

# MFT FOR KINETIC MODELS

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## PLAN

1. LD FOR Poisson Point Process
2. Stochastic models associated to homogeneous Boltzmann eq.
3. LD: possible energy non conservation
4. Somov theorem for microcanonical ensemble
5. Improved upper bound for Wac's walk
6. Total number of collisions: a dynamical phase transition
7. Further directions

# Large deviations for Poisson point processes

$S$  measurable space [ I think  $S = \mathbb{R}^2$  ]

$\lambda$  positive measure on  $S$ ,  $\lambda$  finite  $\lambda(S) < \infty$

$Z \sim \text{PPP}(\lambda)$  points thrown at random on  $S$  with intensity  $\lambda$

[ hole falling from the sky ]

$Z$  : (random) atomic measure on  $S$  s.t.:

$$Z(B) \sim \text{Poisson}(\lambda(B))$$

$$B_1 \cap B_2 = \emptyset \Rightarrow Z(B_1) \text{ independent } Z(B_2)$$

$$\lambda \mapsto N\lambda \quad Z_N \sim \text{PPP}(N\lambda) \quad \text{Large deviations!}$$

[ Easy from independence : the rest for Poisson random variables carries out ]

$Q \in \mathcal{M}_+(S)$  positive measure on  $S$  (weak topology)

$$\mathbb{P}(Z_N \approx NQ) \asymp e^{-N I_X(Q)}$$

$$I_X(Q) = \begin{cases} \int d\lambda \left\{ \frac{dQ}{d\lambda} \log \frac{dQ}{d\lambda} - \left( \frac{dQ}{d\lambda} - 1 \right) \right\} & Q \ll \lambda \\ +\infty & \text{otherwise} \end{cases}$$

= relative entropy of  $Q$  w.r.t.  $\lambda$

## 2. STOCHASTIC MODELS ASSOCIATED TO HOMOGENEOUS BOLTZMANN EQ. [Kac's works]

$v = (v_1, \dots, v_N) \quad v_i \in \mathbb{R}^d \quad N \text{ velocities, } \quad \underline{H_0} \text{ space structure}$

Binary collisions with conservation of momentum and energy  
 Markov process (continuous time) with space state  $(\mathbb{R}^d)^N$  and generator

$$L_N f = \frac{1}{N} \sum_{i,j \neq i} L_{ij} f \quad f: \mathbb{R}^{dN} \rightarrow \mathbb{R}$$

$$L_{ij} f(v) = \int_{S^{d-1}} dv \, B(v_i - v_j, \omega) [f(-, v_i^1, \dots, v_j^1) - f(v)]$$

$$\begin{cases} v_i^1 = v_i + \omega \cdot (v_j - v_i) \, \omega \\ v_j^1 = v_j - \omega \cdot (v_j - v_i) \, \omega \end{cases} \quad \text{out going velocities}$$

$$B(v - v_*, \omega) = [ (v - v_*) \cdot \omega ]_- \quad \text{collision kernel (hard sphere)}$$

On a Fixed time interval

$$\# \text{ collisions} = O(N) \quad \# \text{ collisions / particle} = o(1)$$

kinetic scaling

# • Law of large numbers (propagation of chaos)

- $t=0$  start from a chaotic state  $\mu_0^N$
- $\mu_0^N$  exchangeable (invariant for permutations of the cases)

(marginal on the first variable)  $(\mu_0^N)_{x_1} \rightarrow \int_{\mathbb{R}} f_0 dv$   
 (probability density on  $\mathbb{R}$ )

(marginal on  $k$  variables)  $(\mu_0^N)_{x_1, \dots, x_k} \rightarrow (f_0 dv)^{\otimes k}$

- $t=t$   $\mu_t^N = \text{Law}(v(t))$  still chaotic

and  $f_t$  computed from  $f_0$  by solving homogeneous Boltz. eq.

$$\left. \begin{aligned} \partial_t F(v) &= \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} dv_0 \int_{\mathbb{S}^{d-1}} dw \, B(v-v_0, w) [F' F'_0 - F F'_0] \\ F|_{t=0} &= f_0 \end{aligned} \right\}$$

$$\begin{aligned} F &= F(v) \\ F' &= F'(v') \\ F'_0 &= F'(v_0) \\ F'_0 &= F'(v'_0) \end{aligned}$$

- GOAL: describe fluctuations in the setting of large deviations  
 $\rightarrow$  still incomplete [Poisson paradigm applies, not Gaussian paradigm]

### 3.1 LARGE DEVIATIONS : EMPIRICAL OBSERVABLES

Fix a time interval  $[0, T]$

• Empirical measure

$$\pi_t^N = \frac{1}{N} \sum_{i=1}^N \delta_{v_i(t)}, \quad t \in [0, T] \quad (\text{Random}) \text{ probability on } \mathbb{R}^d$$

In fact LLN equivalent to  $\pi_t^N \xrightarrow{P} f_t \frac{dv}{R}$  (deterministic limit)

• Empirical flow : records the details of the collisions:

times, incoming/outgoing velocities

$\omega^N$  (Random) positive measure on  $[0, T] \times (\mathbb{R}^d)^4$

$d\omega^N = \frac{1}{H} \#$  jumps in  $(t, t+dt)$  with incoming velocities in  $(v, v+dv)$ ,  $(v_*, v_*+dv_*)$  outgoing velocities in  $(v', v'+dv')$ ,  $(v'_*, v'_*+dv'_*)$

REN  $\omega^N(d\epsilon, \cdot)$  supported on  $v+v_* = v'+v'_*$ ,  $|v|^2 + |v_*|^2 = |v'|^2 + |v'_*|^2$

LLN  $\omega^N \xrightarrow{P} d\mathbb{F} \quad d\mathbb{F} = dt f_t(v) f_t(v_*) \frac{dv dv_*}{(2\pi)^d} B(v-v_*, w) dw$   
 $\xrightarrow{\text{SOLUTION TO BE}}$

• By conservation of the number of particles

if  $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ ,  $s < t$

"continuity equation"

$$\pi_t^N(\phi) - \pi_s^N(\phi) = \int_{[s, t] \times (\mathbb{R}^d)^4} d\omega^N [\phi' + \phi'_* - \phi - \phi_*]$$

### 3.2. LARGE DEVIATIONS: CANDIDATE RATE FUNCTION

Fix  $\mu_0^N$  initial (chaotic) state. Aim

Law of  $\mu_0^N$  (microscopic dynamics)  $\rightarrow \mu_0^N(\pi^N, \alpha^N) \approx (\pi, \alpha) \approx e^{-N I(\pi, \alpha)}$  (functions in initial state)

$$I(\pi, \alpha) = I_0(\pi_0) + I_{\text{dyn}}(\pi, \alpha) \quad \text{dynamic contribution}$$

How to guess  $I_{\text{dyn}}$ ?

- Suppose  $\pi_t^N(dv) \approx F_t(v) dv$ , for some path  $F_t$
- then the statistics of collisions will be essentially as a Poisson point process with intensity  $N R^F$
- If we know the statistics of collisions we recover  $\pi_t^N$  from the continuity eq.

$$I_{\text{dyn}}(\pi, \alpha) = \int dv dF \left[ \frac{\partial \alpha}{\partial F} \log \frac{\partial \alpha}{\partial F} - \left( \frac{\partial \alpha}{\partial F} - 1 \right) \right] + \infty$$

$\pi_t = F_t dv$  + continuity eq  
otherwise

Recall  $\dot{Q}^F = dt F(v) dv F_t^*(v_0) dv_0 B(v, v_0, \omega) d\omega$

## Remarks

[9]

•  $(\pi, Q) \mapsto I_{\text{eff}}(\pi, Q)$  NOT convex [  $Q^F$  is quadratic ]

• If we disregard  $\partial^N$

$$P_{k_0}^{(N)}(\pi^N \approx \pi) \asymp e^{-N \hat{I}(\pi)}$$

$$\hat{I}(\pi) = \inf_Q I(\pi, Q)$$

No explicit formula, just a variational representation

## 3.3 LARGE DEVIATIONS : RESULTS

• Deterministic (Newtonian) dynamics

Confort's theorem (derivation of Boltzmann eq. from Newton):

propagation of chaos holds with probability converging to 1 in the Boltzmann-Grad limit ( $N \rightarrow \infty$  --)

Large deviations require this probability to be in fact superexponentially close to one



• Heuristic argument and implications [Boudet, '20]

• Rigorous results in [Bodineau, Gallagher, Saint-Raymond, Simondon, '23]

they compute log moment generating function via cluster expansion (small time as in Confort)

# Stochastic dynamics

UB: [Leonard '85] (without  $Q^W$ ), [BBB02a]

[Rezakhalov '88] with discrete and bonded velocities, also a matching lower bound

→ Role of energy conservation for large deviation [Heydecker '23]  
has to be clarified

Analytical side: homogeneous Boltzmann equation

• ! energy conserving solution

•  $\exists$  solutions not energy conserving [LU, WENNERGER '02]

LLN:  $\mathbb{P}^N \rightarrow$  ! energy conserving solution

but  $I_{\text{dym}}(\text{LU-Wennergger}) = 0$

Heydecker:  $P_{\mu_0}^N(\text{LU-Wennergger}) \approx e^{-cN}$

→ Need a better candidate rate function!

#### 4. SANOV THEOREM FOR MICROCANONICAL ENSEMBLES

(11)

LU-WERNEBERG is really a static effect:

we have to understand the cost for sending to  $\infty$  a fraction of energy

- Sanov Thm.  $v_1, v_2, \dots, v_N$  iid with  $Q_{\text{aw}}$  on  $(\mathbb{R}^d)$

$$\pi^N = \frac{1}{N} \sum_{i=1}^N \delta_{v_i} \quad \text{large deviations with} \quad H_{\text{can}}(\pi) := \overline{\text{Ent}}(\pi | m) \\ = \int dm \frac{d\pi}{dm} \log \frac{d\pi}{dm}$$

- Microcanonical ensemble:

$$v_1, v_2, \dots, v_N \text{ sampled according to } m^{\otimes N} \left( \bullet \mid \frac{1}{N} \sum_i \frac{|v_i|^2}{2} = e \right)$$

We can observe (with exp. small probability)

$\pi$  with energy  $< e$

[Klein, Raman '15]

$$H_{\text{micro}}(\pi) = \begin{cases} \overline{\text{Ent}}(\pi | m) + C_e \left[ e - \pi\left(\frac{|v|^2}{2}\right) \right] & \text{if } \pi\left(\frac{|v|^2}{2}\right) \leq e \\ +\infty & \text{otherwise} \end{cases}$$

In fact:

(weak closure)

$$\big\{ \pi : \pi\left(\frac{|v|^2}{2}\right) = e \big\} = \big\{ \pi : \pi\left(\frac{|v|^2}{2}\right) \leq e \big\}$$

## 5. IMPROVED UPPER BOUND FOR KAC'S WALKS

(12)

- Start with microcanonical distribution of velocities

$$m^{\otimes N}(\cdot) \mid \frac{1}{N} \sum_i \frac{|v_i|^2}{2} = e, \quad \frac{1}{N} \sum_i v_i = 0$$

Then [BBBC '24]

$(\pi^N, \alpha^N)$  large deviations upper bound with

$$I(\pi, \alpha) = \begin{cases} H_{\text{micro}}(\pi_0) + I_{\text{dyn}}(\pi, \alpha) & \text{if } \pi_e(v) = 0 \\ +\infty & \text{otherwise} \end{cases} \quad \pi_e(v) = 0 \quad \forall v \in \mathbb{R}^d$$

$$\rightarrow \text{Now } I(\text{W-WENDEBERG}) > 0$$

- Matching lower bound proven in some cases (including W-Wenberger) but open in general

Recall

$$I_{\text{dyn}}(\pi, \alpha) = \int d\alpha^F \left\{ \frac{d\alpha}{d\alpha^F} \log \frac{d\alpha}{d\alpha^F} - \left( \frac{d\alpha}{d\alpha^F} - 1 \right) \right\}$$

$$\pi_e = f_e dv + \text{continuity equation}$$

## 6. TOTAL NUMBER OF COLLISIONS: a dynamical phase transition

(13)

- Observable to be analyzed

$$g_{H,T} = \frac{1}{NT} \# \text{ collisions in } [0, T]$$

Random variable with values in  $[0, \infty)$

→ joint limit  $H \rightarrow \infty \quad T \rightarrow \infty$  (in this order)

- Low of large numbers

$$\bar{q} = \bar{q}_e = \int m_e(\omega) m_e(\omega') B(v, \omega, \omega') d\omega$$

[typical value]

$$M_e = \text{Maxwellian with energy } e$$

$$\propto e^{-\frac{1}{2T} v^2} dv$$

$T = T(e)$

$$g_{H,T} \rightarrow \bar{q}$$

- Large deviations exhibit ~~an~~ interesting features (PHASE TRANSITIONS)

Due to possible energy non conservation  
and Lu-Weninger self solutions [BBBH '25]

# Initial distribution of velocities

Uniform measure on  $\{v\} = \frac{1}{N} \sum_{i=1}^N v_i = 0, \quad \frac{1}{N} \sum_{i=1}^N \frac{|v_i|^2}{2} = e$

i.e. we look at the stationary process

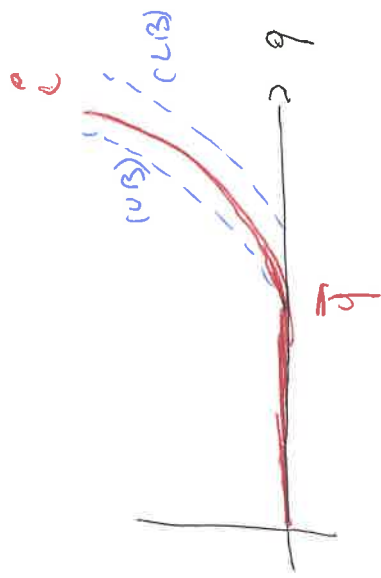
## Large deviations at scale $NT$

$$P_{NT}(q_{NT} \approx q) \propto e^{-NT \tilde{c}(q)}$$

$\tilde{c}$  given by a variational formula

$$\tilde{c}(q) \Rightarrow q \in [q, \bar{q}]$$

due to energy non conservation  
 Same microcanonical  
 or LU-WernerSeg



$\tilde{c}$  convex For thermodynamic reasons  
 [subadditivity]

(space / time)

Problem when  $NT \rightarrow \infty$  then  $T \rightarrow \infty$  but should be general.  
 Initial condition not relevant (ergodicity)

• Large deviations at scale  $N$

$$P_{st}^N(q_{N,T} \approx q) \approx e^{-N \tilde{I}(q)}$$

a simple explicit formula for  $\tilde{I}$



- $\tilde{I}$  convex, but an accident, depends on the form of  $B(u, w)$
- here stationary process is crucial:  
rate function would depend on initial condition
- here: first  $N \rightarrow \infty$ , then  $T \rightarrow \infty$  [No large deviations for  $T \rightarrow \infty$ ]

• Results obtained by analyzing  $I(\pi, \alpha)$  when  $T \rightarrow \infty$   
 they do not depend on the details of microscopic dynamics,  
 only on large deviations - (in principle, they apply also  
 to the deterministic case -

## 7. FURTHER DIRECTIONS

- Gradient flow formulation of homogeneous Boltzmann eq. and entropic propagation of chaos

[Ensaar '24] [BBO '26]

Natural connection between large deviations and gradient flows.

It can be exploited to prove convergence of microscopic entropy to the macroscopic one "Sandier - Gerfaty scheme"

For non homogeneous, but linear Boltzmann eq. it has been exploited in [BBB '20] to prove the diffusive limit

- Schrödinger problem in this context of binary collisions

[Bacukhoff, Contat, Leung '20] for  $10^6$  Nekean

- Large deviations for non equilibrium stationary states

Many results in the hydrodynamical regime