

Entropic repulsion and metastability in the solid-on-solid (SOS) model

P. Caputo,
joint with F.Martinelli, E.Lubetzky, F.L.Toninelli, A.Sly

Roscoff - June 27, 2012

Plan

- SOS: a random interface model
- Heat Bath Dynamics: Poincaré inequality
- Open problems and conjectures
- SOS with a wall. Entropic repulsion
- Dynamics of entropic repulsion: Metastability
- Exponentially large relaxation times
- Methods

(2+1)Dimensional SOS model

Discrete height: $\varphi = \{\varphi_x, x \in \mathbb{Z}^2\}$, with $\varphi_x \in \mathbb{Z}$.

Λ square of side L in \mathbb{Z}^2 centered at 0.

0 boundary condition: $\varphi_x = 0$ for all $x \in \mathbb{Z}^2 \setminus \Lambda$.

Gibbs measure: $\beta > 0$

$$\pi(\varphi) = \pi_{\beta,L}(\varphi) = \frac{1}{Z_{\beta,L}} \exp\left(-\beta \sum_{x \sim y} |\varphi_x - \varphi_y|\right)$$

(2+1)Dimensional SOS model

Discrete height: $\varphi = \{\varphi_x, x \in \mathbb{Z}^2\}$, with $\varphi_x \in \mathbb{Z}$.

Λ square of side L in \mathbb{Z}^2 centered at 0.

0 boundary condition: $\varphi_x = 0$ for all $x \in \mathbb{Z}^2 \setminus \Lambda$.

Gibbs measure: $\beta > 0$

$$\pi(\varphi) = \pi_{\beta,L}(\varphi) = \frac{1}{Z_{\beta,L}} \exp\left(-\beta \sum_{x \sim y} |\varphi_x - \varphi_y|\right)$$

Roughening transition:

Low temperature (large β , rigid phase): localization

$\pi_{\beta,L}(\varphi_0^2) \leq C_\beta$ (exponential tails, via Peierls argument)

High temperature (small β , rough phase): delocalization

$\pi_{\beta,L}(\varphi_0^2) \sim \log L$ (very hard ! see Frohlich-Spencer CMP 1981).

[One expects Gaussian fluctuations]

Heat bath dynamics of SOS model

Cont. time π -reversible Markov chain with generator

$$\mathcal{L}f(\varphi) = \sum_{x \in \Lambda} [\pi(f | \varphi_{\Lambda \setminus \{x\}}) - f(\varphi)].$$

Dirichlet form $\mathcal{E}(f, f) = \sum_{x \in \Lambda} \pi [\text{Var}_x(f)]$

where $\text{Var}_x(f) = \text{Var}_\pi(f | \varphi_{\Lambda \setminus \{x\}})$.

[Glauber dynamics, Gibbs sampler]

Heat bath dynamics of SOS model

Cont. time π -reversible Markov chain with generator

$$\mathcal{L}f(\varphi) = \sum_{x \in \Lambda} [\pi(f | \varphi_{\Lambda \setminus \{x\}}) - f(\varphi)].$$

Dirichlet form $\mathcal{E}(f, f) = \sum_{x \in \Lambda} \pi [\text{Var}_x(f)]$

where $\text{Var}_x(f) = \text{Var}_\pi(f | \varphi_{\Lambda \setminus \{x\}})$.

[Glauber dynamics, Gibbs sampler]

Poincaré inequality: find $\gamma(L, \pi) > 0$ such that for all $f \in L^2(\pi)$:

$$\text{Var}_\pi(f) \leq \gamma(L, \pi) \mathcal{E}(f, f)$$

$\gamma(L, \pi)$ is the *Relaxation Time*, inverse of *Spectral Gap*.

Heat bath dynamics of SOS model

Cont. time π -reversible Markov chain with generator

$$\mathcal{L}f(\varphi) = \sum_{x \in \Lambda} [\pi(f | \varphi_{\Lambda \setminus \{x\}}) - f(\varphi)].$$

Dirichlet form $\mathcal{E}(f, f) = \sum_{x \in \Lambda} \pi [\text{Var}_x(f)]$

where $\text{Var}_x(f) = \text{Var}_\pi(f | \varphi_{\Lambda \setminus \{x\}})$.

[Glauber dynamics, Gibbs sampler]

Poincaré inequality: find $\gamma(L, \pi) > 0$ such that for all $f \in L^2(\pi)$:

$$\text{Var}_\pi(f) \leq \gamma(L, \pi) \mathcal{E}(f, f)$$

$\gamma(L, \pi)$ is the *Relaxation Time*, inverse of *Spectral Gap*.

Open problem: prove that $\gamma(L, \pi)$ is polynomial in L

Remarks on the continuous SOS model

Same problem, but now $\varphi_x \in \mathbb{R}$ and

$$\pi(\varphi) = \frac{1}{Z_{\beta,L}} \exp\left(-\beta \sum_{x \sim y} |\varphi_x - \varphi_y|\right)$$

is a **log-concave** probability on \mathbb{R}^Λ .

No roughening transition in the continuous model:

Surface is always rough in 2D. Expected: $\pi(\varphi_0^2) \sim \log L$.

Remarks on the continuous SOS model

Same problem, but now $\varphi_x \in \mathbb{R}$ and

$$\pi(\varphi) = \frac{1}{Z_{\beta,L}} \exp\left(-\beta \sum_{x \sim y} |\varphi_x - \varphi_y|\right)$$

is a **log-concave** probability on \mathbb{R}^Λ .

No roughening transition in the continuous model:

Surface is always rough in 2D. Expected: $\pi(\varphi_0^2) \sim \log L$.

Dynamics:

Langevin diffusion (SDE): $\mathcal{E}(f, f) = \sum_{x \in \Lambda} \pi [(\nabla_x f)^2]$

Poincaré inequality:

$$\text{Var}_\pi(f) \leq \gamma(L, \pi) \mathcal{E}(f, f)$$

Expected: $\gamma(L, \pi) = O(L^2)$.

As in Gaussian free field case.

Similar bound expected for heat bath dynamics

(as in discrete model): $\mathcal{E}(f, f) = \sum_{x \in \Lambda} \pi [\text{Var}_x(f)]$

(1 + 1)D SOS Model

$$\varphi = \{\varphi_i, i = 1, \dots, L\}: \quad \nu_i(d\eta_i) = \frac{e^{-\beta\eta_i}}{Z} d\eta_i,$$

$$\pi = \otimes_{i=1}^{L-1} \nu_i \left(\cdot \mid \sum_i \eta_i = 0 \right), \quad \eta_i := \varphi_{i+1} - \varphi_i.$$

Continuous heights: $\varphi_i \in \mathbb{R}$, then $\gamma(L, \pi) = O(L^2)$
[Barthe-E.Milman; Barthe-Cordero Erasquin, Barthe-Wolff]

Discrete heights: $\varphi_i \in \mathbb{Z}$, then $\gamma(L, \pi) = O(L^2)$
[Martinelli-Sinclair]

Metropolis chain with ± 1 height updates:

$$\mathcal{E}(f, f) = \sum_x \pi [c_x (\nabla_x f)^2] \quad (\text{discrete gradient})$$

C-Martinelli-Toninelli: $\gamma(L, \pi) = O(L^2(\log L)^c)$
(motion by mean curvature).

$(2 + 1)$ D SOS (discrete) with a wall: Entropic repulsion

$\varphi_x \in \mathbb{Z}$ and

$$\pi_+(\varphi) = \pi(\varphi \mid \varphi_x \geq 0 \quad \forall x \in \Lambda)$$

Entropic repulsion **heuristics** (β large):

- shift heights $h \rightarrow h + 1$ at **energy loss** $-4\beta L$ (boundary)
- full downward spikes at x give the **gain in entropy** $+L^2 e^{-4\beta h}$.
- surface grows until $4\beta L \approx L^2 e^{-4\beta h}$ or $h \approx H(L) := \frac{1}{4\beta} \log L$.

$(2 + 1)$ D SOS (discrete) with a wall: Entropic repulsion

$\varphi_x \in \mathbb{Z}$ and

$$\pi_+(\varphi) = \pi(\varphi \mid \varphi_x \geq 0 \ \forall x \in \Lambda)$$

Entropic repulsion **heuristics** (β large):

- shift heights $h \rightarrow h + 1$ at **energy loss** $-4\beta L$ (boundary)
- full downward spikes at x give the **gain in entropy** $+L^2 e^{-4\beta h}$.
- surface grows until $4\beta L \approx L^2 e^{-4\beta h}$ or $h \approx H(L) := \frac{1}{4\beta} \log L$.

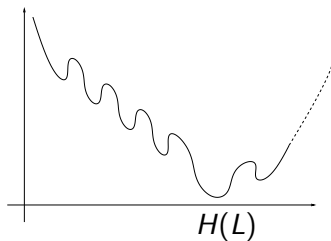
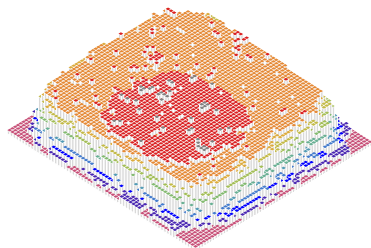
Theorem

For any $\beta \geq \beta_0$, $k \geq k_0$:

$$\pi_+ \left(\#\left\{x \in \Lambda : \varphi_x \notin [H(L) - k, H(L) + k]\right\} > e^{-2\beta k} L^2 \right) \leq e^{-cL}.$$

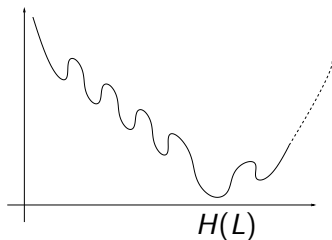
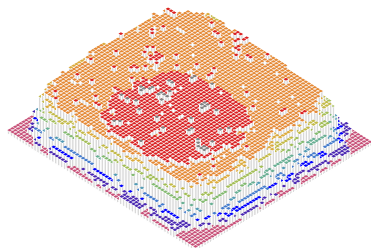
Metastability

A deeper analysis of the **free energy** landscape reveals **metastable** behavior:



Metastability

A deeper analysis of the **free energy** landscape reveals **metastable** behavior:



Theorem

Start heat bath dynamics at $\varphi \equiv 0$.

For $a \in (0, 1]$, let $\tau_a = \min\{t > 0 : \varphi(t) \in \Omega_a\}$ where $\Omega_a = \{\varphi : \#\{x : \varphi_x \geq aH(L)\} > 0.9L^2\}$.

Then $\lim_{L \rightarrow \infty} \pi_+(\Omega_a) = 1$ and yet

$$\lim_{L \rightarrow \infty} \mathbb{P}\left(e^{cL^a} \leq \tau_a \leq e^{(1/c)L^a}\right) = 1.$$

Mixing time bounds

SOS model with wall and ceiling

$$\pi_{+,b}(\varphi) = \pi(\varphi \mid 0 \leq \varphi_x \leq L, \forall x \in \Lambda)$$

Heat bath is then a Markov chain with finite state space.

$$T_{\text{mix}}(L) = \inf \left\{ t > 0 : \max_{\varphi} \|p_t(\varphi, \cdot) - \pi_{+,b}\|_{\text{TV}} \leq \frac{1}{2} \right\}$$

From standard bounds:

$$\gamma(L, \pi_{+,b}) \leq c T_{\text{mix}}(L) \leq c' L^3 \gamma(L, \pi_{+,b}).$$

Mixing time bounds

SOS model with wall and ceiling

$$\pi_{+,b}(\varphi) = \pi(\varphi \mid 0 \leq \varphi_x \leq L, \forall x \in \Lambda)$$

Heat bath is then a Markov chain with finite state space.

$$T_{\text{mix}}(L) = \inf \left\{ t > 0 : \max_{\varphi} \|p_t(\varphi, \cdot) - \pi_{+,b}\|_{\text{TV}} \leq \frac{1}{2} \right\}$$

From standard bounds:

$$\gamma(L, \pi_{+,b}) \leq c T_{\text{mix}}(L) \leq c' L^3 \gamma(L, \pi_{+,b}).$$

Theorem

For any $\beta \geq \beta_0$, $\exists c > 0$:

$$e^{cL} \leq T_{\text{mix}}(L) \leq e^{(1/c)L}.$$

Spectral gap bounds

Without ceiling (π_+). Suitable recursive analysis shows that

$$\gamma(L, \pi_+) \approx \gamma(L, \pi_{+,b})$$

Then from previous theorem, one has

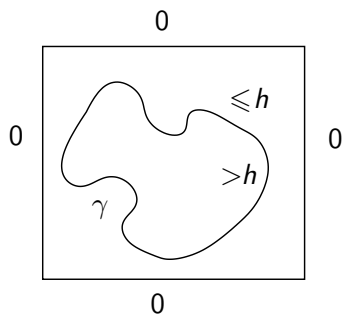
$$e^c L \leq \gamma(L, \pi_+) \leq e^{(1/c)L}.$$

Without wall (π). Expect **polynomial** $\gamma(L, \pi)$. We prove
Theorem

$$\gamma(L, \pi) \leq e^{L^{5/6}}.$$

Methods 1

Equilibrium estimates for $\pi, \pi_+, \pi_{+,b}$: Monotonicity, FKG inequalities, Peierls type estimates (contour estimates)



$$\pi_+(\gamma \text{ is an } h\text{-contour}) \leq \exp \left\{ -\beta|\gamma| + c \text{Area}(\gamma)e^{-4\beta h} \right\}.$$

Methods 2

Metastability analysis and lower bounds on mixing times:

Refined equilibrium bounds to quantify bottlenecks

Main idea: Fix $h = aH(L) = \frac{a}{4\beta} \log L$.

Restricted ensemble $\pi_A = \pi_+(\cdot | A)$, where A is the event that all h contours γ have $\text{Area}(\gamma) \leq \delta L^{2a}$, δ small.

Then in π_A :

- 1) all h contours have area less than $(\log L)^2$ w.h.p.
- 2) $\pi_A(\partial A) \leq e^{-cL^a}$
- 3) $\pi_A(\text{large density of heights at least } h + 1) \leq e^{-cL^a}$

This establishes bottleneck:

$\tau_a \geq e^{cL^a}$ w.h.p. when started from $\varphi \equiv 0$.

Methods 3

Upper bounds on mixing times: coupling arguments, with monotonicity and a *standard canonical paths* technique yield the upper bound

$$T_{\text{mix}}(L) \leq e^{cL \log L}$$

To obtain $T_{\text{mix}}(L) \leq e^{cL}$ much more work is needed.

Main steps:

- Improved *canonical paths* argument: define reduced space $G \subset \Omega$ such that on G canonical paths gives $T_{\text{mix}}(L; G) \leq e^{cL}$.
- If T_G is time needed to enter G with probab. α , then $T_{\text{mix}}(L) \leq c(\alpha)(T_G^2 + T_{\text{mix}}(L, G))$.
- Show that uniformly in initial condition, the process enters G within time $e^{cL} \sim T_G$ with probab. at least $1/2 \sim \alpha$.
- *Cluster expansion* tools to have fine control of the statistics of SOS contours.