Phase transition in kinetically constrained dynamics

T. Bodineau, C. Toninelli

INHOMOGENEOUS RANDOM SYSTEMS – January 2011

Outline

- Kinetically constrained dynamics
- Non-equilibrium phase transitions
- Analogy with Ising model
- Proofs

Glasses

Key properties.

- huge increase of relaxation time as the temperature decays
- dynamical heterogeneities
- ageing

Kinetically constrained dynamics

➪ Simple lattice models of glass forming systems at high density
➪ Rich dynamical behavior (cooperative relaxation ...)
➪ Trivial thermodynamics

Glasses

Key properties.

- huge increase of relaxation time as the temperature decays
- dynamical heterogeneities
- ageing

Kinetically constrained dynamics

➪ Simple lattice models of glass forming systems at high density
➪ Rich dynamical behavior (cooperative relaxation ...)
➪ Trivial thermodynamics

Glasses

Key properties.

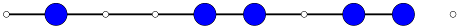
- huge increase of relaxation time as the temperature decays
- dynamical heterogeneities
- ageing

Kinetically constrained dynamics

➪ Simple lattice models of glass forming systems at high density
➪ Rich dynamical behavior (cooperative relaxation ...)
➪ Trivial thermodynamics

East model

Markov chain: $\eta(t) = \{\eta_i(t)\}_{1 \leq i \leq N}$ with $\eta_i \in \{0,1\}$

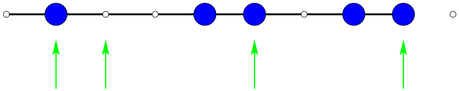


Transition rules.

- A site can be updated **only if** its East neighbor is empty
- Update rates : $0 \xrightarrow{\rho} 1$ and $0 \xleftarrow{1-\rho} 1$

East model

Markov chain: $\eta(t) = \{\eta_i(t)\}_{1 \le i \le N}$ with $\eta_i \in \{0, 1\}$

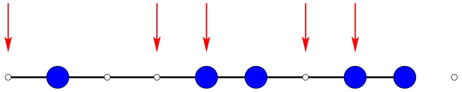


Transition rules.

- A site can be updated **only if** its East neighbor is empty
- Update rates : $0 \stackrel{\rho}{\longrightarrow} 1$ and $0 \stackrel{1-\rho}{\longleftarrow} 1$

East model

Markov chain: $\eta(t) = \{\eta_i(t)\}_{1 \le i \le N}$ with $\eta_i \in \{0, 1\}$

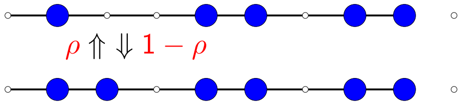


Transition rules.

- A site can be updated **only if** its East neighbor is empty
- Update rates : $0 \xrightarrow{\rho} 1$ and $0 \xleftarrow{1-\rho} 1$

East model

Markov chain: $\eta(t) = \{\eta_i(t)\}_{1 \le i \le N}$ with $\eta_i \in \{0,1\}$



Transition rules.

- A site can be updated **only if** its East neighbor is empty
- Update rates : $0 \overset{\rho}{\to} 1$ and $0 \overset{1-\rho}{\leftarrow} 1$

The markov chain is reversible wrt

$$\mu_N = \bigotimes_{i=1}^{N} \nu_\rho(\eta_i) \quad \text{with} \quad \nu_\rho(1) = 1 - \nu_\rho(0) = \rho$$

Works on kinetically constrained models

Huge class of models, with various constrained.

Many results on

- Ergodicity (➪ phase transition)
- Spectral gap
- Relaxation to equilibrium
- .....

Question.
Can we find a **dynamical free energy** characterizing glassiness?

[Garrahan, Jack, Lecomte, Pitard, van Duijvendijk, van Wijland]

Works on kinetically constrained models

Huge class of models, with various constrained.

Many results on

- Ergodicity (➪ phase transition)
- Spectral gap
- Relaxation to equilibrium
- .....

Question.
Can we find a **dynamical free energy** characterizing glassiness?

[Garrahan, Jack, Lecomte, Pitard, van Duijvendijk, van Wijland]

Activity

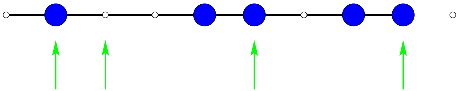
Dynamical parameter to characterize the

- dynamical heterogeneities
- jammed configurations

$\mathcal{A}_i(t) = \{$ Number of flips at site i during the time interval $[0,t]\}$

Total activity : $$\mathcal{A}(t) = \sum_i \mathcal{A}_i(t)$$

East model: $$\mathbb{E}_{\mu_N}\big(\mathcal{A}(t)\big) = t(N-1)\rho(1-\rho)^2 + t\rho(1-\rho)$$



Large deviations

Mean activity: $\mathbb{A} = \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{N}\mathbb{E}_{\mu_N}\big(\mathcal{A}(t)\big)$

Question.

$$a \neq \mathbb{A}, \qquad \mathbb{E}_{\mu_N}\Big(\frac{1}{t}\mathcal{A}(t) \simeq a\Big) \approx \exp(-Nt\,\mathcal{F}(a))$$

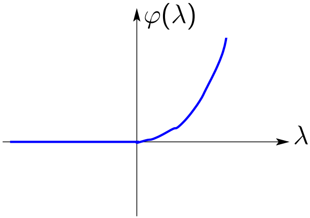
Large deviations

Mean activity: $\mathbb{A} = \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{N}\mathbb{E}_{\mu_N}\big(\mathcal{A}(t)\big)$

Question.

$$a \neq \mathbb{A}, \qquad \mathbb{E}_{\mu_N}\Big(\frac{1}{t}\mathcal{A}(t) \simeq a\Big) \approx \exp(-Nt\,\mathcal{F}(a))$$

$$\text{For}\lambda \in \mathbb{R}, \qquad \varphi(\lambda) = \lim_{N\to\infty}\lim_{t\to\infty}\frac{1}{Nt}\log\mathbb{E}_{\mu_N}\Big(\exp\big(\lambda\mathcal{A}(t)\big)\Big)$$



Phase transition.

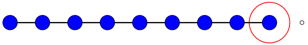
[Garrahan, Jack, Lecomte, Pitard, van Duijvendijk, van Wijland]

Heuristics

$$\lambda \in \mathbb{R}, \qquad \varphi(\lambda) = \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{Nt} \log \mathbb{E}_{\mu_N} \left(\exp\left(\lambda \mathcal{A}(t) \right) \right)$$

First order phase transition.

- $\lambda > 0$ then the activity is increased : no singularity
- $\lambda < 0$ then the activity is suppressed



$t = 0$: configuration totally filled

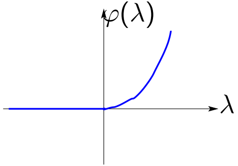
$t > 0$: system is forbidden to move

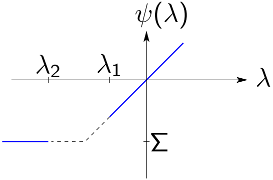
$$\mathbb{E}_{\mu_N} \left(\mathcal{A}(t) = 0 \right) \approx \rho^N \exp(-(1-\rho)t)$$

Finite size scaling

$$\lambda \in \mathbb{R}, \qquad \varphi(\lambda) = \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{Nt} \log \mathbb{E}_{\mu_N} \left(\exp\left(\lambda \mathcal{A}(t) \right) \right)$$

$$\psi(\lambda) = \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}_{\mu_N} \left(\exp\left(\frac{\lambda}{N} \mathcal{A}(t) \right) \right)$$





Theorem.

There are $\lambda_2 \leq \lambda_1 < 0$ such that

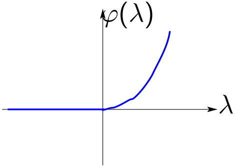
$$\forall \lambda > \lambda_1, \qquad \psi(\lambda) = \mathbb{A}\lambda,$$

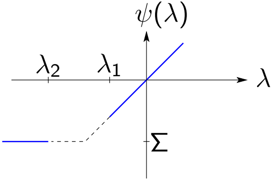
$$\forall \lambda < \lambda_2, \qquad \psi(\lambda) = \Sigma\,.$$

Finite size scaling

$$\lambda \in \mathbb{R}, \qquad \varphi(\lambda) = \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{Nt} \log \mathbb{E}_{\mu_N} \left(\exp\left(\lambda \mathcal{A}(t)\right)\right)$$

$$\psi(\lambda) = \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}_{\mu_N} \left(\exp\left(\frac{\lambda}{N} \mathcal{A}(t)\right)\right)$$





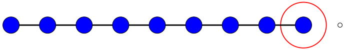
If there was no transition, then

$$\psi(\lambda) \simeq N\varphi(\frac{\lambda}{N}) = N\left[\varphi(0) + \varphi'(0)\frac{\lambda}{N} + O\left(\frac{1}{N^2}\right)\right] = \varphi'(0)\lambda + O\left(\frac{1}{N}\right)$$

As $\varphi'(0) = \mathbb{A} \quad \Rightarrow \qquad \psi(\lambda) \simeq \mathbb{A}\lambda$

Surface tension

$$\lambda < \lambda_2, \qquad \psi(\lambda) = \lim_{N \to \infty} \lim_{t \to \infty} \frac{1}{t} \log \mathbb{E}_{\mu_N} \Big(\exp \big(\frac{\lambda}{N} \mathcal{A}(t) \big) \Big)$$

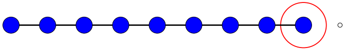


Blocking the whole system :

$$\mathbb{E}_{\mu_N} \left(\mathcal{A}(t) = 0 \right) \approx \rho^N \exp(-(1-\rho)t)$$

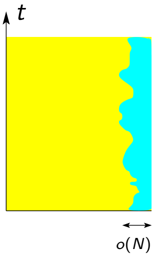
Surface tension

$$\lambda < \lambda_2, \qquad \psi(\lambda) = \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}_{\mu_N}\left(\exp\left(\frac{\lambda}{N}\mathcal{A}(t)\right)\right)$$



Blocking the whole system :

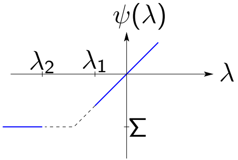
$$\mathbb{E}_{\mu_N}\left(\mathcal{A}(t)=0\right) \approx \rho^N \exp(-(1-\rho)t)$$



Surface tension : $\Sigma \in]0, 1-\rho[$

$$\mathbb{E}_{\mu_N}\left(\exp\left(\frac{\lambda}{N}\mathcal{A}(t)\right)\right) \approx \exp(-\Sigma t)$$

Cost of maintaining an interface during time t



Tilted measures.

$$\mu_{N,\lambda,t}(\,\cdot\,) = \frac{\mathbb{E}_{\mu_N}(\cdot\ \exp(\frac{\lambda}{N}\mathcal{A}(t)))}{\mathbb{E}_{\mu_N}(\exp(\frac{\lambda}{N}\mathcal{A}(t)))}$$

Theorem: density profiles

There are $\lambda_2 \leq \lambda_1 < 0$ such that

$$\forall \lambda > \lambda_1, \qquad \mu_{N,\lambda,T}\Big(\frac{1}{NT}\int_0^T dt \sum_i \eta_i(t) \in [\rho - \delta_N, \rho + \delta_N]\Big) \overset{T\to\infty}{\longrightarrow} 1$$

$$\forall \lambda < \lambda_2, \qquad \mu_{N,\lambda,T}\Big(\frac{1}{NT}\int_0^T dt \sum_i \eta_i(t) \geq (1 - \delta_N)\Big) \overset{T\to\infty}{\longrightarrow} 1$$

with $\delta_N \to 0$ as $N \to \infty$.

Consequence : anomalous large deviation scaling

Large deviations for reducing the activity. Fix $0 \le u < 1$

$$-\Sigma(1-u) \le \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{t} \log \mathbb{P}_{\mu_N}\left(\frac{\mathcal{A}(t)}{N\ t} \approx u\mathbb{A} \right) \le \lambda_1 \mathbb{A}(1-u)$$

Dynamics without constraints

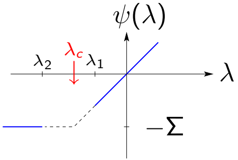
$$\lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{tN} \log \mathbb{P}_{\mu_N}\left(\frac{\mathcal{A}(t)}{N\ t} \approx u\mathbb{A} \right) = F(u) \neq 0$$

Other dynamics

Theorem valid for a larger class of 1D dynamics.

Fredrickson Andersen model (FA-1f)

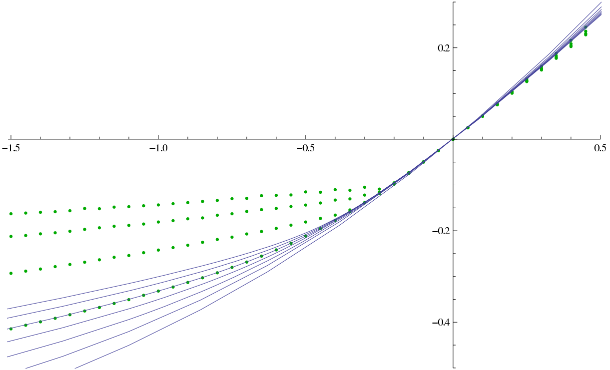
- A site can be updated **only if** a neighbor is empty
- Update rates : $0 \xrightarrow{\rho} 1$ and $0 \xleftarrow{1-\rho} 1$



Question. Extending the results up to λ_c ?

$$\lambda_c = -\frac{\Sigma}{\mathbb{A}}$$

Simulations FA-1f



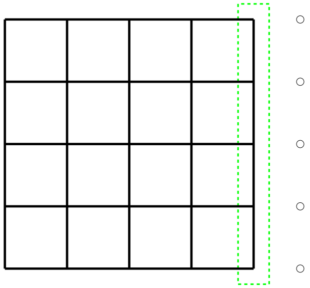
Sizes : 4, 5, 6, 7, 8, 10 and 16, 32, 64

Work in progress [B., Lecomte, Toninelli]

Higher Dimensions

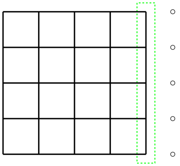
East Model in $\{1, N\}^2 \Leftrightarrow N$ independent East Models in $\{1, N\}$

$$\psi^{(2D)}(\lambda) = \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{tN} \log \mathbb{E}_{\mu_N}\left(\exp\left(\frac{\lambda}{N}\mathcal{A}(t)\right)\right) = \psi^{(1D)}(\lambda)$$

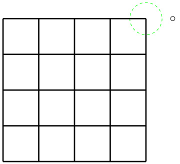


FA-1f in higher Dimensions

Finite size scaling is sensitive to boundary conditions



$$\lim_{N\to\infty}\lim_{t\to\infty}\frac{1}{tN}\log\mathbb{E}_{\mu_N}\left(\exp\left(\frac{\lambda}{N}\mathcal{A}(t)\right)\right)$$

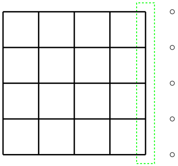


$$\lim_{N\to\infty}\lim_{t\to\infty}\frac{1}{t}\log\mathbb{E}_{\mu_N}\left(\exp\left(\frac{\lambda}{N^2}\mathcal{A}(t)\right)\right)$$

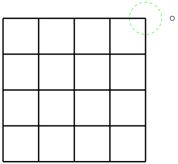
Only partial results on the inactive regime.

FA-1f in higher Dimensions

Finite size scaling is sensitive to boundary conditions



$$a < \mathbb{A}, \qquad \lim_{N \to \infty} \lim_{t \to \infty} \frac{1}{t N} \log \mathbb{P}_{\mu_N} \left(\frac{\mathcal{A}(t)}{N^2 t} \approx a \right)$$



$$a < \mathbb{A}, \qquad \lim_{N \to \infty} \lim_{t \to \infty} \frac{1}{t} \log \mathbb{P}_{\mu_N} \left(\frac{\mathcal{A}(t)}{N^2 t} \approx a \right)$$

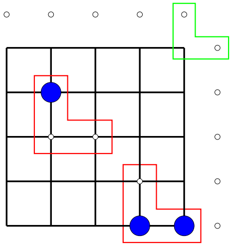
Consequence

Different large deviation scalings

The constraint matters

North-East model.

- North and East sites empty
- $0 \xrightarrow{\rho} 1$ and $0 \xleftarrow{1-\rho} 1$



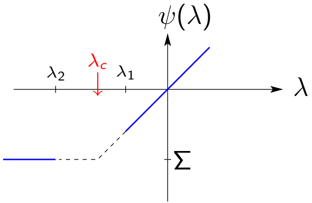
$$\psi^{(NE)}(\lambda) \stackrel{?}{=} \lim_{N\to\infty} \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}_{\mu_N} \left(\exp\left(\frac{\lambda}{N^2} \mathcal{A}(t) \right) \right) .$$

What did we learn ?

Question.

Can we find a **dynamical free energy** characterizing glassiness?

First order phase transition.



Finite size scaling :

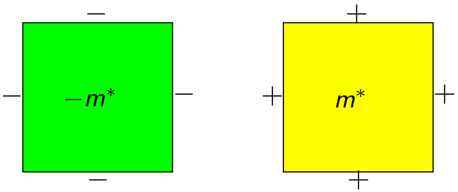
Shift of the critical value

Can one predict something by looking at the activity at $\lambda = 0$?

Box: $\Lambda_N = \{-N, N\}^2$,
Spins : $\sigma = \{\sigma_i\}_{i \in \Lambda_N}$ with $\sigma_i \in \{-1, 1\}$

Hamiltonian: $$\mathcal{H}(\sigma) = - \sum_{\substack{i \sim j \\ i,j \in \Lambda_N}} \sigma_i \sigma_j - \sum_{i \in \Lambda_N} h_i \, \sigma_i$$

Gibbs measure: $$\mu_{T,N}(\sigma) = \frac{1}{Z_{T,N}} \exp\left(-\frac{1}{T} \mathcal{H}(\sigma) \right)$$

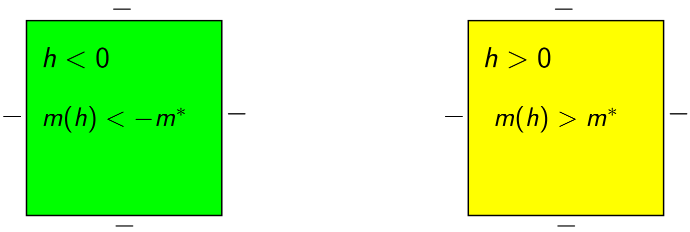


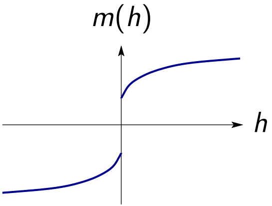
$T < T_c$: phase transition

$h_i = 0$ for i away from the boundary.

First order phase transition

For $T < T_c$

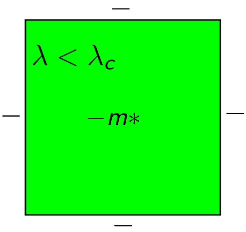


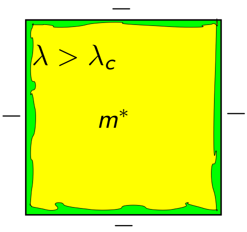


$m(h)$: magnetization in the infinite volume with field h.

Finite size scaling

For $T < T_c$. Rescaled magnetic field $h = \frac{\lambda}{N} > 0$





Shift of the free energy :

$$-N^2 m^* \frac{\lambda}{N}$$

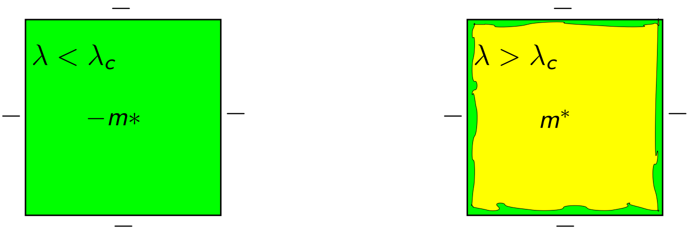
Shift of the free energy :

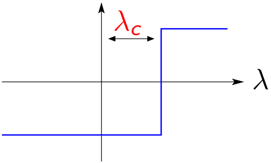
$$N^2 m^* \frac{\lambda}{N} - \tau N$$

Critical parameter : $\lambda_c = \frac{\tau}{2m^*}$

Finite size scaling

For $T < T_c$. Rescaled magnetic field $h = \frac{\lambda}{N} > 0$





[Schonmann, Shlosman]
[Borgs, Kotecky]
[Borgs, Imbrie] ...

Ingredients of the proof

- Donsker-Varadhan large deviation principle
- Local equilibrium (Hydrodynamic theory)
- Surface tension (Equilibrium phase coexistence)

Large deviation principle

The flip rate at $i \neq N$ is :

$$c_i(\eta) = (1 - \eta_{i+1})\Big(\rho(1-\eta_i) + (1-\rho)\eta_i\Big)$$

The time changed dynamics with rates : $c_i^\lambda(\eta) = \exp(\lambda) c_i(\eta)$.

Probability measure on trajectories $\{\eta_s\}_{s \leq t}$: $\mathbb{P}, \mathbb{P}_\lambda$

Radon-Nykodim derivative :

$$\frac{d\mathbb{P}_\lambda}{d\mathbb{P}} = \exp\left(\lambda \mathcal{A}_t - \int_0^t (\exp(\lambda) - 1) \sum_{i=1}^N c_i(\eta_s)\, ds\right)$$

Correspondence between the activity and the path density

$$\mathbb{E}\big(\exp\left(\lambda \mathcal{A}_t\right)\big) = \mathbb{E}_\lambda\Big(\exp\Big((\exp(\lambda) - 1)\int_0^t \sum_i c_i(\eta_s)\, ds\Big)\Big) .$$

Large deviation principle

The flip rate at $i \neq N$ is :

$$c_i(\eta) = (1 - \eta_{i+1})\Big(\rho(1-\eta_i) + (1-\rho)\eta_i\Big)$$

The time changed dynamics with rates : $c_i^\lambda(\eta) = \exp(\lambda) c_i(\eta)$.

Probability measure on trajectories $\{\eta_s\}_{s \leq t}$: $\mathbb{P}, \mathbb{P}_\lambda$

Radon-Nykodim derivative :

$$\frac{d\mathbb{P}_\lambda}{d\mathbb{P}} = \exp\left(\lambda \mathcal{A}_t - \int_0^t (\exp(\lambda) - 1) \sum_{i=1}^N c_i(\eta_s)\, ds\right)$$

Correspondence between the activity and the path density

$$\mathbb{E}\big(\exp\left(\lambda \mathcal{A}_t\right)\big) = \mathbb{E}_\lambda\Big(\exp\left((\exp(\lambda) - 1)\int_0^t \sum_i c_i(\eta_s)\, ds\right)\Big).$$

$$\mathbb{E}\Big(\exp\big(\lambda \mathcal{A}_t\big)\Big) = \mathbb{E}_{\lambda}\Big(\exp\Big((\exp(\lambda) - 1) \int_0^t \sum_i c_i(\eta_s)\, ds \Big)\Big) \,.$$

Donsker-Varadhan theory (in the reversible case)

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}\Big(\exp\big(\lambda \mathcal{A}_t\big)\Big)$$

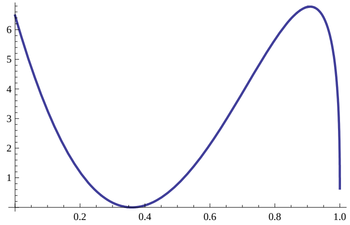
$$= \exp(\lambda) \; \sup_f \left\{ (1 - \exp(-\lambda)) \mu_N\Big(f \sum_{i=1}^N c_i(\eta) \Big) - \mathcal{D}_N(\sqrt{f}) \right\}$$

with $f \geq 0$, $\mu_N(f) = 1$ and the Dirichlet form

$$\mathcal{D}_N(f) = \sum_{i=1}^N \mu_N\Big(c_i(\eta) \big(f(\eta^i) - f(\eta) \big)^2 \Big) \,.$$

For N large

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}\Big(\exp\Big(\frac{\lambda}{N} \mathcal{A}_t\Big)\Big) \simeq \sup_f \Big\{ \lambda \mu_N \Big(f \, \frac{1}{N} \sum_{i=1}^{N} c_i(\eta) \Big) - \mathcal{D}_N(f) \Big\}$$

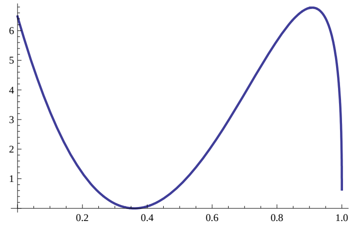


Dirichlet form evaluated for Bernoulli with density in $[0, 1]$.

➪ Almost minimum at density 1

For N large

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}\Big(\exp\big(\frac{\lambda}{N} \mathcal{A}_t \big) \Big) \simeq \sup_f \Big\{ \lambda \mu_N \Big(f \ \frac{1}{N} \sum_{i=1}^{N} c_i(\eta) \Big) - \mathcal{D}_N(f) \Big\}$$



Dirichlet form evaluated for Bernoulli with density in $[0, 1]$.

➪ Almost minimum at density 1

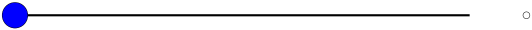
Dirichlet form ➪ Local equilibrium : density close to ρ or 1.

Surface tension

Definition.

$\Sigma_L = \inf_f \mathcal{D}_L(f)$ for densities such that $\mu_L(f(\eta)\eta_1) = 1$.

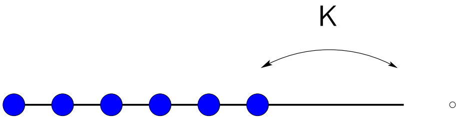
$$\Sigma = \lim_{L \to \infty} \Sigma_L \, .$$



Existence of Σ : $\quad L > L'$ then $\Sigma_L < \Sigma_{L'}$.

Surface tension : Lower Bound

$$\mathcal{C} = \{\eta_i(s) = 1, i \leq N - K, s \leq t\}$$

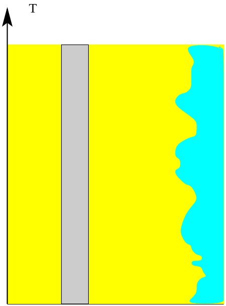


$$\mathbb{E}\Big(\exp\big(\frac{\lambda}{N}\mathcal{A}_t\big)\Big) \geq \mathbb{E}\Big(\exp\big(\frac{\lambda}{N}\mathcal{A}_t\big) 1_{\mathcal{C}}\Big)$$

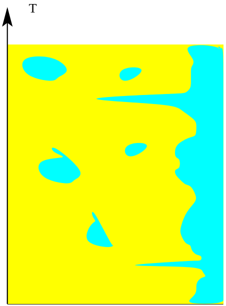
$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}\Big(\exp\big(\frac{\lambda}{N}\mathcal{A}_t\big)\Big) \geq - \inf_{f \rightsquigarrow \mathcal{C}} \Big\{ \mathcal{D}_K(f) \Big\} + O(K/N)$$

Surface tension

Existence of a barrier of 1 ?



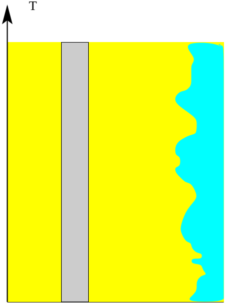
Coexistence of the two phases



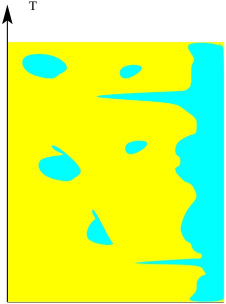
1. Prove that for $\lambda < \lambda_2$ the inactive phase dominates
2. Approximate the surface tension

Surface tension

Existence of a barrier of 1 ?



Coexistence of the two phases



1. Prove that for $\lambda < \lambda_2$ the inactive phase dominates
2. Approximate the surface tension

Active phase

For $\lambda > \lambda_1$ the active phase dominates :

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}\Big(\exp\big(\frac{\lambda}{N}\mathcal{A}_t\big)\Big) \simeq \sup_f \Big\{ \lambda \mu_N \Big(f \, \frac{1}{N} \sum_{i=1}^N c_i(\eta) \Big) - \mathcal{D}_N(f) \Big\}$$

If $f \simeq 1$ in the variational principle :

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}\Big(\exp\big(\frac{\lambda}{N}\mathcal{A}_t\big)\Big) \simeq \lambda \mu_N \Big(\frac{1}{N} \sum_{i=1}^N c_i(\eta) \Big) \simeq \lambda \mathbb{A}$$

Conclusion

- First order phase transitition
- Finite size scaling
- Surface cost Σ

Open questions.

- Existence of λ_c
- Description of the interface
- Higher dimensions
- Conservative dynamics