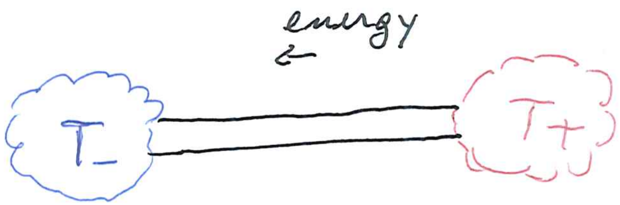
Thermodynamic potentials for stationary non-equilibrium states

PLAN

- Large deviations for Gibbs measures
- Non-equilibrium
  - Basic model : stochastic lattice gases
  - Hydrodynamical limits and large deviations
  - Quasi potential
  - Lagrangian phase transitions
- Process level large deviations

1. Stationary non-equilibrium states



N = # degrees of freedom

if $T_- = T_+$ $\qquad \mu^N \propto e^{-\beta H_N} \qquad \beta = \frac{1}{T}$

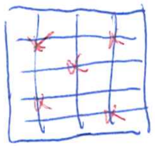
we can obtain all equilibrium information without looking at the dynamics

when $T_- \neq T_+$ $\qquad \mu^N = ?$ $\qquad$ interested in the large N behaviour

Microscopic dynamics $\xrightarrow[t \to \infty]{}$ μ^N $\longrightarrow$ large N limit

Macroscopic dynamics in a finite window $[0, T]$ $(N \to \infty)$ $\longrightarrow$ statistics of fluctuations [large deviations] $\longrightarrow$ behaviour of μ^N for large N [variational problems]

2. Large deviations in equilibrium statistical mechanics [Lattice gases]



$\Lambda \subset \mathbb{Z}^d$

$$\Omega_\Lambda = \{0,1\}^\Lambda \qquad \text{configuration space}$$

$$\mathcal{H}_\Lambda(\eta) = \sum_{x \subset \Lambda} \phi_x(\eta) + \text{b.c.} \qquad \text{Energy}$$

$$\mathcal{N}_\Lambda(\eta) = \sum_{x \in \Lambda} \eta_x \qquad \#\text{ of particles in } \Lambda$$

$$\mu_\Lambda^\lambda(\eta) = \frac{1}{Z_\Lambda^\lambda} \frac{1}{2^{|\Lambda|}} e^{-\mathcal{H}_\Lambda(\eta) + \lambda \mathcal{N}_\Lambda(\eta)} \qquad \text{Gibbs measure (Finite volume)}$$

$$p(\lambda) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log Z_\Lambda^\lambda \qquad \text{pressure}$$

$$f(\rho) = \sup_\lambda \{ \lambda \rho - p(\lambda) \} \qquad \text{free energy}$$

(Here starts the thermodynamics)

Q: "full" statistics of the density $\frac{\mathcal{N}_\Lambda}{|\Lambda|}$ as $\Lambda \uparrow \mathbb{Z}^d$

A: provided by the free energy

Boltzmann/Einstein fluctuations formula

Lanford

Comets, Ellis, Olla

(mathematical side)

$\bar\lambda \in \mathbb{R}$ fixed, $\bar e \in (0,1)$ associated density $\bar\lambda = f'(\bar e)$, $\bar e = p'(\bar\lambda)$

$$\mu^{\bar\lambda}_\Lambda\left(\frac{W_\Lambda}{|\Lambda|} \sim e\right) \asymp e^{-|\Lambda| F(e|\bar e)}$$

$$F(e|\bar e) = f(e) - \bar\lambda(e-\bar e) - f(\bar e)$$

affine tilt (thermodynamic) free energy

In the sense that $\forall B$ measurable

$$-\inf_{e\in \mathring{B}} F(e|\bar e) \le \varliminf_\Lambda \frac{1}{|\Lambda|} \log \mu^{\bar\lambda}_\Lambda\left(\frac{W_\Lambda}{|\Lambda|} \in B\right) \le \varlimsup_\Lambda \frac{1}{|\Lambda|} \log \mu^{\bar\lambda}_\Lambda(\cdot) \le -\inf_{e\in \bar B} F(e|\bar e)$$

Also

$$F(e|\bar e) = \lim_{\Lambda\uparrow\mathbb{Z}^d} \frac{1}{|\Lambda|} \operatorname{Ent}(\mu^{\lambda}_\Lambda \,|\, \mu^{\bar\lambda}_\Lambda)$$

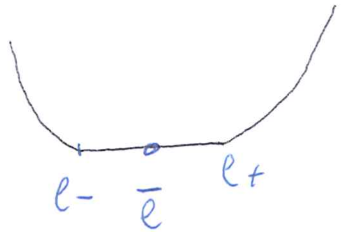
$\beta \ll 1$ $\quad p$ smooth (analytic), $F(\cdot|\bar e)$ smooth and uniformly convex

$\beta \gg 1$ (phase transitions) $\quad p$ with corners, $F(\cdot|\bar e)$ with flat parts

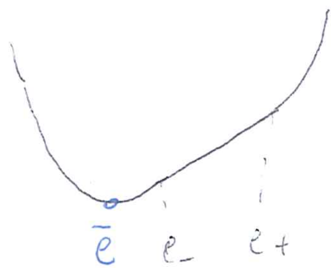
$F(\cdot|\bar e)$

$\beta \ll 1$

$F(\cdot|\bar e)$



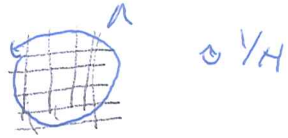
$F(\cdot|\bar e)$



$\beta \gg 1$ (phase transition)

We will eventually describe space inhomogeneous systems
Need to record the spatial structure in the observable

$\Lambda \in \mathbb{R}^d$ macroscopic domain, $\frac{1}{N}$ lattice mesh, $\Lambda_N = \frac{1}{N}\mathbb{Z}^d \cap \Lambda$



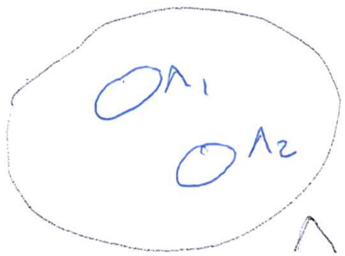
$\pi^N = \frac{1}{N^d} \sum_{x \in \Lambda_N} \eta_x \delta_x$ empirical density $\in$ positive measures on Λ

then

$$\mu^{\bar{\lambda}}_{\Lambda_N} (\pi^N \sim \pi) \asymp e^{-N^d \mathcal{F}(\pi)}$$

$$\mathcal{F}(\pi) = \int_\Lambda f(\rho(x) | \bar{\rho})\, dx \qquad \pi(dx) = \rho(x)\, dx$$

$\longrightarrow$ local functional

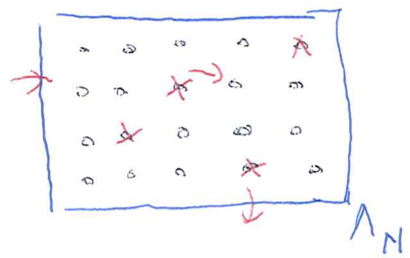


macroscopic fluctuations of the density
in Λ_1, Λ_2 (disjoint macroscopic regions)
are independent

QUEST In non-equilibrium $\mathcal{F} \longrightarrow$?
(everything in the high temperature regime)

3. Non-equilibrium models : stochastic lattice gases

- inhomogeneous boundary reservoirs
- applied external field (charged particles)



Markov process on $\Omega_{\Lambda_N} = \{0,1\}^{\Lambda_N}$

$c^{E}_{x,y}$ = jump ~~r~~ rate from x to y (nearest neighbours)

local detailed balance w.r.t. Gibbs measure

At boundary sites

$c^{\pm}_{x}$ entrance / exit rates corresponding to boundary reservoir at chemical potential λ_x

E applied field $\propto \frac{1}{N}$

$\lambda = \{\lambda_x\}_{x \in \partial\Lambda_N}$ chemical potential of the boundary reservoirs

$E = 0$, λ = constant model for equilibrium dynamics (reversible w.r.t. the Gibbs measure)

- $\exists !$ invariant probability $\mu^{\lambda, E}_{\Lambda_N}$

want to understand its (macroscopic) fluctuations properties

4. Hydrodynamical description [Varadhan, ...]

Diffusive rescaling: microspace $\propto \frac{1}{N}$ microtime $\propto \frac{1}{N^2}$

$$\eta(t) = \{\eta_x(t)\}_{x \in \Lambda_N} \quad \text{microscopic process}$$

$$\pi_t^N = \frac{1}{N^d} \sum_{x \in \Lambda_N} \eta_x(N^2 t)\, \delta_x \qquad t \in [0,T]$$ empirical density at time t

Assume $t=0$ $\quad \pi_0^N \to \rho_0\, dx$ (weak topology)

Then $t=t$ $\quad \pi_t^N \to \rho_t\, dx$

where $\{\rho_t\}_{t \in [0,T]}$ solves (non-linear) driven diffusion eq.

$$\begin{cases} \partial_t \rho + \nabla \cdot \sigma(\rho) E = \nabla \cdot D(\rho) \nabla \rho & (0,T) \times \Lambda \\ f'(\rho) = \lambda & (0,T] \times \partial\Lambda \\ \rho|_{t=0} = \rho_0 & \Lambda \end{cases}$$

Transport coefficients: σ mobility, D diffusion coefficient

[Green-Kubo formula]

Einstein relationship: $\boxed{D = f'' \sigma}$ $\quad f$: equilibrium free energy

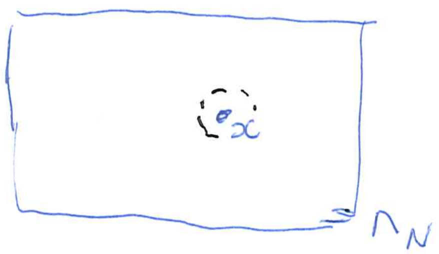
(counterpart of the microscopic local detailed balance)

- Typical behaviour stationary non-equilibrium state : local equilibrium

$\bar{e} = \bar{e}(x)$ stationary solution hydrodynamic eq

$$\begin{cases} \nabla \cdot \sigma(e) E = \nabla \cdot D(e) \nabla e & \Lambda \\ f'(e) = \lambda & \partial\Lambda \end{cases}$$

Fix $x \in \Lambda$



$\mu_{\Lambda_N}^{\lambda, \bar{E}} \Big|_{\text{(microscopic) neighborhood of } x} \rightarrow \mu^{\lambda_x}$ Gibbs measure with chemical potential $\lambda_x = f'(\bar{e}(x))$

- If we look at local (micro) observables the system behaves as it were at equilibrium

→ what about macroscopic correlations ?

→ what happens for spatially extended observables ?

Answer will depend only on the transport coefficients σ, D

5. Hydrodynamical large deviations [KOV, ..]

Fix macroscopic time window $[0,T]$

η^N deterministic initial configuration s.t. $\pi^N(\eta^N) \longrightarrow \rho_0\, dx$

$\mathbb{P}^N_{\eta^N}$ distribution microscopic process $\eta(t)$, $t \in [0, N^2 T]$

Then

$$\mathbb{P}^N_{\eta^N}\left(\pi^N_\cdot \sim \pi_\cdot \right) \simeq e^{-N^d I_{[0,T]}(\pi_\cdot)}$$

$$I_{[0,T]}(\pi) = \begin{cases} \dfrac{1}{4}\displaystyle\int_0^T \| \partial_t \rho + \nabla\cdot\sigma E - \nabla\cdot D\nabla\rho \|^2_{-1,\sigma(\rho)} & \text{if } \pi_\cdot = \rho_\cdot\, dx,\ \rho|_{t=0} = \rho_0 \\ +\infty & \text{otherwise} \end{cases}$$

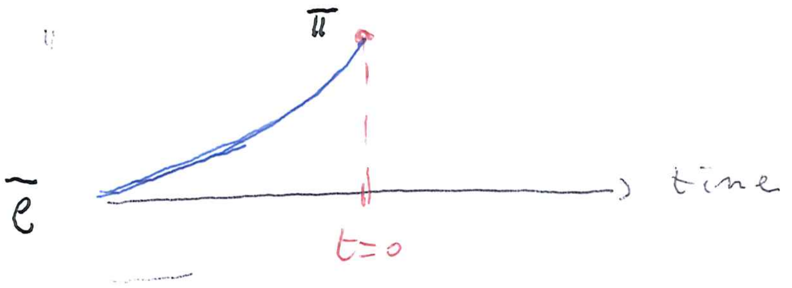
$$\frac{1}{2}\| g \|^2_{-1,\sigma(\rho)} = \sup_H \left\{ \int_\Lambda g H\, dx - \frac{1}{2}\int_\Lambda \langle \sigma(\rho) \nabla H, \nabla H \rangle\, dx \right\}$$

[Wasserstein if $\sigma(\rho) = \rho$, independent particles]

Now $T \to \infty$. Freidlin - Wentzell quasipotential

$$V(\pi) = \lim_{T\to\infty} \inf_{\substack{\pi_\cdot :\\ \pi_{-T} = \bar{e}\,dx \\ \pi_0 = \pi}} I_{[-T,0]}(\pi_\cdot) =$$

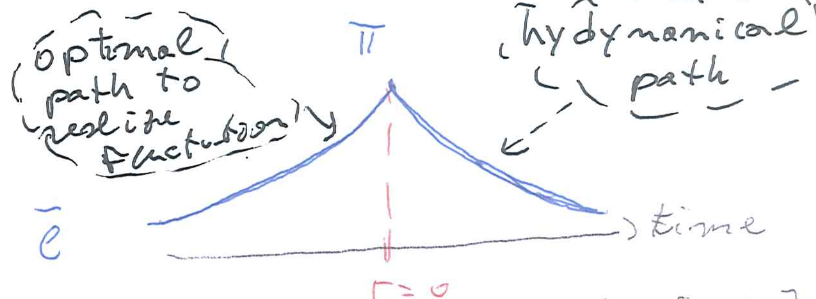
minimal cost to produce the fluctuation π at time $t=0$ starting from the stationary density at time $t = -\infty$



- In equilibrium

$$V(\pi) = \mathcal{F}(\pi) = \int_\Lambda f(e(x)|\bar{e})\,dx$$

and



[Onsager - Machlup principle]

- In non-equilibrium:

- $\mu^{\lambda,\tau}_{\Lambda_N}(\pi_N \sim \pi) \asymp e^{-N^d V(\pi)}$ describes the full statistics of the empirical density for the SNS [FW, BG]

- V is a Lypunov functional for the hydrodynamic evolution (H theorem)

- V solves a stationary Hamilton - Jacobi equation

6. Computing non-equilibrium potentials : $V(\pi) = ?$

A first guess

$$\mathcal{F}_{loc\,eq}(\pi) = \int_\Lambda F(\rho(x)\,|\,\bar\rho(x))\,dx \qquad \pi(dx) = \rho(x)\,dx$$

$\bar\rho(x)$ stationary solution hydrodynamic equation

Correct for independent particles and few other models, but wrong in general

- Generic Fact : V is non-local

  macroscopic correlations of SNS, as predicted by

  Fluctuating hydrodynamics [Spohn]

- In specific models we can really put our hands on V

WASEP $d=1$

$$c_{x,x+1} = \frac{1}{2} + \frac{E}{2N}$$

$$c_{x,x-1} = \frac{1}{2} - \frac{E}{2N}$$

if $E=0$

$$V(\pi) = \sup_{F\uparrow} \int_0^1 \Big\{ \rho \log\frac{\rho}{F} + (1-\rho)\log\frac{1-\rho}{1-F} + \log\frac{F'}{\rho_+-\rho_-} \Big\}\,dx \qquad [DLS]$$

achieved when F solves

$$\begin{cases} F(1-F)\dfrac{F''}{F'^2} + F = \rho \\ F(0) = \rho_-\,,\quad F(1) = \rho_+ \end{cases}$$

manifest non-locality

7. Lagrangian phase transitions [geometry of phase space]

Think of $I_{[0,T]}(\pi)$ as an action functional

$$I_{[0,T]}(\pi) = \int_0^T \mathcal{L}(\pi, \dot{\pi})\, dt$$

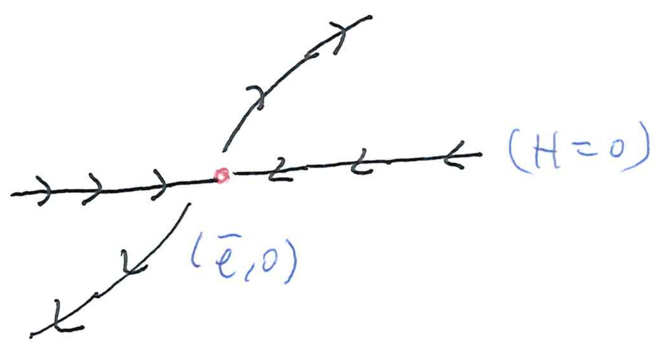
the corresponding Hamiltonian is

$$\mathcal{H}(e, H) = \langle \nabla H, \sigma(e) \nabla H \rangle_{L^2(\Lambda)} - \langle \nabla H, D\nabla e - \sigma(e) \rangle_{L^2(\Lambda)}$$

Canonical equations

$$\begin{cases} \dot{e} = \dfrac{\delta \mathcal{H}}{\delta H} & \text{parabolic} \\ \dot{H} = -\dfrac{\delta \mathcal{H}}{\delta e} & \text{anti-parabolic} \end{cases}$$

$(\bar{e}, 0)$ stationary solution



stable manifold

$\mathcal{M}_s = \{(e,0)\}$

Here lives the hydrodynamical flow

[$\bar{e}$ globally attractive]

$\mathcal{M}_u$ unstable manifold

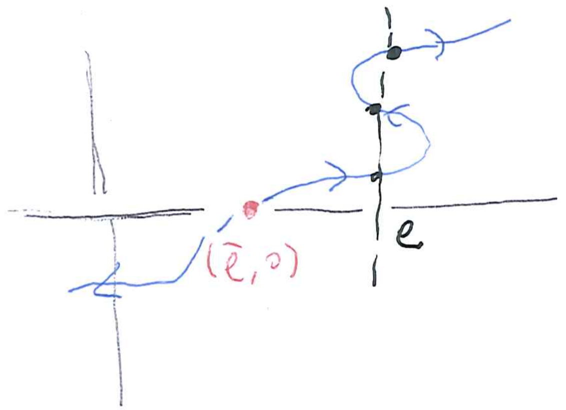
Here we look for the optimal path defining the quasipotential

- In equilibrium: $\mathcal{M}_u$ is a graph

$$\mathcal{M}_u = \{ (e, H) : H = -\frac{\delta \mathcal{F}}{\delta e} \}$$

counterpart of the reversibility of microscopic dynamics

- Out of equilibrium: no need to



  - we have few critical points of the action as candidates for the optimal path

  - for special e (caustic points) different branches will have the same cost

$\Rightarrow$ phase transitions
[corners in V]

Interpretation: at caustic points the optimal exit path is not unique
[varying e a little, the exit path changes by a finite amount]

- What can be proven. For WASEP the Hamiltonian flow can be constructed on $\mathcal{M}_u$ - Special e that are caustic points are then exhibited (a perturbative argument around $E = +\infty$) - [BDGJL]

8. Process level large deviations [BGL]

different point of view $\mathbb{P}^N_{\eta^N}$ as a probability on space/time paths

joint limit $N, T \to \infty$

- Donsker – Varadhan level 3 large deviations.

Fix N. $\eta(t)$ microscopic path $\in D([0,T]; \Omega_{N})$

extend it by periodizing to a path on $D(\mathbb{R}; \Omega_{N})$

$$R_T = \frac{1}{T}\int_0^T \delta_{\theta_s \eta(\cdot)}\, ds \quad \text{empirical process} \quad \in \mathcal{P}_{stat}\big(D(\mathbb{R}; \Omega_N)\big)$$

θ_s ← time translation

then

$$\mathbb{P}^N_{\eta^N}\left(R_T \sim R\right) \simeq e^{-T H_N(R)}$$

$$H_N(R) = ent\left(R \mid \mathbb{P}^N_{\mu^{\lambda,\varepsilon}_N}\right) = \lim_{T\to\infty} \frac{1}{T}\, Ent\left(R|_{[0,T]} \mid \mathbb{P}^N_{\mu^{\lambda,\varepsilon}_N}|_{[0,T]}\right)$$

affine functional

→ what happens as $N \to \infty$?

Project to hydrodynamical observable

$$\pi^N : D(\mathbb{R}; \Omega_{\Lambda_N}) \longrightarrow D(\mathbb{R}; \mathcal{M}_+(\Lambda))$$

$$\mathcal{R}^N_T = R_T \circ (\pi^N)^{-1} \in \mathcal{P}_{stat}(D(\mathbb{R}; \mathcal{M}_+(\Lambda)))$$

$$\mathcal{R}^N_T = \frac{1}{T}\int_0^T \delta_{\theta_s \pi^N_\cdot} \, ds$$

<u>then</u>

$$\mathbb{P}^N_{\eta^N}(\mathcal{R}^T_N \sim R) \asymp e^{-N^d T \, H(R)}$$

joint limit $N, T \to \infty$

$$H(R) = \int R(d\pi_\cdot) \, I_{[0,1]}(\pi_\cdot)$$

- What is it good for?

  - Statistics of the occupation measure

    $A \subset \Lambda$ $$\frac{1}{T}\int_0^T \pi^N_t(A)\, dt$$ time averaged density in A

  - Statistics of currents [not described here]