LARGE FLUCTUATIONS OF PARTICLE SYSTEMS, AN OVERVIEW

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Stochastic Particle Systems

- Continuous time Markov processes
- State space = Configurations of indistinguishable particles on a lattice
- Lattice: $\Lambda_\epsilon \subseteq (\epsilon\mathbb{Z})^d$
- Example: $\{0,1\}^{\Lambda_\epsilon}$, exclusion rule
- Example: $\mathbb{N}^{\Lambda_\epsilon}$, no exclusion rule
- η = Configuration of particles
- $\eta_t(x)$ =number of particles at site $x \in \Lambda_\epsilon$ at time t.

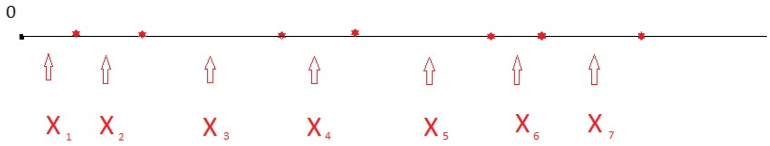
Poisson Processes

Parameter $\lambda \in \mathbb{R}^+$, X_i i.i.d. exponential random variables with parameter λ

$$\mathbb{P}(X_i \in [a,b]) = \lambda \int_a^b e^{-\lambda u} d\,u \qquad 0 \leq a < b$$

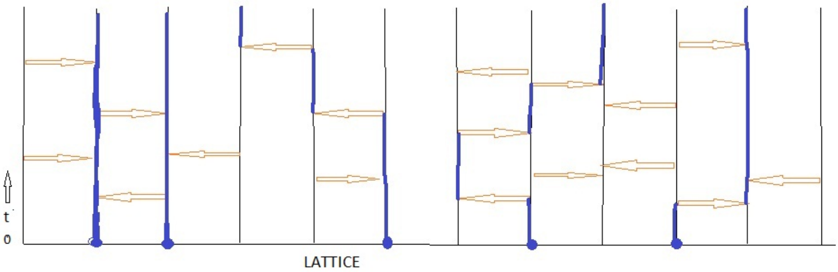
$$Y_i = \sum_{j=1}^{i} X_j$$

Locally finite random configuration of points $\sum_{i=1}^{+\infty} \delta_{Y_i}$



Harris graphical construction

Example: Symmetric simple exclusion



Generator

$$Lf(\eta) = \sum_{\eta'} c(\eta, \eta') \left[f(\eta') - f(\eta) \right]$$

It means that the jump from configuration η to configuration η' is driven by a Poisson process of parameter $c(\eta, \eta')$

$c(\eta, \eta')$= Rate of jump from η to η'

Other examples

Zero Range: particles perform variable speed simple random walks. Particles at x jump with rate depending on $\eta_t(x)$

$$Lf(\eta)=\sum_x\sum_{y\sim x}g(\eta(x))\left[f(\eta^{x,y})-f(\eta)\right]$$

$$\eta^{x,y}=\eta-\delta_x+\delta_y$$

KMP: $\eta_t(x)\in\mathbb{R}^+$ (Energies). If $x\sim y$ at rate 1

$$\Big(\eta(x),\eta(y)\Big)\Longrightarrow\Big(U(\eta(x)+\eta(y)),(1-U)(\eta(x)+\eta(y))\Big)$$

U = uniform random variable in $[0,1]$

Empirical measure

Lattice embedded in $\mathbb{R}^d$, given $\Lambda \subseteq \mathbb{R}^d$

$$\Lambda_\epsilon = \Lambda \cap (\epsilon\mathbb{Z})^d$$

$$\eta \Longrightarrow \pi_\epsilon(\eta) = \text{Empirical measure}, \ \pi_\epsilon(\eta) \in \mathcal{M}(\Lambda, \mathbb{R}^+)$$

$$\pi_\epsilon(\eta) = \epsilon^d \sum_{x \in \Lambda_\epsilon} \eta(x)\delta_x$$

$$\int_\Lambda \phi(u) d\left[\pi_\epsilon(\eta)\right](u) = \epsilon^d \sum_{x \in \Lambda_\epsilon} \eta(x)\phi(x)$$

Empirical current

$(\eta_t)_{t\in[0,T]}$= trajectory, τ_i= jump times, at time τ_i 1 particle jumps from x^i to y^i

$(\eta_t)_{t\in[0,T]} \Longrightarrow \mathcal{J}_\epsilon$=empirical current, $\mathcal{J}_\epsilon \in \mathcal{M}(\Lambda \times [0,T], \mathbb{R}^d)$

$$\mathcal{J}_\epsilon = \epsilon^d \sum_i (y^i - x^i)\delta_{(x^i,\tau_i)}$$

$$\int_0^T \int_\Lambda \phi(u,t) \cdot d\left[\mathcal{J}_\epsilon\right](u) = \epsilon^d \sum_i \phi(x^i,\tau^i)\cdot(y^i - x^i)$$

Continuity equation

$$\partial_t \pi_\epsilon + \nabla \cdot \mathcal{J}_\epsilon = O(\epsilon^2)$$

Hydrodynamic scaling limit

$c(\eta, \eta')$ satisfy detailed balance with respect to a Gibbs measure

$$\frac{1}{Z} e^{-H(\eta)}$$

high temperature regime

$$e^{-H(\eta)} c(\eta, \eta') = e^{-H(\eta')} c(\eta', \eta)$$

Finite range interactions, conservative dynamics, local changes

$L \Longrightarrow \epsilon^{-2} L$ Diffusive rescaling

$$\pi_\epsilon(\eta_0) \stackrel{\epsilon \to 0}{\to} \rho_0(u) d\, u$$

Hydrodynamic scaling limit

$$\pi_\epsilon(\eta_t) \stackrel{\epsilon\to 0}{\to} \rho(u,t)du \qquad \mathcal{J}_\epsilon(\eta) \stackrel{\epsilon\to 0}{\to} j(u,t)dudt$$

$$\begin{cases} \partial\rho + \nabla\cdot j = 0 \\ j(u,t) = -D(\rho(u,t))\nabla\rho(u,t) = J(\rho(u,t)) \\ \rho(u,0) = \rho_0(u) \\ \rho(u,t) = \gamma(u)\,, \qquad u \in \partial\Lambda \end{cases}$$

Boundary conditions arises from Glauber dynamics at the boundary that destroy reversibility

$D = d \times d$ diffusion matrix, symmetric and positive definite

Observing just the density

$$\begin{cases} \partial\rho = \nabla\cdot(D(\rho)\nabla\rho) \\ \rho(u,0) = \rho_0(u) \\ \rho(u,t) = \gamma(u)\,, \qquad u \in \partial\Lambda \end{cases}$$

Large deviations

$$\mathbb{P}\big((\pi_\epsilon, \mathcal{J}_\epsilon) \sim (\rho, j)\big)\big) \simeq e^{-\epsilon^{-d} I(\rho,j)}$$

$$I(\rho, j) = \frac{1}{4} \int_0^T dt \int_\Lambda du \big(j - J(\rho)\big) \cdot \sigma(\rho)^{-1} \big(j - J(\rho)\big)$$

if $\partial_t \rho + \nabla \cdot j = 0$ and $\rho = \gamma$ on $\partial\Lambda$. Assumes value $+\infty$ otherwise.

$\sigma(\rho) = d \times d$ mobility matrix symmetric and positive definite

Einstein relation

$$D(\rho) = \sigma(\rho) f''(\rho)$$

Free energy

f = density of free energy for the Gibbs measure

fixed $\lambda \in \mathbb{R}$ chemical potential consider

$$\frac{1}{Z_\epsilon(\lambda)} e^{-H(\eta)+\lambda \sum_{x\in\Lambda_\epsilon} \eta(x)}$$

Pressure

$$p(\lambda) = \lim_{\epsilon\to 0} \frac{\epsilon^d}{|\Lambda|} \log Z_\epsilon(\lambda)$$

strictly convex, smooth, independent from boundary conditions

$$f(\rho) = \sup_\lambda \{\lambda\rho - p(\lambda)\}$$

Examples

SSEP: $D(\rho) = \mathbb{I}$, $\sigma(\rho) = \rho(1-\rho)\mathbb{I}$

$$f(\rho) = \rho \log \rho + (1-\rho)\log(1-\rho)$$

Hydrodynamics $\partial_t \rho = \Delta \rho$ heat equation

Zero Range: $D(\rho) = \phi'(\rho)\mathbb{I}$, $\sigma(\rho) = \phi(\rho)\mathbb{I}$

$$f(\rho) = \rho \log \phi(\rho) - \log \mathcal{Z}\big(\phi(\rho)\big)$$

Hydrodynamics $\partial_t \rho = \Delta \phi(\rho)$ non linear diffusion

Invariant measure

$\mu_\epsilon(\eta)$ probability measure on configuration space such that

$$\mathbb{P}(\eta_t = \eta) = \mu_\epsilon(\eta)\,, \qquad \text{for any t}$$

Irreducibility $\Longrightarrow$ invariant measure is unique $\Longrightarrow$ stationary state
Boundary conditions $\Longrightarrow$ no reversibility $\Longrightarrow$ stationary non equilibrium state

No Gibbsian structure, combinatorial representations

Large deviations for μ_ϵ

$$\mathbb{P}_{\mu_\epsilon}\left(\pi_\epsilon(\eta) \sim \rho\right) \simeq e^{-\epsilon^{-d} V(\rho)}$$

$V(\rho) =$ large deviations rate functional for the invariant measure. Macroscopic variational approach.

$\bar{\rho} =$ stationary density profile

$$\begin{cases} \nabla \cdot (D(\bar{\rho}) \nabla \bar{\rho}) = 0 \\ \bar{\rho}(u) = \gamma(u) \qquad u \in \partial\Lambda \end{cases}$$

$$V = V_\gamma \qquad V(\rho) \geq 0 \qquad V(\bar{\rho}) = 0$$

Quasipotential

$$V(\rho^*) = \inf_T \inf_{\left\{\substack{\rho(u,t):\\ \rho(u,0)=\rho^*(u)\\ \rho(u,-T)=\bar{\rho}(u)}\right\}} I_{[-T,0]}(\rho, j)$$

Easy in the reversible cases, challenging in the non reversible ones

From the variational characterization we get that $V(\rho)$ solves the stationary $\infty-$dimensional Hamilton-Jacobi equation

$$\int_\Lambda \nabla \frac{\delta V}{\delta \rho} \cdot \left(\sigma(\rho) \nabla \frac{\delta V}{\delta \rho} + J(\rho) \right) du = 0$$

$\frac{\delta(\cdot)}{\delta\rho}$ = functional derivative

Geometric interpretation

The Hamilton-Jacobi equation is equivalent to the following orthogonality condition

$$\int_\Lambda J^A(\rho) \cdot \sigma(\rho)^{-1} J^S(\rho)\, du = 0$$

where

$$J^S(\rho) = -\sigma(\rho)\nabla \frac{\delta V}{\delta \rho} \qquad J^A(\rho) = J(\rho) - J^S(\rho)$$

An example

SSEP $\Lambda = [0,1]$

1) $\gamma(0) = \gamma(1) = \gamma \Longrightarrow$ reversible

$$V(\rho) = \int_0^1 \left(\rho \log \frac{\rho}{\gamma} + (1-\rho) \log \frac{1-\rho}{1-\gamma} \right) du$$

2) $\gamma(0) \neq \gamma(1) \Longrightarrow$ not reversible

$$V(\rho) = \sup_{\varphi} \int_0^1 \left(\rho \log \frac{\rho}{\varphi} + (1-\rho) \log \frac{1-\rho}{1-\varphi} + \log \frac{\varphi'}{\bar{\rho}'} \right) du$$

$$\begin{cases} \frac{\varphi'' \varphi (1-\varphi)}{(\varphi')^2} + \varphi = \rho \\ \varphi(0) = \gamma(0), \varphi(1) = \gamma(1) \\ \varphi \text{ monotone} \end{cases}$$

Time dependent models

Non homogeneous in time Markov models

Time dependent boundary conditions $\gamma = \gamma(u,t)$

Add also a weak external field

$$c^E(\eta,\eta') = c(\eta,\eta') + \epsilon \ell_{\eta,\eta'}(E) + o(\epsilon)$$

$$E = (E_1(u,t), \dots, E_d(u,t))$$

Hydrodynamics

$$\begin{cases} \partial\rho + \nabla \cdot j = 0 \\ j = -D(\rho)\nabla\rho + \sigma(\rho)E = J_E(\rho) \\ \rho(u,t) = \gamma(u,t) \qquad u \in \partial\Lambda \end{cases}$$

Work

Given (ρ, j) satisfying a time dependent Hydrodynamics

$$W = \int_{T_1}^{T_2} d\,t \left(\int_\Lambda d\,u \; (j \cdot E) - \int_{\partial\Lambda} \left(f'(\gamma) j \cdot n \right) \, dS(u) \right)$$

after integrations by parts

$$\begin{aligned} W &= \int_\Lambda f\big(\rho(u,T_2)\big)\, du - \int_\Lambda f\big(\rho(u,T_1)\big)\, du \\ &+ \int_{T_1}^{T_2} dt \int_\Lambda j \cdot \sigma(\rho)^{-1} j \, du \end{aligned}$$

Clausius Inequality $W \geq \Delta F$

$$F(\rho) = \int_\Lambda f\big(\rho(u)\big)\, du$$

Stationary non equilibrium states

$$(\gamma, E) \to \bar\rho_{\gamma,E} \qquad \nabla \cdot J_E(\bar\rho_{\gamma,E}) = 0$$

SNS if $J_E(\bar\rho_{\gamma,E}) \neq 0$

Work necessary to maintain a SNS

if $(\gamma(t), E(t)) = (\gamma, E)$, $\rho(t) = \bar\rho_{\gamma,E}$, $t \in [T_1, T_2]$

$$\begin{aligned} W &= \int_{T_1}^{T_2} dt \int_\Lambda J(\bar\rho_{\gamma,E}) \cdot \sigma(\bar\rho_{\gamma,E})^{-1} J(\bar\rho_{\gamma,E})\, du \\ &= \int_{T_1}^{T_2} dt \int_\Omega J^A(\bar\rho_{\gamma,E}) \cdot \sigma(\bar\rho_{\gamma,E})^{-1} J^A(\bar\rho_{\gamma,E})\, du \end{aligned}$$

since $J^S(\bar\rho_{\gamma,E}) = -\sigma(\bar\rho_{\gamma,E}) \nabla \frac{\delta V_{\gamma,E}}{\delta \rho}(\bar\rho_{\gamma,E}) = 0$

Thermodynamic transformations

(γ^i, E^i), $i = 1, 2$ SNS; consider $(\gamma(t), E(t))$ such that

$$(\gamma(0), E(0)) = (\gamma^1, E^1) \qquad \lim_{t \to +\infty} (\gamma(t), E(t)) = (\gamma^2, E^2)$$

Consider $(\rho(t), j(t))$ satisfying time dependent hydrodynamics with $\rho(0) = \bar{\rho}_{\gamma^1, E^1}$, then $\lim_{t \to +\infty} \rho(t) = \bar{\rho}_{\gamma^1, E^1}$

$$+\infty = W \geq \Delta F$$

Renormalized work

Oono-Paniconi; Hatano-Sasa

Renormalized work

$$W^{ren} = W - \int_{T_1}^{T_2} dt \int_{\Lambda} J^A(\rho(t)) \cdot \sigma(\rho(t))^{-1} J^A(\rho(t))\, du$$

after integrations by parts

$$\begin{aligned} W^{ren} &= F(\rho(T_2)) - F(\rho(T_1)) \\ &+ \int_{T_1}^{T_2} dt \int_{\Omega} J^S(\rho(t)) \cdot \sigma(\rho(t))^{-1} J^S(\rho(t))\, du \end{aligned}$$

Clausius inequality for SNS

Thermodynamic transformation from SNS 1 to SNS 2

$$+\infty > W^{ren} = F(\bar{\rho}_{\gamma^2,E^2}) - F(\bar{\rho}_{\gamma^1,E^2})$$
$$+ \int_0^{+\infty} dt \int_\Omega J^S(\rho(t)) \cdot \sigma(\rho(t))^{-1} J^S(\rho(t)) du \geq \Delta F$$

Meaningful Clausius inequality

Excess of renormalized work

$$\big(\gamma^\delta(t), E^\delta(t)\big) = \big(\gamma(\delta t), E(\delta t)\big) \Longrightarrow W_\delta^{ren}$$

Minimal work

$$\lim_{\delta \to 0} W_\delta^{ren} = \Delta F$$

$\delta \to 0 \Longrightarrow$ Quasistatic Transformations

Excess of renormalized work

$$W_{ex}^{ren} = W^{ren} - \Delta F$$

Relation with the Quasipotential

$$W_{ex}^{ren} = \int_{T_1}^{T_2} dt \int_{\Omega} J^S(\rho(t)) \cdot \sigma(\rho(t))^{-1} J^S(\rho(t)) du$$

Take SNS $\bar{\rho}_{\gamma^1, E^1}$ and put in contact with time independent environment (γ^2, E^2)

From Hamilton-Jacobi equation

$$W_{ex}^{ren} = V_{\gamma^2, E^2}(\bar{\rho}_{\gamma^1, E^1})$$