-\lambda|\gamma| - \beta \sum_{\ell=1}^{n} V^{\omega}(\gamma(\ell))\},$$

where $\lambda > \lambda_0 = \log(2d)$, $\beta > 0$, and the random environment $\{V^{\omega}(x)\}_{x\in\mathbb{Z}^d}$ is assumed to be i.i.d. and s.t.

- $0 \in \mathrm{supp}(V^{\omega}) \subset [0,\infty]$;
- $p = \mathbb{P}(V^{\omega} = \infty)$ is sufficiently small.

Quenched disorder

We associate to $\gamma \in \mathcal{D}_N$ the weight

$$W^{\omega}_{\lambda,\beta}(\gamma) = \exp\Big\{-\lambda|\gamma| - \beta \sum_{\ell=1}^{n} V^{\omega}(\gamma(\ell))\Big\},$$

where $\lambda > \lambda_0 = \log(2d)$, $\beta > 0$, and the random environment $\{V^{\omega}(x)\}_{x\in\mathbb{Z}^d}$ is assumed to be i.i.d. and s.t.

- $0 \in \operatorname{supp}(V^{\omega}) \subset [0,\infty]$;
- $p = \mathbb{P}(V^{\omega} = \infty)$ is sufficiently small.

In particular, the annealed weight $\mathbb{E}(W^{\omega}_{\lambda,\beta}(\gamma))$ is attractive, and the vertices x at which $V^{\omega}(x) = \infty$ do not percolate (a.s.).

Quenched disorder

We introduce the quenched and annealed partition functions

$$\mathfrak{D}_N^\omega = \mathfrak{D}_N^\omega(\lambda, \beta) = \sum_{\gamma \in \mathcal{D}_N} W_{\lambda,\beta}^\omega(\gamma),$$

$$\mathbf{D}_N(\gamma) = \mathbb{E}\mathfrak{D}_N^\omega.$$

For this model, it was shown in [Flury '08, Zygouras '09], under somewhat stronger assumptions on the potential, that the corresponding free energies coincide

$$-\lim_{N\to\infty} \frac{1}{N} \log \mathfrak{D}_N^\omega = \xi = -\lim_{N\to\infty} \frac{1}{N} \log \mathbf{D}_N^\omega,$$

when $d \geq 4$ and β is small enough (and $p = 0$).

Quenched disorder

Our first result is the following strengthening of the latter statement (under our weaker assumptions on V):

Assume that $d \geq 4$, and β and p are small enough. Then the limit

$$\mathfrak{d}^\omega = \lim_{N\to\infty} \frac{\mathfrak{D}_N^\omega}{\mathbf{D}_N}$$

exists $\mathbb{P}$-a.s. and in L^2.
Moreover, $\mathfrak{d}^\omega > 0$, $\mathbb{P}$-a.s., on the event that $0 \in \mathrm{Cl}_\infty(V)$.

Above, $\mathrm{Cl}_\infty(V)$ is the (unique) infinite cluster of vertices for which $V^\omega(x) < \infty$.

Quenched disorder

Our second result extends results for the directed polymer by [Imbrie, Spencer '88] and [Bolthausen '89] to our setting:

Assume that $d \geq 4$, and β and p are small enough. Then, for any bounded continuous function f on $\mathbb{R}^{d-1}$,

$$\mathbb{P}^*\text{-}\lim_{N\to\infty} \sum_{x\in\mathbb{Z}^{d-1}} \mu_N^\omega\big(\pi^\perp(\gamma) = x\big) f(x/\sqrt{N}) = \frac{1}{\sqrt{\det(2\pi\Sigma)}} \int_{\mathbb{R}^{d-1}} f(x) \mathrm{e}^{-\frac{1}{2}\langle \Sigma^{-1}x, x\rangle} \mathrm{d}x.$$

Here Σ is the diffusion matrix of the corresponding annealed polymer model, and $\mathbb{P}^*(\cdot) = \mathbb{P}(\cdot \,|\, 0 \in \mathrm{Cl}_\infty(V))$.

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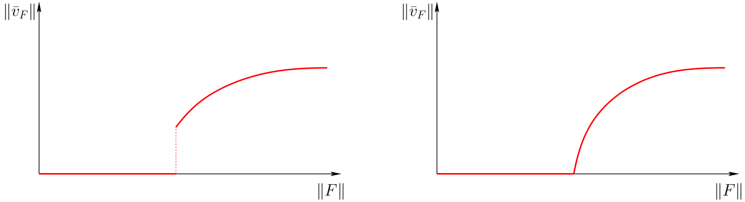
Order of the phase transition in the attractive case

We have seen that, in the attractive case, there is a phase transition between a collapsed and stretched phase. Some related questions (still under investigation):

- Order of the phase transition: apparently always 1st order when $d \geq 2$, but sometimes second order when $d = 1$ (seems to depend on ϕ and even on the temperature!).
- Behaviour at the critical force, when $d \geq 2$.



Quenched random environment

Diffusivity at very high temperature and $d \geq 4$ is OK, but *much* remain to be understood. In particular, it would be very desirable to

- prove diffusivity in the whole weak disorder regime (not only very high temperatures);

Quenched random environment

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- prove diffusivity in the whole weak disorder regime (not only very high temperatures);
- analyze the strong disorder regime: path localization (macroscopic atoms, etc.), effective random walk representation;

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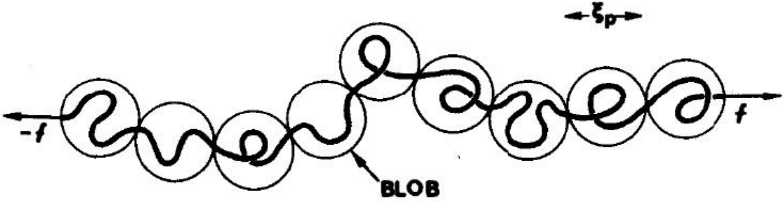
- prove diffusivity in the whole weak disorder regime (not only very high temperatures);
- analyze the strong disorder regime: path localization (macroscopic atoms, etc.), effective random walk representation;
- Extend these results to the stretched case (rather than point-to-plane).

Pincus blob picture

In 1976, when studying the scaling properties of stretched polymers (SAW), Pincus introduced a heuristic "**blob picture**", which has turned out to be very useful in analyzing polymer systems (see de Gennes' book *Scaling Concepts in Polymer Physics*).



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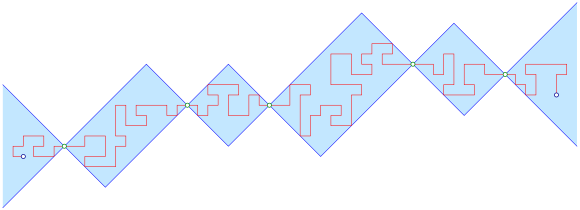

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The main properties assumed by Pincus are

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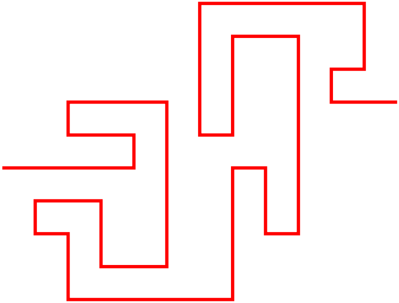
Models with mixed interactions

A widely used model of polymers is that of a SAW with attractive interactions between spatially nearest-neighbour bonds.



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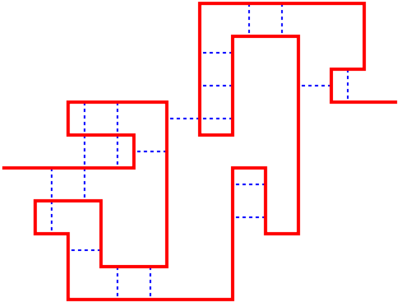

Models with mixed interactions

A widely used model of polymers is that of a SAW with attractive interactions between spatially nearest-neighbour bonds.

- Currently: only SAW with weak attraction.
- Desirable: systems with competing attraction/repulsion.
- Main difficulty: decomposition into irreducible pieces.

The end

Thank you!