Scaling limit for Polymer dynamics in the pinned phase

Hubert Lacoin

CNRS and Université Paris Dauphine

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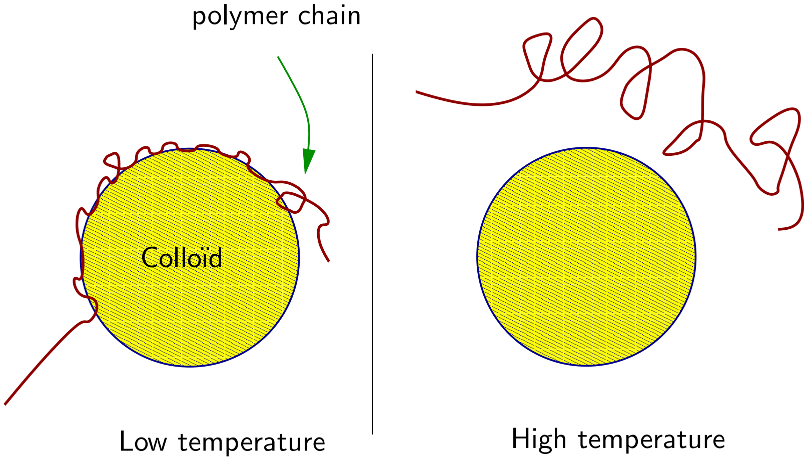
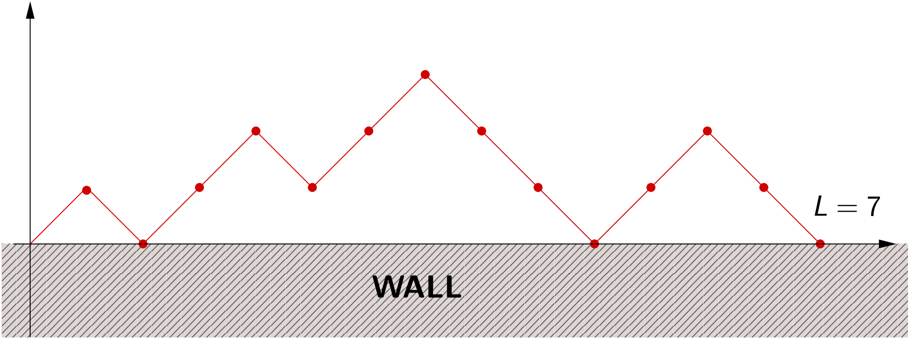
One example for physical motivation : polymers in a solution with colloids

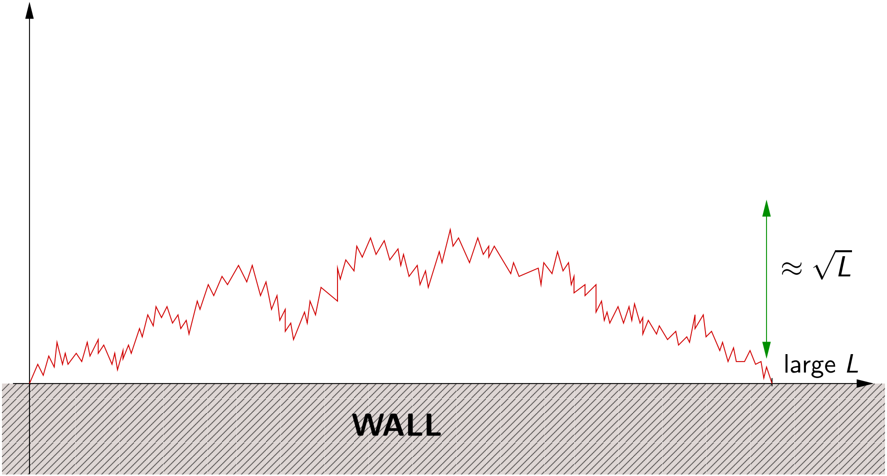


Model with wall



The trajectory is chosen uniformly at random among the $(\eta(x))_{n\in[-L,L]}$ satisfying $(\eta(x+1)-\eta(x))=\pm 1$ and $\eta(x)\geq 0$ for all x and $\eta_{-L}=\eta_L=0$.

Entropic repulsion



Taking into account the polymer/interface interaction

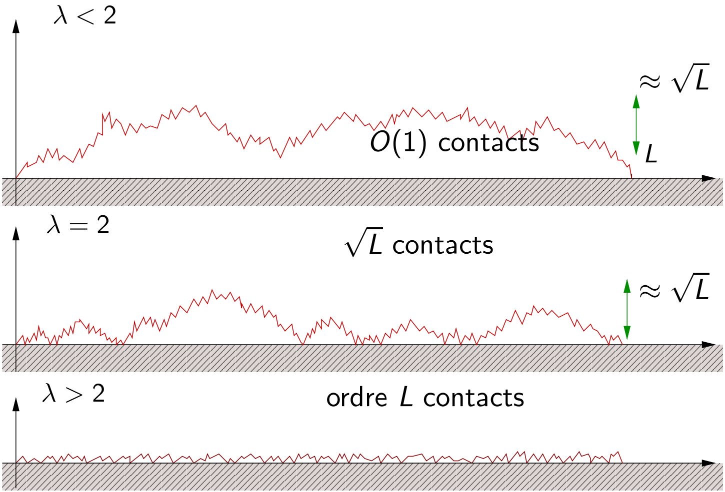
For fixed $\lambda > 0$. We give to each to each trajectory S a weight

$$\pi_L^\lambda(\eta) = \frac{\lambda^{\#\{\text{ contacts of } \eta \text{ with the wall }\}}}{\sum_{\eta' \in \Omega_L} \lambda^{\#\{\text{ contacts of } \eta' \text{ with the wall }\}}}. \tag{1}$$

- $\lambda > 1$ for an attractive interface.
- $\lambda < 1$ for a repulsive interface.

In the case of an attractive interface there is an energy/entropy competition

Typical behaviors



Rescaling

After isotropic space rescaling, at equilibrium, the polymer chain is macroscopically flat.

We wonder what is the macroscopic time-evolution (after proper time rescaling) when starting from a macroscopically non-flat profile, of the polymer measure. For this question to make sense mathematically, we need to introduce a dynamical version of the model, chosen in a way that it is a plausible modelization of the physical evolution.

What a dynamic is

We have to consider a Markov chain on the space of polymer configuration whose equilibrium measure is the polymer measure π_L^λ.

The dynamic

(i) The dynamic we study moves the polymer paths by flipping corners.
(ii) It has been introduced by theorical physicist to model DNA loops evolution.
(iii) Its mixing time properties have been studied by Caputo, Martinelli and Toninelli '08 and CMT+ L, Simenhaus '12.

Scaling limit

We want to start from an η that approximate a macroscopic profile $u_0 : [-1,1] \to \mathbb{R}$:

$$\frac{1}{L}\eta(Lx,0) = u_0(x) + o(1), \forall x \in [-1,1]$$

and one want to find a time scale θ_L and a non-trivial process $u(x,t)$ (deterministic or random) such that

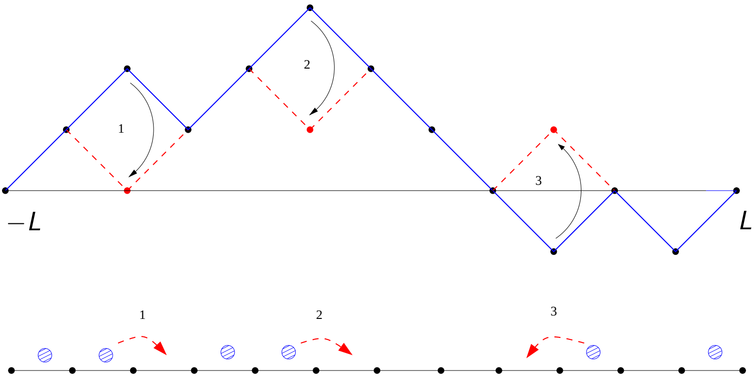
$$\frac{1}{L}\eta(Lx,\theta_L t) = u(x,t) + o(1)$$

with high probability for all $t \in [0, T]$.

Influence of λ

The answer to the question may depend on λ, in particular, it might be qualitatively different when $\lambda < 2$ and $\lambda > 2$ as the equilibrium states differs a lot.

A simpler model : Corner-flip dynamics and correspondance with particle systems



Theorem (L, Simenhaus, Toninelli '12)

Consider u_0 a function $[-1,1] \to \mathbb{R}$, and a sequence of initial condition η_0^L satisfying

$$\lim_{L\to\infty} \max_{x\in[-1,1]} \left| \frac{1}{L} g\eta_0^L(Lx) - u_0(x) \right| = 0$$

Then time scaling is L^2 scaling limit of $\eta^L(t,x)$ is given by u the solution of

$$\begin{cases} \partial_t u & = (\partial_x)^2 u, \quad \forall t \geq 0, x \in (-1,1), \\ u(-1,t) & = u(1,t) = 0, \quad \forall t \geq 0, \\ u(x,0) & = u_0(x), \quad \forall x \geq 0. \end{cases}$$

In the sense that with probability going to one, for all choice of T and ε,

$$\max_{t\leq L^2 T} \max_{x\in[-1,1]} \left| \frac{1}{L} \eta_0^L(Lx, L^2 t) - u(x,t) \right| \leq \varepsilon.$$

Proof of the scaling limit

(i) Show that $(x,t) \mapsto \mathbb{E}[\eta(x,t)]$ satisfies the discrete heat equation, and that once rescaled in time and space this is close to the continuous one.

(ii) Show that

$$L^{-2} \max_{t\in[O,L^2T} \sum_{x=-L}^{L} [\mathbb{E}[\eta(x,t)] - \eta(x,t)]^2$$

goes to zero in probability.

Intuition for the scaling limit with the wall

(i) Time scaling should be the same.

(ii) Around point that do not touch the interface, one should have $\partial_t u = (\partial_x)^2 u$.

(iii) When the polymer is delocalized at equilibrium ($\lambda \leq 2$), the wall is globally repulsive so that one should observe should be macroscopically identical to the case with no wall.

(iv) When the wall is attractive, part of the polymer might want to stick to the wall. and things become harder to guess.

Theorem (The repulsive phase (L 2012))

For the polymer dynamics with wall and and $\lambda \le 1$ (energegetic repulsion), the scaling limit is given by the 1D heat equation with Dirichlet boundary condition as in the case without wall.

$$\begin{cases} \partial_t u & = (\partial_x)^2 u, \quad \forall t \ge 0, x \in (-1,1), \\ u(-1,t) & = u(1,t) = 0, \quad \forall t \ge 0, \\ u(x,0) & = u_0(x), \quad \forall x \ge 0. \end{cases}$$

The attractive phase $\lambda = \infty$

Proposition (inspired from Caputo Martinelli Toninelli '06)

Let $A(\eta)$ be the area below the curve i.e.

$$A(\eta) := \sum_{x=-L}^{L} \eta_x(t) \tag{2}$$

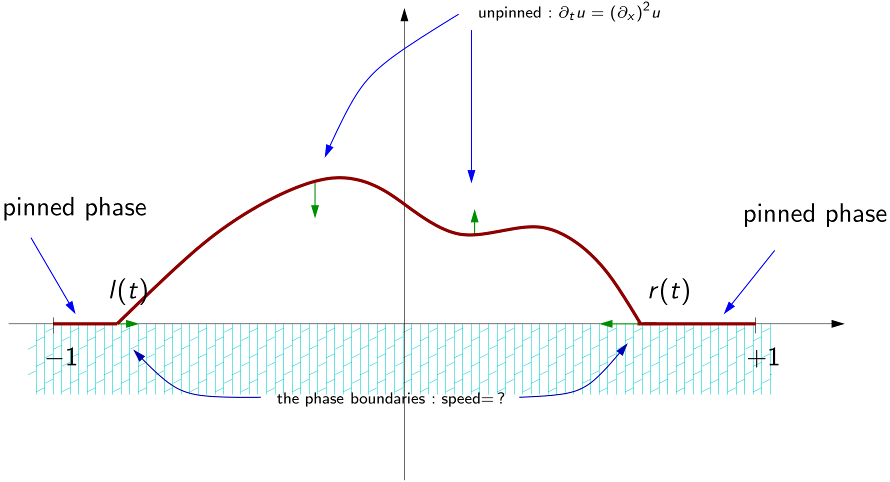
then one has w.h.p for all time

$$A(\eta(t)) \leq \min\left(A(\eta_0) - 2t + L^{7/4}, L\right). \tag{3}$$

In particular w.h.p the dynamics terminates before time

$$A(\eta(0))/2 + L^{3/4} = O(L^2)$$

On the other side if the dynamics start from an initial condition with $A(\eta(0)) = \Omega(L^2)$, the dynamics takes a time $\Omega(L^2)$ to stop.


unpinned : $\partial_t u = (\partial_x)^2 u$
pinned phase
pinned phase
$l(t)$
$r(t)$
-1
$+1$
the phase boundaries : speed= ?

Consider the following free boundary problem

$$\begin{cases} \partial_t u & = (\partial_x)^2 u, \quad \forall t \geq 0, x \in (l(t), r(t)), \\ u(t,x) & = 0 \quad \forall t \geq 0, x \in [-1,1] \setminus (l(t), r(t)), \\ \partial_x u(l(t),t) & = -\partial_x u(r(t),t) = -1, \\ \partial_t l(t) & = -(\partial_x)^2 u(l(t),t), \quad \partial_t r(t) = (\partial_x)^2 u(r(t),t), \\ u(x,0) & = u_0(x), \quad -l(0) = r(0) = 1. \end{cases} \tag{4}$$

This problem seems hill-posed, and in particular there seems to be too many boundary condition. However, with some condition on the initial condition there exist a unique smooth solution to it.

Theorem (Corollary of a result from Chayes, Kim '08)

If $u : [-1, 1] \to \mathbb{R}$ is continuous, 1-Lipshitz, positive on $(-1, 1)$ and symetric and unimodal. Then there exists a unique solution to the considered Stefan Problem, until positive time. Moreover, in that case u, r and l are $\mathcal{C}^\infty$ (in time and space).

The solution exists until time $T_0 := \int_{-1}^{1} u(x)\,\mathrm{d}x/2$, at which $r(t)$ and $l(t)$ join.

Remark

Existence of solution should hold in a much more general setup. The only condition that is essencial is positivity : this can be seen from the expression of T_0.

Theorem (L '12)

Let us consider the dynamics with wall and $\lambda = \infty$, started from a sequence of initial condition satisfying

$$\lim_{L\to\infty} \max_{x\in[-1,1]} \left| \frac{1}{L}\eta_0^L(Lx) - u_0(x) \right| = 0$$

Then with probability going to one, for all choice of ε,

$$\max_{t\geq 0} \max_{x\in[-1,1]} \max_{x\in[-1,1]} \left| \frac{1}{L}\eta_0^L(Lx, L^2 t) - u(x,t) \right| \leq \varepsilon. \tag{5}$$

and further more the dynamic stops after a time $L^2 \int_{-1}^{1} u_0(x)\,\mathrm{d}x(1+o(1))$.

Conjectures : the repulsive phase

Our reasonning concerning the repulsive phase does not work when delocalization holds because of entropic repulsion. However we believe that this case $\lambda \in (1, 2]$ is not different from the case where $\lambda \leq 1$ and that we should observe the same scaling limit.

Conjectures : the attractive phase

When $\lambda > 2$, the dynamic belong to the same university class than when $\lambda = \infty$. The scaling limit should essentially be the same except that

(i) The slope at the interphase should not be one but the slope corresponding to local equilibrium of the polymer.

(ii) The drift of the boundary should be equal to $\pm(\partial_x)^2 u/d(\lambda)$.

However the proof of the case $\lambda = \infty$ cannot adapt because the special argument concerning the volume is specific to that case.