Static large deviations for reaction-diffusion models

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Motivation: Statistical Mechanics

1. Define a Gibbs measure
   - $\mathbb{T}_N = \left\{0, 1_N, \dots, 1 - 1_N\right\}$ $\quad 1_N = 1/N$
   - $\{0,1\}^{\mathbb{T}_N} \quad \eta \quad \eta(x) \in \{0,1\}$

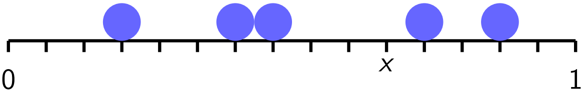
$$\mathbb{H}(\eta) = -\sum_{x \in \mathbb{T}_N} [1 - 2\,\eta(x + 1_N)]\,[1 - 2\,\eta(x)]$$

$$\mu_\beta(\eta) \;=\; \frac{1}{Z_\beta}\, e^{-\beta\,\mathbb{H}(\eta)}$$

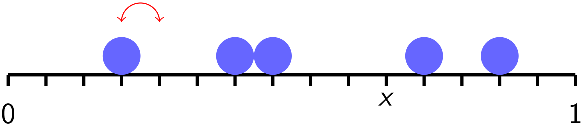
2. Define dynamics
   - Invariant for Gibbs measure (usually reversible)
   - Here we start from the dynamics
   - The invariant measure is not known explicitly

Kawasaki dynamics

- $\mathbb{T}_N = \left\{0, 1/N, \ldots, 1 - 1/N\right\} \quad \{0,1\}^{\mathbb{T}_N} \quad \eta \quad \eta(x) \in \{0,1\}$



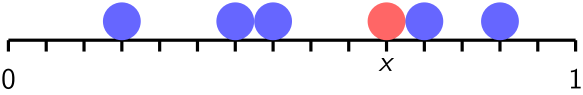
Kawasaki dynamics:



- Conservative dynamics
- Stationary states ν_α, $0 \leq \alpha \leq 1$
- Mixing time N^2.

Glauber dynamics

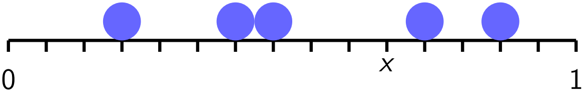
Glauber dynamics: $c(\eta)$ local function $c(\tau_x \eta)$ $\eta(x) \to 1 - \eta(x)$



- Non-conservative dynamics
- stationary states not known explicitly
- $\sigma(x) = 1 - 2\eta(x)$
- $c(\eta) = 1 - \gamma\, \sigma(0) \,[\, \sigma(1) + \sigma(-1) \,] + \gamma^2 \, \sigma(1)\, \sigma(-1) \qquad 0 \le \gamma < 1$
- $\mathbb{H}(\sigma) = - \sum_x \sigma(x)\, \sigma(x+1)$
- $\mu_\gamma(\sigma) \sim \exp\{-\beta \mathbb{H}(\sigma)\} \qquad \gamma = \tanh \beta$
- Mixing time 1

The problem

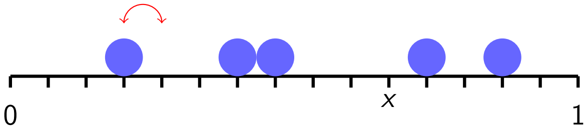
- $\mathcal{F} = \{u : \mathbb{T} \to [0,1]\}$
- $u^{(k)} \to u \quad \int_{\mathbb{T}} G(x)\, u^{(k)}(x)\, dx \longrightarrow \int_{\mathbb{T}} G(x)\, u(x)\, dx \quad G \in C(\mathbb{T})$
- $d(u, v)$



- $\eta \mapsto \rho_N \in \mathcal{F}$
- $\rho_N = \sum_{x \in \mathbb{T}_N} \eta(x)\, \chi_{(x, x+1_N]} \quad 1_N = 1/N$
- Glauber + N^2-Kawasaki
- μ_N stationary state   not known
- Problem: $\mathcal{A} \subset \mathcal{F}$ s.t. $\mu_N(\mathcal{A}) \longrightarrow 1$

Kawasaki hydrodynamics

- $u_0 : \mathbb{T} \to [0,1] \qquad \rho_N(\cdot) \sim u_0(\cdot)$
- $\rho_N(t) \sim u(t)$

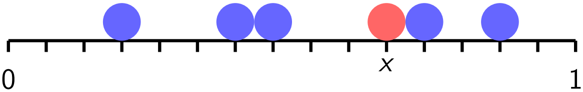


$$\frac{d}{dt}\eta_t(x) = \eta_t(x-1_N)\,[\,1-\eta_t(x)\,] + \eta_t(x+1_N)\,[\,1-\eta_t(x)\,] - \eta_t(x)\,[\,1-\eta_t(x+1_N)\,] - \eta_t(x)\,[\,1-\eta_t(x-1_N)\,]$$

$$\frac{d}{dt}\frac{1}{N}\sum_{x\in\mathbb{T}_N} G(x)\,\eta_t(x) = \frac{1}{N^2}\,\frac{1}{N}\sum_{x\in\mathbb{T}_N}(\Delta_N G)(x)\,\eta_t(x)$$

$$(\Delta_N G)(x) = N^2[\,G(x+1_N) + G(x-1_N) - 2G(x)\,]$$

Glauber hydrodynamics



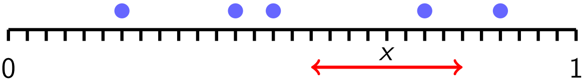
$$\frac{d}{dt}\eta_t(x) \;=\; c(\tau_x\eta_t)[\,1-\eta_t(x)\,] \;-\; c(\tau_x\eta_t)\,\eta_t(x)$$

$$\frac{d}{dt}\frac{1}{N}\sum_{x\in\mathbb{T}_N} G(x)\,\eta_t(x) \;=\; \frac{1}{N}\sum_{x\in\mathbb{T}_N} G(x)\,c(\tau_x\eta_t)[\,1-2\eta_t(x)\,]$$

$$\langle\,\rho_N(t)\,,\;G\rangle \;=\; \frac{1}{N}\sum_{x\in\mathbb{T}_N} G(x)\,\eta_t(x)$$

Hydrodynamics Glauber + Kawasaki

$$\frac{d}{dt}\langle \rho_N(t)\,,\, G\rangle \;=\; \frac{1}{N}\sum_{x\in\mathbb{T}_N}\Big\{ (\Delta_N G)(x)\,\eta_t(x) \;+\; G(x)\,c(\tau_x\eta_t)[\,1-2\eta_t(x)\,]\Big\}$$



- Exclusion speeded-up N^2 $\quad \mu_N(t,x) \sim \nu_\alpha \quad \alpha \sim \rho_N(t,x)$
- $F(\alpha) = E_{\nu_\alpha}[c(\eta)\,[\,1-2\eta(0)\,]]$
- $c(\tau_x\eta_t)[\,1-2\eta_t(x)\,] \sim F(\rho_N(t,x))$

$$\partial_t\rho \;=\; \Delta\rho \;+\; F(\rho)$$

Reaction-diffusion equations

- $F(\alpha) = -\,V'(\alpha)$

$$\begin{cases} \partial_t u \;=\; \Delta u \;-\; V'(u) \\ u(0,\cdot\,) = u_0(\cdot) \end{cases}$$

- $F(\alpha) = E_{\nu_\alpha}\big[\, c(\eta)\,[\,1 - 2\eta(0)\,]\,\big]$ polynomial
- Exists unique solution and $u \in C^\infty((0,\infty) \times \mathbb{T})$
- $u \le v \Longrightarrow u(t) \le v(t)$
- $V'(0) = -\,F(0) = -\,c(\mathbf{0}) < 0 \qquad V'(1) = -\,F(1) = c(\mathbf{1}) > 0$

$$0 \;=\; \Delta\rho \;-\; V'(\rho)$$

- $\mathcal{S}$ solutions

Theorem: Chen, Matano (89) $\forall\, u_0,\ \exists\, \rho \in \mathcal{S}$ s.t. $u(t) \longrightarrow \rho$.

Stationary state

- $\mathfrak{N}_\epsilon(\mathcal{S}) \quad \mu_N\big[\,\mathfrak{N}_\epsilon(\mathcal{S})^c\,\big] \to 0$

$$\mu_N\big[\,\rho_N \notin \mathfrak{N}_\epsilon(\mathcal{S})\,\big] \;=\; \mathbf{P}_{\mu_N}\big[\,\rho_N(0) \notin \mathfrak{N}_\epsilon(\mathcal{S})\,\big] \;=\; \mathbf{P}_{\mu_N}\big[\,\rho_N(t) \notin \mathfrak{N}_\epsilon(\mathcal{S})\,\big]$$

- $\rho_N(t) \to u(t)$

$$\begin{cases} \partial_t u \;=\; \Delta u \;-\; V'(u) \\ u(0,\cdot\,) = u_0(\cdot) \end{cases}$$

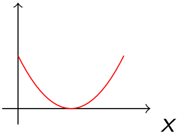
- $u(t) \to \gamma \in \mathcal{S}$
- $u(t) \in \mathfrak{N}_\epsilon(\mathcal{S}) \qquad t$ large

Solutions of the elliptic equation

$$0 \ = \ \Delta u \ - \ V'(u)$$

- $V'(\alpha) = 0 \quad \gamma(x) = \alpha$ solution.

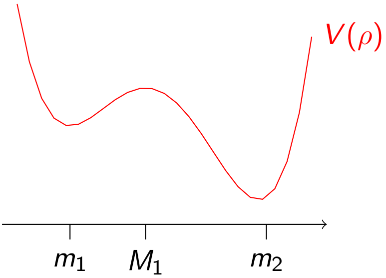
- V polynomial degree 2.
- $V'(0) < 0 \quad V'(1) > 0$
- $u_0(x) = a \quad u(t,x) = a(t) \quad \dot{a}(t) = -V'(a(t))$
- $u^{(a)}(x) = a \quad u^{(0)} \leq u \leq u^{(1)} \quad u^{(0)}(t) \leq u(t) \leq u^{(1)}(t)$
- $u(t) \to \mathfrak{m} \quad \mathfrak{m}$ minima of V.



Solutions of the elliptic equation

$$0 < m_1 < M_1 < m_2 < \cdots < m_{\mathfrak{n}-1} < M_{\mathfrak{n}-1} < m_{\mathfrak{n}}$$

- $\Delta\rho - V'(\rho) = 0$
- $\partial_t^2 \rho - V'(\rho) = 0$



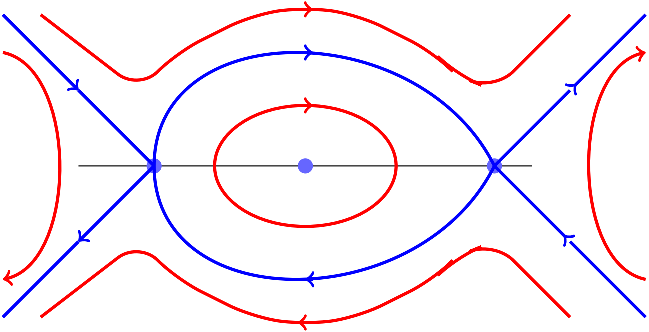
Hamiltonian dynamics

- $(q(t)\,,\, p(t)) \quad q(t) = \rho(t)$

$$\begin{cases} \dot{q}(t) = p(t) \\ \dot{p}(t) = V'(q(t)) \end{cases}$$

Hamiltonian dynamics

- $\dot{q}(t) = p(t) \quad \dot{p}(t) = V'(q(t))$



- Periodic solutions

Hamiltonian dynamics

$$\begin{cases} \dot{q}(t) = p(t) \\ \dot{p}(t) = V'(q(t)) \end{cases} \qquad E(p,q) = \frac{1}{2}p^2 \; - \; V(q)$$

$$\dot{E}(t) \;=\; p(t)\,\dot{p}(t) - V'(q(t))\,\dot{q}(t) \;=\; p(t)\,V'(q(t)) - V'(q(t))p(t) \;=\; 0$$

$$\frac{1}{2}p(t)^2 \; - \; V(q(t)) \;=\; C_0 \qquad p(t) \;=\; \pm\sqrt{2V(q(t)) + C_0}$$

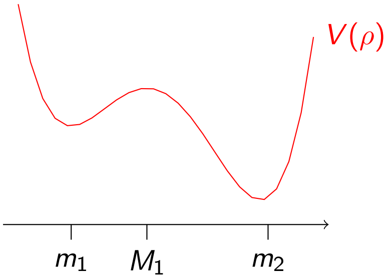
Theorem:

- Zeros of F are real numbers
- Critical points of V are maxima or minima
- Then, at most finite number of solutions [up to translations].

Unstable solutions

$\mathcal{S}$ solutions $\qquad \mu_N(\mathfrak{N}_\epsilon(\mathcal{S})) \to 1$

- Unstable solutions
- $\partial_t u = \Delta u - V'(u)$
- $u(0) = a \qquad u(t) = a(t)$
- $\dot{a}(t) = -V'(a(t))$
- $u(0) = M_j \pm \epsilon \quad u(t) \to m_{j\pm 1}$



$\mathcal{U}$ "unstable" solutions $\qquad \mu_N(\mathfrak{N}_\epsilon(\mathcal{U})) \to 0$

Dynamical large deviations

Kipnis, Olla, Varadhan (89) Donsker, Varadhan (89)
Jona-Lasinio, L, Vares (93) Bodineau, Lagouge (10, 12) L, Tsunoda (15)

- initial state η^N $\rho_N(\eta^N) \to \gamma$

Hydrodynamical limit:

$$\mathbb{P}_{\eta^N}\left[\rho_N(t) \sim u(t)\ ,\ 0 \le t \le T\right] \ \to\ 1 \qquad \begin{cases} \partial_t u = \Delta u + F(u) \\ u(0,\cdot) = \gamma(\cdot) \end{cases}$$

Large deviations:

- $u(t) = u(t,x) \quad 0 \le t \le T$

$$\mathbb{P}_{\eta^N}\left[\rho_N(t) \sim u(t)\ ,\ 0 \le t \le T\right] \ \approx\ e^{-N\, I_{[0,T]}(u)}$$

Large Deviations rate function

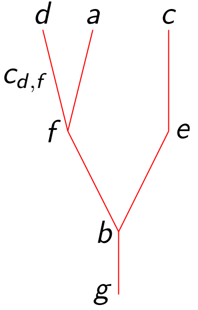
- $B(\alpha) = E_{\nu_\alpha}\left[\{1 - \eta(0)\}\, c(\eta)\right] \quad D(\alpha) = E_{\nu_\alpha}\left[\eta(0)\, c(\eta)\right]$
- $F(\alpha) = B(\alpha) - D(\alpha)$
- $\sigma(\alpha) = \alpha(1 - \alpha)$
- B, D concave functions

$$\partial_t u = \Delta u + F(u) - \partial_x[\sigma(u)\partial_x H] + B(u)(e^H - 1) - D(u)(e^{-H} - 1)$$

$$\begin{aligned} I_T(u) \;&=\; \frac{1}{2}\int_0^T dt \int_{\mathbb{T}} dx\, \sigma(u)\,(\nabla H)^2 \\ &\quad + \int_0^T dt \int_{\mathbb{T}} dx \left\{ B(u)\,(1 - e^H + He^H) + D(u)\,(1 - e^{-H} - He^{-H}) \right\} \end{aligned}$$

Quasi-potential

- $\bar\rho_1, \dots, \bar\rho_p$ stationary solutions $\mathcal{M}_1, \dots, \mathcal{M}_p$
- $V_i(\gamma) = \inf_{T>0} \inf\{ I_{[0,T]}(u) : u_0 \in \mathcal{M}_i \,, \; u(T) = \gamma\}$
- $c_{i,j} = V_i(\bar\rho_j)$
- $T(i)$ trees i root
- $\mathfrak{g} \in T(i) \quad \kappa(\mathfrak{g}) = \sum_{(a,b)\in\mathfrak{g}} c_{a,b}$
- $w_i = \min_{\mathfrak{g}\in T(i)} \kappa(\mathfrak{g})$
- $v_i = w_i - \min_k w_k$
- $\mu_N(\mathcal{N}_\epsilon(\mathcal{M}_i)) \approx e^{-N v_i}$



$\kappa(\mathfrak{g}) \quad \mathfrak{g} \in T(g)$

$$W(\gamma) = \min_i \{ v_i + V_i(\gamma) \}$$

Static large deviations (Farfán, L, Tsunoda)

- $B(\rho) = E_{\nu_\rho}\big[[1-\eta(0)]\, c(\eta)\big]$
- $D(\rho) = E_{\nu_\rho}\big[\eta(0)\, c(\eta)\big]$
- $-V'(\rho) = F(\rho) = B(\rho) - D(\rho)$
- $\Delta\rho = V'(\rho)$ has finite number of solutions
- $B \quad D$ concave functions
- $\mathcal{C}$ closed $\quad \mathcal{O}$ open

$$\limsup_{N\to\infty} \frac{1}{N} \log \mu_N(\rho_N \in \mathcal{C}) \;\le\; -\inf_{\vartheta\in\mathcal{C}} W(\vartheta)\;,$$

$$\liminf_{N\to\infty} \frac{1}{N} \log \mu_N(\rho_N \in \mathcal{O}) \;\ge\; -\inf_{\vartheta\in\mathcal{O}} W(\vartheta)\;.$$

W quasi-potential

Static large deviations (Farfán, L, Tsunoda)

- $\Delta\rho = V'(\rho)$ has finite number of solutions
- $B \quad D$ concave functions

$$\mu_N(\rho_N \sim \gamma) \;\approx\; e^{-NW(\gamma)}$$

- W bounded, lower semicontinuous, compact level sets
- $\mu_N(\mathcal{N}_\epsilon(\mathcal{M}_i)) \approx e^{-Nv_i}$
- $\mathcal{S}_{\rm unst} = \{\bar\rho_j : v_j > 0\}$
- $\mathcal{S}_0 = \mathcal{S} \setminus \mathcal{S}_{\rm unst}$

$$\mu_N\big(\,\mathfrak{N}_\epsilon(\mathcal{S}_0)\,\big) \;\to\; 1$$

- Difficult to characterize unstable solutions
- Analytical problem $\quad$ optimal formulation

Stabile states

$$\mu_N(\mathcal{N}_\epsilon(\mathcal{M}_i)) \approx e^{-Nv_i}$$

- $\mathcal{M}_i$ is stabile if $\forall\, \epsilon > 0 \;\; \inf_{\gamma \notin \mathcal{N}_\epsilon(\mathcal{M}_i)} V_i(\gamma) > 0$
- If $\mathcal{M}_i$ stabile, then $c_{i,j} > 0 \;\forall\, j \neq i$
- $\mathcal{M}_i$ stabile does not imply that $v_i = 0$
- All minima m_k are stabile

Unstable condition:

- Let j such that $c_{j,k} = 0$ for some k
- Suppose that $c_{k,\ell} > 0$ for all $\ell \neq k$.
- Then, $v_j > 0$

Heteroclinic orbits

- $\phi \to \psi \quad \lim_{t\to+\infty} u(t) = \psi \quad \lim_{t\to-\infty} u(t) = \phi$
- $\rho_j \to \rho_k \implies c_{j,k} = 0$
- $M_j \to m_{j+1} \quad M_j \to m_j \quad \implies v(M_j) > 0$

Fiedler, Rocha, Wolfrum (04)

- $V''(M_j) \neq 0$
- ϕ non-constant solution $\quad m_i < \phi(x) < m_{i+1}$
- There are heteroclinic orbits $\phi \to \bar{\rho}_i$, $\phi \to \bar{\rho}_{i+1}$
- $v(\phi) > 0$

Conclusion

- Remains to remove local minima