Energy non-conserving paths for the Kac's walk

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Contents

Introduction

General framework: microscopic (stochastic) dynamics with energy/momentum conservation.

Large deviations: asymptotic probability of "atypical" paths, exponentially small with the size of the systems.

Asymptotic probability of paths that violate the conservation laws? (Spoiler: for the homogeneous Boltzmann equation this problem is related to the existence of weak solutions with increasing energy (Lu and Wennberg solutions))

The homogeneous Boltzmann equation

$$\partial_t f_t(v) = \int_{\mathbb{R}^d} \mathrm{d}v_* \int_{S_{d-1}} \mathrm{d}\omega\, B(v - v_*, \omega) \big[f_t(v') f_t(v'_*) - f_t(v) f_t(v_*) \big]$$

v, v_* pre-collision velocities, v', v'_* post-collision velocities,

$$v' = v + (\omega \cdot (v_* - v))\omega, \quad v'_* = v_* - (\omega \cdot (v_* - v))\omega$$

Collision kernel $B(v - v_*, \omega) = \frac{1}{2} |\omega \cdot (v - v_*)|$ (hard sphere)

The homogeneous Boltzmann equation

$$\partial_t f_t(v) = \int_{\mathbb{R}^d} \mathrm{d}v_* \int_{S_{d-1}} \mathrm{d}\omega \, B(v - v_*, \omega) \big[f_t(v') f_t(v'_*) - f_t(v) f_t(v_*) \big]$$

- Uniqueness in the class of solutions which conserve the energy [Mischler, Wennberg '99]
- Existence of (weak) solutions with increasing energy [Lu, Wennberg '02]
- Any solution has not decreasing energy [Lu, Wennberg '02]
- Bounded collision kernel B: existence and uniqueness [Arkeryd '72]

Microscopic dynamics: the Kac's walk

$\{v_1, ..., v_N\}$, $v_i \in \mathbb{R}^d$. At exponentially distributed random times

$$(v_i, v_j) \to (v_i', v_j')$$

with $v_i + v_j = v_i' + v_j'$ and $|v_i|^2 + |v_j|^2 = |v_i'|^2 + |v_j'|^2$

Microscopic dynamics: the Kac's walk

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Continuous time Markov chain on $\left(\mathbb{R}^d\right)^N$

$$\mathcal{L}_N G(\boldsymbol{v}) = \frac{1}{N} \sum_{\{i,j\}} \int_{\mathbb{S}_{d-1}} \mathrm{d}\omega \, B\big(v_i - v_j, \omega\big)\big[G\big(T_{i,j}^{\omega}\boldsymbol{v}\big) - G(\boldsymbol{v})\big]$$

$$\left(T_{i,j}^{\omega}\boldsymbol{v}\right)_i = v_i + (\omega \cdot (v_j - v_i))\omega, \ \left(T_{i,j}^{\omega}\boldsymbol{v}\right)_j = v_j - (\omega \cdot (v_j - v_i))\omega$$

Kinetic limit and propagation of chaos

Initial distribution $F_0^N = f_0^{\otimes N}$. As $N \to \infty$

$$F_t^{N,j}(v_1, .., v_j) \to \prod_{i=1}^{j} f_t(v_i)$$

with f_t solution to the HBE (propagation of chaos).

[Kac '56] bounded collision kernel.

Empirical measure $\pi_t^N = \frac{1}{N} \sum_{i=1}^N \delta_{v_i(t)}$

(LLN) $\mathrm{d}\pi_t^N \to f_t \, \mathrm{d}v$ f solution to the HBE

[Sznitman '84] Hard sphere collision kernel, initial distribution with finite > 2 moment.

Discrete energy model

$\{\epsilon_1, .., \epsilon_N\}$, $\epsilon_i \in \mathbb{N}$

Collision $(\epsilon_i, \epsilon_j) \to (\epsilon_i', \epsilon_j')$, with $\epsilon_i + \epsilon_j = \epsilon_i' + \epsilon_j'$

Uniform collision kernel (bounded)

$$B(\epsilon, \epsilon_*, \epsilon', \epsilon_*') = \frac{1}{\epsilon + \epsilon_* + 1} \mathbb{1}_{\{\epsilon + \epsilon_* = \epsilon' + \epsilon_*'\}} \mathbb{1}_{\left\{\{\epsilon, \epsilon_*\} \neq \{\epsilon', \epsilon_*'\}\right\}}$$

LLN for the empirical measure: discrete HBE

$$\partial_t f_t(\epsilon) = \sum_{\epsilon_*, \epsilon', \epsilon_*'} B(\epsilon, \epsilon_*, \epsilon', \epsilon_*') \left[f_t(\epsilon') f_t(\epsilon_*') - f_t(\epsilon) f_t(\epsilon_*) \right].$$

LDP

Probability of "atypical paths"

$$P(\pi^N \sim \pi) \sim e^{-N\mathcal{I}(\pi)}$$

Rate function $\mathcal{I}(\pi) = \mathcal{E}(\pi_0) + \mathcal{J}(\pi)$

- $\mathcal{E}(\pi_0)$ "static contribution " (the initial distribution is not the prescribed one).
- $\mathcal{J}$ "dynamical contribution" (the path is not the solution to HBE). The zero level set is the set of solutions to HBE.

Large deviation results

- C.Léonard (1995): LD upper bound for Kac's walk
- F.Rezakhanlou (1998): LDP for non-homogeneous case, finite set of velocities (conservation of momentum, not of energy)
- B.B., D.Benedetto, L.Bertini, C.Orrieri (2021): LDP$^{(*)}$ for a Kac's like walk (conservation of momentum, not of energy)
- D.Heydecker (2022): LDP$^{(*)}$ for Kac's walk;
- T.Bodineau, I.Gallagher, L.Saint-Raymond, S.Simonella (2022);F. Bouchet (2020): newtonian dynamics (hard sphere interaction)

Rate function

Fix a one-particle distribution m. Léonard rate function

$$\mathcal{I}(\pi) = \mathrm{Ent}(\pi_0|m) + \mathcal{J}(\pi)$$

- Ent relative entropy
- $\mathcal{J}$ dynamical rate function

$$\mathcal{J}(\pi) = \sup_{\phi} \Big\{ \pi_T(\phi_T) - \pi_0(\phi_0) - \int_0^T \mathrm{d}t\, \pi_t(\partial_t \phi) \\ -\frac{1}{2} \int_0^T \mathrm{d}t \int \mathrm{d}\pi_t \otimes \mathrm{d}\pi_t \, \mathrm{d}\omega B \big(e^{\bar{\nabla}\phi} - 1\big) \Big\},$$

where $\bar{\nabla}\phi = \phi(v') + \phi(v'_*) - \phi(v) - \phi(v_*)$

Comments

$\mathcal{J} = 0$ iff $\mathrm{d}\pi_t = f_t \, \mathrm{d}v$, with f any solution to the HBE. In particular, the rate function $\mathcal{I}$ is zero on the Lu and Wennberg solutions while the probability of these paths is exponentially small with the number of particles N [Heydecker'22].

LDP in microcanonical ensemble

Static case

$(v_1, ..., v_N) \in \mathbb{R}^N$ uniformly distributed on

$$\Sigma^N_{e,0} := \{ \sum_{i=1}^N v_i^2 = Ne, \quad \sum_{i=1}^N v_i = 0 \}$$

$$\text{(LLN)} \quad \pi^N(du) := \frac{1}{N} \sum_{i=1}^N \delta_{v_i}(du) \to M_{e,0}$$

Sanov theorem for microcanonical ensemble

$$(\text{LDP}) \quad P(\pi^N \sim \tilde{m}) \sim e^{-NH_{e,0}(\tilde{m})}$$

where

$$H_{e,0}(\tilde{m}) = \begin{cases} Ent(\tilde{m}|M_{e,0}) + \frac{1}{2e}[e - \tilde{m}(v^2)] & \text{if } \tilde{m}(v) = 0, \tilde{m}(v^2) \leq e \\ +\infty & \text{otherwise} \end{cases}$$

[Chatterjee '17], [Kim, Ramanan '18], [Nam '20]

Kac's walk, empirical observable

Kac's walk on $\Sigma^N_{e,u}$.

empirical observable: empirical measure and flux;

$\{\tau_k^{(i,j)}\}_{k\geq 0}$ random collision times of the pair (v_i, v_j)

empirical flux: map $Q^N\colon D([0,T]\to\Sigma^N_{e,u})\to\mathcal{M}$ defined by

$$Q^N(F) := \frac{1}{N}\sum_{\{i,j\}}\sum_{k\geq 1} F\big(\tau_k^{i,j}; v_i(\tau_k^{i,j}-), v_j(\tau_k^{i,j}-), v_i(\tau_k^{i,j}), v_j(\tau_k^{i,j})\big)$$

Q^N records the collision

Balance equation

$\forall \phi \in C_b(\mathbb{R}^d)$

$$\pi^N_T(\phi_T) - \pi^N_0(\phi_0) - \int_0^T \mathrm{d}t\, \pi^N_t(\partial_t \phi_t) - \int Q^N(\bar{\nabla}\phi) = 0,$$

where $\bar{\nabla}\phi := \phi(v') + \phi(v'_*) - \phi(v) - \phi(v_*)$.

We call (π^N, Q^N) a **measure-flux pair**

Microcanonical initial data

Fix $u \in \mathbb{R}^d$, $e > 0$. Choose a probability measure m on $\mathbb{R}^d$ s.t.

- $m(e^{\gamma_0 |v|^2}) < +\infty$ for $\gamma_0 \in (-\infty, \gamma_0^*)$
- $\lim_{\gamma_0 \to \gamma_0^*} m(e^{\gamma_0 |v|^2}) = +\infty$.

Microcanonical initial distribution

$$\nu^N_{e,u}(\cdot) = m^{\otimes N}(\cdot | \sum_{i=1}^N v_i = Nu, \quad \sum_{i=1}^N |v_i|^2 = Ne)$$

tilted measure

$$m_{e,u}(\mathrm{d}u) = \frac{m(\mathrm{d}u) e^{\gamma_0(e,u)|v|^2 + \gamma(e,u)\cdot v}}{m\left(e^{\gamma_0(e,u)|v|^2 + \gamma(e,u)\cdot v}\right)}$$

with $\gamma_0(e,u), \gamma(e,u)$ s. t $m_{e,u}(v) = u$, $m_{e,u}(|v|^2) = e$.

LDP

Theorem (B., Benedetto, Bertini, Caglioti (2022))

Let (π^N, Q^N) be a measure-flux pair for the Kac's walk with microcanonical initial distribution $\nu^N_{e,u}$.

- *For any closed $C \subset \mathcal{S}$*

$$\overline{\lim_{N\to+\infty}} \frac{1}{N} \log \mathbb{P}^N_{\nu^N_{e,u}} \Big((\pi^N, Q^N) \in C \Big) \leq - \inf_{(\pi,Q)\in C} I_{e,u}(\pi, Q)$$

- *Under some extra assumption on m, for each open $O \subset \mathcal{S}$*

$$\underline{\lim_{N\to+\infty}} \frac{1}{N} \log \mathbb{P}^N_{\nu^N_{e,u}} \Big((\pi^N, Q^N) \in O \Big) \geq - \inf_{(\pi,Q)\in O\cap\hat{\mathcal{S}}} I_{e,u}(\pi, Q)$$

where
$\hat{\mathcal{S}} = \{(\pi, Q) \in \mathcal{S} : Q(|v|^2 + |v_*|^2 + |v'|^2 + |v'_*|^2) < +\infty\}$

The rate function $I_{e,u}$: warm up

$\mathrm{d}Q^{\pi\otimes\pi} := \frac{1}{2}\,\mathrm{d}\pi_t \otimes \mathrm{d}\pi_t\, B\,\mathrm{d}\omega\,\mathrm{d}t$ "typical flow"

$J(\pi, Q)$: relative entropy of Q w.r.t. $Q^{\pi\otimes\pi}$

$$J(\pi, Q) = \int \Big\{ \mathrm{d}Q \log \frac{\mathrm{d}Q}{\mathrm{d}Q^{\pi\otimes\pi}} - \mathrm{d}Q + \mathrm{d}Q^{\pi\otimes\pi} \Big\}.$$

$J = 0$ iff $(\pi, Q) = (\pi, Q^{\pi\otimes\pi})$, i.e. iff $\mathrm{d}\pi_t = f_t\,\mathrm{d}v$, with f solution to the HBE

The rate function $I_{e,u}$

$$I_{e,u}(\pi, Q) = H_{e,u}(\pi_0) + J_{e,u}(\mu, Q),$$

where

$$H_{e,u}(\pi_0) = \begin{cases} \mathrm{Ent}(\pi|m_{e,u}) + \left[\gamma_0^* - \gamma_0(e,u)\right]\left[e - \pi_0\left(|v|^2\right)\right] \text{ if } \pi_0 \in C_{e,u} \\ +\infty \, \text{otherwise} \end{cases}$$

$$J_{e,u}(\pi, Q) = \begin{cases} J(\pi, Q) & \text{if } \sup_t \pi_t(|v|^2) \leq e, \ \pi_t(v) = u \\ +\infty & \text{otherwise.} \end{cases}$$

Remarks

- LB for paths s.t. $Q(|v|^2 + |v_*|^2 + |v'|^2 + |v'_*|^2) < +\infty$ (non varying energy paths)
- the zero level set of $I_{e,u}$ is (π, Q^π) with $\pi_0 = m_{e,u}$ and $\mathrm{d}\pi = f\,\mathrm{d}v$, with f the **unique energy conserving solution** to the HBE with initial value $\mathrm{d}m_{e,u}/\,\mathrm{d}v$.
- $J(\pi, Q)$ (without constrain) is the one obtained in Léonard
- Same results for the discrete energy model.
- (Spoiler) Matching lower bound for a class of Lu& Wennberg solutions

Increasing energy solutions

Construction of Lu and Wennberg solutions.

Sequence of initial one particle density f_0^n:

- $f_0^n \to f_0$ weakly
- $\lim_{n\uparrow+\infty} \int f_0^n(v)|v|^2 \,\mathrm{d}v = e > \int f_0(v)|v|^2 \,\mathrm{d}v$

  (a fraction of energy evaporates at $+\infty$)

f_t evolves following the Boltzmann equation (typical behavior).
$\mathcal{E}(0^+) = e$, i.e. energy has a jump at $t = 0$.

Theorem (B., Benedetto, Bertini, Caglioti,(2022))

Given a non decreasing energy profile $\mathcal{E}(t)$ $t \in [0, T]$ piece-wise constant, with $\mathcal{E}(T) \le e$, there exists a Lu and Wennberg solution with an energy profile $\mathcal{E}$ and its asymptotic probability is

$$e^{-NI_{e,u}(f\,\mathrm{d}v, Q^{f\otimes f})} = e^{-NH_{e,u}(f\,\mathrm{d}v)}$$

Remark: the cost is due only to the initial distribution

LDP in canonical setting

LDP$^{(*)}$ with canonical rate function

$$I(\pi, Q) = \inf_{e,u} \left(A(e,u) + I_{e,u}(\pi, Q) \right)$$

where

$$A(e,u) = \sup_{\gamma} \left\{ \gamma_0 e + \gamma \cdot u - \log m\left(e^{\gamma_0 |v|^2 + \gamma \cdot v}\right) \right\}$$

(rate function for the energy and momentum of the sum of i.i.d. m-distributed random variables (Cramér))

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(rate function for the energy and momentum of the sum of i.i.d. m-distributed random variables (Cramér))

Asymptotic probability of the Lu and Wennberg solution

$$e^{N \gamma_0^* (\mathcal{E}(T) - \mathcal{E}(0))}$$

Discrete energy model

Trajectory with modified collision kernel

$$\tilde{B}(\epsilon, \epsilon_*, \epsilon', \epsilon'_*) = \frac{1}{2}\delta_{\epsilon,\epsilon_*}\delta_{\epsilon+\epsilon_*,\epsilon'+\epsilon'_*}\left[\delta_{\epsilon',\epsilon+\epsilon_*}+\delta_{\epsilon'_*,\epsilon+\epsilon_*}\right]\mathbb{1}_{\left\{\{\epsilon,\epsilon_*\}\neq\{\epsilon',\epsilon'_*\}\right\}},$$

(only particles with the same energy collide; in each collision the whole energy is transferred to a single particle)

Stationary state

$$t \to \infty \quad f_t \to \delta_0, \qquad \text{weakly}$$

Condensation to the zero energy state

Condensation in finite time

Time reparametrization: $t^* \in (0, T)$, $\alpha(t) = \frac{t}{1-t/t^*}$,

$$\bar{f}_t(\epsilon) = \begin{cases} f_{\alpha(t)}(\epsilon) & t \in [0, t^*) \\ \delta_{\epsilon,0} & t \in [t^*, T], \end{cases}$$

flux $d\bar{Q} = \mathrm{d}t\, \bar{q}_t$

$$\bar{q}_t(\epsilon, \epsilon_*, \epsilon', \epsilon'_*) = \frac{1}{2}\bar{f}_t(\epsilon)\bar{f}_t(\epsilon_*)\tilde{B}_t(\epsilon, \epsilon_*, \epsilon', \epsilon'_*),$$

Asymptotic probability

Theorem (B., Benedetto, Bertini, Caglioti,(2021))

$$P\big((\pi^N, Q^N) \sim (\bar{f}_t(\epsilon)\,\mathrm{d}\epsilon, d\bar{Q})\big) \sim e^{-Nc}$$

Entropy dissipation formulation of HBE

Entropy production

$\pi(\mathrm{d}v) = f(v)\,\mathrm{d}v$; entropy $H(\pi) = \int \mathrm{d}v\, f \log f$

For any measure-flux pair (π, Q)

$$\frac{\mathrm{d}}{\mathrm{d}t} H(\pi_t) = \int \mathrm{d}v\ \dot{f}_t \log f_t = Q(\bar{\nabla} \log f)$$
$$= \iint \mathrm{d}v\, \mathrm{d}v_*\, \mathrm{d}\omega q_t \log \frac{f_t' f_t'^*}{f_t f_t^*}$$

Then

$$H(\pi_t) - H(\pi_0) = J(\pi, Q) - J(\pi, \mathcal{Y}Q)$$

or

$$H(\pi_t) - H(\pi_0) + J(\pi, \mathcal{Y}Q) = J(\pi, Q) \geq 0$$

Entropy dissipation inequality

Since $J = 0$ iff (π, Q) solves HBE, we have the following characterization of the solution to HBE

$$H(\pi_t) - H(\pi_0) + J(\pi, \mathcal{Y}Q) \leq 0$$

Entropy dissipation inequality

Since $J = 0$ iff (π, Q) solves HBE, we have the following characterization of the solution to HBE

$$H(\pi_t) - H(\pi_0) + J(\pi, \mathcal{Y}Q) \leq 0$$

(equivalently)

$$H(\pi_t) - H(\pi_0) + J(\pi, \mathcal{Y}Q) + J(\pi, Q) \leq 0$$

and $J(\pi, \mathcal{Y}Q) + J(\pi, Q) = \int_0^T \mathrm{d}t \mathcal{D}(\pi_t) + \mathcal{R}(\pi, Q)$

See B,Benedetto, Bertini, Orrieri '21. Uniqueness problem.

EDI of HBE

Set $e_0 = \pi_0(|v|^2)$. The measure-flux pair $(\pi, Q) \in \mathcal{S}_{\mathrm{be}}$ is a solution to the HBE iff

$$\begin{aligned} \mathcal{H}(\pi_T) + \int_0^T \mathrm{d}t\, \mathcal{D}(\pi_t) + \mathcal{R}(\pi, Q) &\leq \mathcal{H}(\pi_0), \\ \sup_{t\in[0,T]} \pi_t(|v|^2) &\leq e_0. \end{aligned}$$

- uniqueness
- related result: M. Erbar'23
- (in progress) convergence of the Kac's walk + entropic propagation of chaos under minimal assumptions.

Thank you!