Asymptotic probability of energy non-conserving paths for binary collision stochastic models

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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?

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

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

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

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

Kinetic limit

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

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

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

$$\partial_t f_t(v) = \frac{1}{2}\int_{\mathbb{R}^d} \mathrm{d}v_* \int_{S_{d-1}} \mathrm{d}\omega\, B(v - v_*, \omega)\big[f_t(v')f_t(v'_*) - f_t(v)f_t(v_*)\big]$$

- (Kac'56) bounded collision kernel.
- (Sznitman'84) hard sphere collision kernel $B = \frac{1}{2}|(v_i - v_j)\cdot\omega|$, initial distribution with finite > 2 moment.

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- Uniqueness in the class of energy conserving solutions (Mischler, Wennberg'99).
- $\exists$ weak solutions with increasing energy (Lu, Wennberg'02)

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)

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

LLN for the empirical measure: discrete HBE

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

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 (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 (variational formula); the zero level set is the set of solutions to HBE.
- $\mathcal{I}$ is zero on the Lu-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

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

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

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

Sanov theorem for microcanonical ensemble

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

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 $\Sigma^N_{e,u}$.

emprirical observable: empirical measure and flow;

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

empirical flow: 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

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

$$\pi_T^N(\phi_T) - \pi_0^N(\phi_0) - \int_0^T \mathrm{d}t\, \pi_t^N(\partial_t \phi_t) - \int Q^N(\bar{\nabla}\phi) = 0,$$

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

LDP for microcanonical initial data

Initial distribution.

$m \in P(\mathbb{R}^d)$ such that $m(e^{\gamma_0 |v|^2}) < +\infty$ for $\gamma_0 \in (-\infty, \gamma_0^*)$ and $\lim_{\gamma_0 \to \gamma_0^*} m(e^{\gamma_0 |v|^2}) = +\infty$.

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

tilted measure

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

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

LDP for microcanonical initial data

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

$J(\pi, Q)$: relative entropy of Q with respect to Q^π

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

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

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

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

where $J_{e,u}(\pi, Q) = J(\pi, Q)$ if $\pi_t(|v|^2) \le e$ and $\pi_t(v) = u$, while $J_{e,u} = +\infty$ otherwise.

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 homogeneous Boltzmann equation with initial value $\mathrm{d}m_{e,u}/\mathrm{d}v$.
- $J(\pi, Q)$ (without constrain) is the one obtained in Léonard, and $J = 0$ on any solution to the homogeneous Boltzmann equation
- Same results for the discrete energy model.

Kac's walk: increasing energy solutions

Construction of Lu and Wennberg solutions.
Sequence of initial densites 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 $\mathcal{E}(t)$ $t \in [0, T]$ piecewise constant, with $\mathcal{E}(T) \leq e$, 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

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))

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

Binary collision models with condensation

Non-reversible discrete energy binary collision models

$\{\epsilon_1, .., \epsilon_N\}$, $\epsilon_i \in \mathbb{N}$; binary collision with $\epsilon_i + \epsilon_j = \epsilon_i' + \epsilon_j'$

Collision kernel, $a \in [0,1)$ ($a \in [0,1]$?)

$$\tilde{B}_a = (1+\epsilon+\epsilon_*)^a \mathbb{1}_{\{\epsilon+\epsilon_*=\epsilon'+\epsilon_*'\}} \frac{1}{2}\Big[\mathbb{1}_{\{\epsilon'=\epsilon+\epsilon_*\}} + \mathbb{1}_{\{\epsilon_*'=\epsilon+\epsilon_*\}}\Big]$$

Non-reversible dynamics; for $a = 0$ $\tilde{B}_a \sim \tilde{B}$. LLN

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

Stationary measure: $\bar{f} = \delta_0$

Non-reversible discrete energy binary collision models II

Collision kernel $B = (1-\alpha)\tilde{B}_a + \alpha B_b$, $\alpha \in [0,1]$, where

$$B_b = \big(1+\epsilon+\epsilon_*\big)^{-b} \mathbb{1}_{\{\epsilon+\epsilon_*=\epsilon'+\epsilon'_*\}},$$

Total collision rate $\lambda = (1-\alpha)\lambda_a + \alpha\lambda_b$

$$\lambda_a = \lambda_a(\epsilon,\epsilon_*) = \big(1+\epsilon+\epsilon_*\big)^a, \qquad \lambda_b = \big(1+\epsilon+\epsilon_*\big)^{(1-b)}$$

Preliminary results (B.,D. Benedetto, S. Marchesani):

- No condensation if $a+b<2$ (ex. λ_a, λ_b of the same order)
- Condensation for $a=b=1$ if $\alpha > \alpha(E)$, with E initial energy.

Thank you!