Large deviations of the current in collisional dynamics

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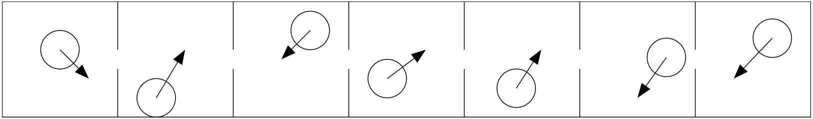
Collaborations

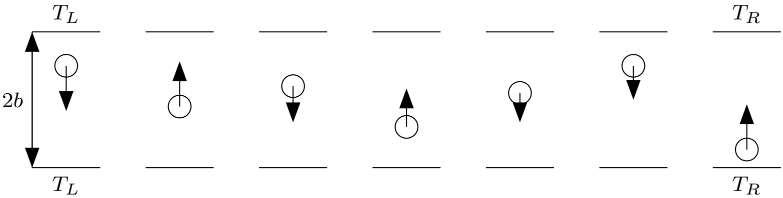
- T. Gilbert, R. Lefevere, Heat conductivity from molecular chaos hypothesis in locally confined billiard systems. Physical Review Letters (2008) 101, 200601
- R.Lefevere, L.Zambotti Hot scatterers and tracers for the transfer of heat in collisional dynamics. Journal of Statistical Physics (2010) 139, 686-713
- R. Lefevere, M. Mariani and L. Zambotti, Macroscopic fluctuations theory of aerogel dynamics. Journal of Statistical Mechanics (2010) L12004
- R. Lefevere, M. Mariani and L. Zambotti, Large deviations of the current in stochastic collisional dynamics. Journal of Mathematical Physics (2011) 52, 033302

Aerogels

Local collision dynamics.

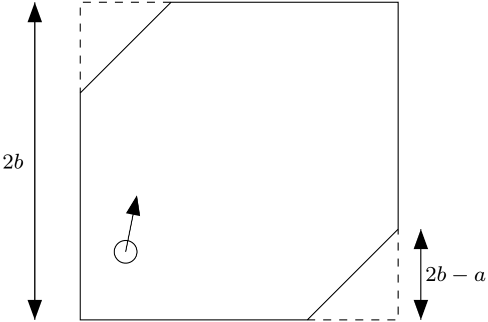


Introduced by Prosen-Campbell



- $T_L \neq T_R$, $b > 0$, $b < a < 2b$.
- $(q_i, p_i)_{1 \leq i \leq N}$, $q_i \in [-b, b]$ et $|q_i - q_{i+1}| \leq a$.
- Ballistic motion+ reflections on the interval's boundaries.
- Interaction if $|q_i - q_{i+1}| = a$ $(p_i = v, p_{i+1} = v') \rightarrow (p_i = v', p_{i+1} = v)$

Local collisions dynamics



$$\mathcal{B} = \{(q_1, q_2) : q_1 \in [-b, b], q_2 \in [-b, b], |q_1 - q_2| \leq a\}$$

Local collision dynamics.

- Energy of particle n at time t :

$$E_n(t) - E_n(0) = J_{n-1}([0,t]) - J_n([0,t])$$

- Time-integrated current:

$$J_n([0,t]) = -\frac{1}{2} \sum_{k=1}^{C_n(t)} [p_{n+1}^2(\tau_n^k) - p_n^2(\tau_n^k)]$$

$(\tau_n^k)_k$ is the sequence of collision times between particles n and $n+1$. $C_n(t)$ number of collisions up to time t.

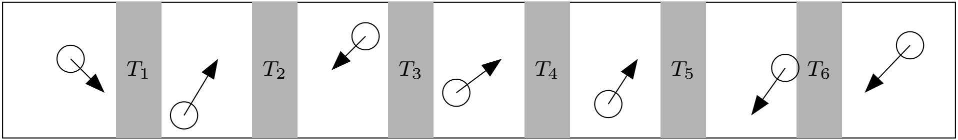
Guess

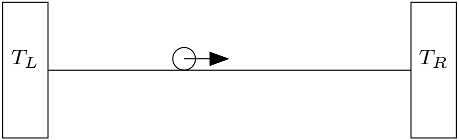
- $$\lim_{t\to+\infty}\frac{1}{t}J_n([0,t]) = -\kappa(T_{n+1}-T_n)$$
- $\kappa = \nu$ the frequency of collision in equilibrium (at temperature, say $\frac{T_i+T_{i+1}}{2}$)

Collaboration with T.Gilbert :

In “many” models, when the collisions become rare and the system large $\kappa \to \nu \sim \sqrt{T}$. *Even for systems having no local chaotic properties !*

Assumption : As $N \to \infty$, separation of scales : $\Delta t_{\text{macro}} >>> \mathbb{E}(\tau_{\text{coll}})$.

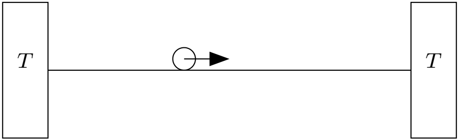




Update of the particle's speed with the law ($\beta = T^{-1}$):

$$\varphi(v) = \beta v e^{-\beta \frac{v^2}{2}}.$$

Stochastic collisions dynamics : equilibrium.



Markov process $(q(s), p(s))$ with invariant measure :

$$\gamma(dq, dp) = \sqrt{\frac{\beta}{2\pi}} \mathbb{1}_{[0,1]}(q) e^{-\beta \frac{p^2}{2}}$$

- Waiting times distributed with ($\beta = T^{-1}$)

$$\frac{\beta_L}{\tau^3}\exp(-\frac{\beta_L}{2\tau^2}) \quad \text{and} \quad \frac{\beta_R}{\tau^3}\exp(-\frac{\beta_R}{2\tau^2}).$$

- Total time elapsed at the $k+1$-st collision :

$$S_k := S_0 + \tau_1 + \cdots + \tau_k$$

- Renewal process :

$$N_t = \sum_{k=1}^{\infty} \mathbf{1}_{(S_k \le t)} = \sup\{k : S_k \le t\}$$

A *Markov renewal process* is a pair of stochastic processes $(X_n, \tau_{n+1})_{n \geq 0}$, such that

1. $(X_n)_{n \geq 0}$ is a Markov chain in some finite state space E with transition density $(t_{ij})_{i,j \in E}$
2. conditionally on $\mathcal{H} = \sigma((X_n)_{n \geq 0})$, $(\tau_{n+1})_{n \geq 0}$ is an independent sequence of positive random variables such that for all $n \geq 1$

$$\mathbb{P}(\tau_n \leq t \,|\, \mathcal{H}) = \mathbb{P}(\tau_n \leq t \,|\, X_n, X_{n+1}) = G_{ij}(t)$$

on the event $\{X_n = i, X_{n+1} = j\}$, where $(G_{ij})_{i,j \in E}$ is a family of distribution functions on $]0, +\infty[$.

$$J[0,t] = \sigma_0 \frac{1}{2} \sum_{k=1}^{N_t} (-1)^k v_k^2$$

Proposition

$$\lim_{t\to\infty} \frac{J[0,t]}{t} = \frac{T_L - T_R}{\left(\frac{\pi}{2T_L}\right)^{\frac{1}{2}} + \left(\frac{\pi}{2T_R}\right)^{\frac{1}{2}}} \quad \text{a.s.}$$

where T_L and T_R are the left and right temperatures.

Proof : Renewal theorem for the (Markov) renewal process N_t with waiting times τ distributed with ($\beta = T^{-1}$)

$$\frac{\beta_L}{\tau^3} \exp(-\frac{\beta_L}{2\tau^2}) \quad \text{and} \quad \frac{\beta_R}{\tau^3} \exp(-\frac{\beta_R}{2\tau^2}).$$

$$\lim_{t\to\infty} \frac{N_t}{t} = \frac{1}{\mathbb{E}_{\beta_L}(\tau) + \mathbb{E}_{\beta_R}(\tau)} = \kappa, \quad \text{a.s.}$$

Back to the spatially extended dynamics

$$\frac{T(n,t+\Delta t)) - T(n,t)}{\Delta t} \sim \frac{1}{\Delta t}\{J(n,[t,(t+\Delta t)]) - J(n-1,[t,(t+\Delta t)])\}$$

We want to look at the limit $\Delta t \to \infty$, $J(n,[t,(t+\Delta t)])$ computed with temperatures $\{T(n,t), T(n+1,t)\}$ at the boundaries of the interval. In the stationary regime

$$\begin{aligned} 0 &= \lim_{\Delta t \to \infty} \frac{1}{\Delta t}\{J(n,[t,(t+\Delta t)]) - J(n-1,[t,(t+\Delta t)]) \\ &= \frac{T_n - T_{n+1}}{(\frac{\pi}{2T_n})^{\frac{1}{2}} + (\frac{\pi}{2T_{n+1}})^{\frac{1}{2}}} - \frac{T_{n-1} - T_n}{(\frac{\pi}{2T_{n-1}})^{\frac{1}{2}} + (\frac{\pi}{2T_n})^{\frac{1}{2}}} = 0 \end{aligned}$$

Compare the stationary solutions between stochastic model and deterministic models (weakly interacting regime and large N)

Stationary solution in the continuum limit

$$T(x) = (T_L^{\frac{3}{2}} + x(T_R^{\frac{3}{2}} - T_L^{\frac{3}{2}}))^{\frac{2}{3}}, \quad x \in [0,1]$$

Good agreement : remember $\kappa = \nu \sim \sqrt{T}$.

Fluctuations of the current

Study LDF of the current $\mathcal{I}(j,\tau,T)$:

$$\mathbb{P}_{\tau,T}\left(\frac{J[0,t]}{t}=j\right)\sim e^{-t\mathcal{I}(j,\tau,T)},\quad t\to\infty.$$

$\mathbb{P}_{\tau,T}$ stochastic dynamics with a fixed temperature difference $\tau=T_L-T_R$, average temperature $T=\frac{T_L+T_R}{2}$.

Theorem

If $\tau\neq 0$ then,

$$\lim_{\varepsilon\downarrow 0}\varepsilon^{-2}\mathcal{I}(\varepsilon j,\varepsilon\tau,T)=\mathcal{G}(j,\tau,T)=\begin{cases}\frac{(j-\kappa\tau)^2}{4\kappa T^2} & \text{if}\quad j\tau>\kappa\tau^2\\ 0 \quad \text{if}\quad j\tau\in[0,\kappa\tau^2] & \\ -\frac{j\tau}{2T^2} & \text{if}\quad j\tau\in[-\kappa\tau^2,0]\\ \\ \frac{j^2+\kappa^2\tau^2}{4\kappa T^2} & \text{if}\quad j\tau<-\kappa\tau^2,\end{cases}$$

where $\kappa=\left(\frac{T}{2\pi}\right)^{\frac{1}{2}}$.

Note : ε will be N in the diffusive scaling limit below.

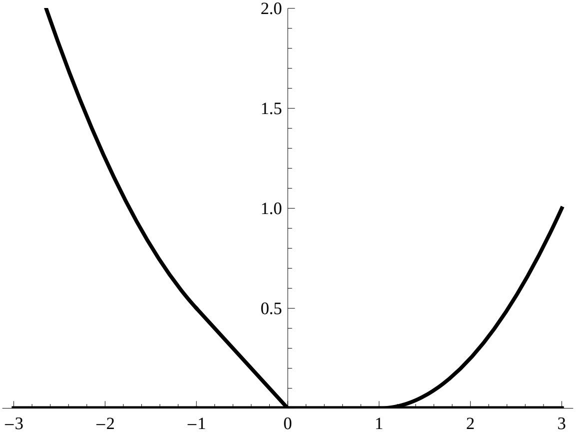


Figure: Plot of $\mathcal{G}$ as a function of j for $\kappa\tau = \kappa T^2 = 1$

Gallavotti-Cohen symmetry:

$$\mathcal{G}(j,\tau,T) - \mathcal{G}(-j,\tau,T) = \frac{j\tau}{2T^2}.$$

Flat part

Origin:

1. Current :

$$J[0,t] = \sigma_0 \frac{1}{2} \sum_{k=1}^{N_t} (-1)^k v_k^2$$

2. Large deviations of N_t for a renewal process whose renewal times $(\tau_k)_{k\in\mathbb{N}}$ are distributed with density :

$$\psi(\tau) = \frac{1}{\tau^3} \exp(-\frac{1}{2\tau^2}).$$

$\forall \alpha > 0$,

$$\begin{aligned} \mathbb{P}\left(\frac{N_t}{t} \leq \alpha\right) &= \mathbb{P}\left(S_{[\alpha t]+1} > t\right) \\ &\geq \mathbb{P}\left(\tau_1 > t\right) \sim t^{-2}, \text{ for } t \text{ large enough.} \end{aligned}$$

Take the Ising model : spin variables $\sigma_i = \pm 1$, $i \in \mathbb{Z}^d$ distributed according to Boltzmann-Gibbs at temperature β^{-1}

$$\mu(\sigma_\Lambda) = \frac{e^{-\beta H_\Lambda(\sigma_\Lambda)}}{Z_\Lambda(\beta, h)}$$

with Hamiltonian:

$$H_\Lambda(\underline{\sigma}) = -\sum_{<i,j>\in\Lambda} \sigma_i \sigma_j + h \sum_{i\in\Lambda} \sigma_i, \quad +\text{b.c.}$$

Large deviations of $\frac{1}{N^d} \sum_{i\in\Lambda} \sigma_i$

$$\mathbb{P}(\frac{1}{N^d} \sum_{i\in\Lambda} \sigma_i \in dm) \sim \exp(-N^d I(m,\beta))$$

$I(m,\beta)$ is the Legendre transform of the Helmholtz free energy :

$$F(h,\beta) = -\lim_{N\to\infty} \frac{1}{N^d} \log Z_\Lambda(h,\beta)$$

- Compute the cumulants (correlation functions)
- See phase transitions (lack of strict convexity of $I(m,\beta)$)

Macroscopic fluctuations theory
Onsager-Machlup 1953
Bodineau,Derrida
Bertini, De Sole, Gabrielli, Jona-Lasinio, Landim

For diffusive systems (i.e ϵ_N and j_N are related to microscopic energy and current by a diffusive scaling):

$$\mathbb{P}\left(\{\epsilon_N \simeq \epsilon, j_N \simeq j\} \text{ on}[0,1] \times [0,\mathrm{S}]\right) \sim \exp[-N\hat{\mathcal{I}}(j,\epsilon)]$$

where $\hat{\mathcal{I}}(j,\epsilon)$ is given by

$$\hat{\mathcal{I}}(j,\epsilon) = \int_0^S dt \int_0^1 dx\, \mathcal{G}(j(x,t), \partial_x \epsilon(x,t), \epsilon(x,t))$$

if j and ϵ satisfy $\partial_s \epsilon(x,s) = -\partial_x j(x,s)$, and $\hat{\mathcal{I}} = +\infty$ otherwise.
"Almost" all known examples :

$$\mathcal{G}(j,\tau,T) = \frac{(j-\kappa\tau)^2}{4\kappa T^2}.$$

Local billard dynamics might be different!

Diffusive scaling

Define $T_N : [0,1] \times \mathbb{R}^+ \to \mathbb{R}^+$ and $\mathcal{J}_n : [0,1] \times \mathbb{R}^+ \to \mathbb{R}$.

$$\begin{aligned} T_N(x,t) &= T([Nx], N^2 t) \\ \mathcal{J}_N(x,t) &= N \cdot \frac{1}{N^2 \Delta t} \cdot J([Nx], [N^2 t, N^2(t+\Delta t)]), \quad \Delta t \text{ arbitrary} \end{aligned}$$

Want to show in the original model :

Proposition

When $N \to \infty$, $\Delta t \to 0$, $(T_N, \mathcal{J}_N)$ converge in L^2 to the unique solution $(\hat{T}, \hat{\mathcal{J}})$ of

- $\partial_t \hat{T}(x,t) = -\partial_x \hat{\mathcal{J}}(x,t)$
- $\hat{\mathcal{J}}(x,t) = -\kappa(\hat{T}(x,t))\partial_x \hat{T}(x,t)$

with $\kappa(T) = (\frac{T}{2\pi})^{\frac{1}{2}}$ and suitable b.c.

One can modify the static model :

$$\begin{aligned} T(n, N^2(t+\Delta t)) - T(n, N^2 t) = \quad & N \quad \cdot \frac{1}{N^2 \Delta t} \{J(n, [N^2 t, N^2(t+\Delta t)]) \\ & - \quad J(n-1, [N^2 t, N^2(t+\Delta t)])\} \Delta t \end{aligned}$$

$$T_N(x, t+\Delta t) - T_N(x,t) = N \left(\mathcal{J}_N(x - \frac{1}{N}, t) - \mathcal{J}_N(x,t) \right) \Delta t$$

Current computed with $\{T([Nx], t), T([Nx]+1, t)\}$.

Fluctuations at finite N

Want to look at :

$$\mathbb{P}\left(\{T_N \simeq T, \mathcal{J}_N \simeq j\} \text{ on}[0,1]\times[0,\mathrm{S}]\right) \sim \exp[-N\,\hat{\mathcal{I}}(j,\epsilon)]$$

At finite N, and for each $(x,t)\in[0,1]\times[0,S]$, $\mathcal{J}_N(x,t)$ is a random variable (and so is $T_N(x,t)$).
Independence over small space-time windows :

$$\mathbb{P}\left(\{T_N \simeq T, \mathcal{J}_N \simeq j\} \text{ on}[0,1]\times[0,\mathrm{S}]\right) = \prod_{k,l} \mathbb{P}(\mathcal{J}_N(x_k,t_l) \simeq j(x_k,t_l))$$

Compute :

$$\begin{aligned} & \log \mathbb{P}[\mathcal{J}_N(x,t) = j(x,t)] \\ = \quad & \Delta t \cdot N^2 \frac{1}{N^2 \Delta t} \log \mathbb{P}[\mathcal{J}_N(x,t) = j(x,t)] \\ = \quad & \Delta t \cdot N^2 \frac{1}{N^2 \Delta t} \log \mathbb{P}[\frac{J([Nx],[N^2 t, N^2(t+\Delta t)])}{N^2 \Delta t} = \frac{j(x,t)}{N}] \end{aligned}$$

Current computed with temperatures $\{T([Nx],N^2 t), T([Nx]+1, N^2 t)\}$.
Remember : the theorem allows to compute:

$$\begin{aligned} & \lim_{\varepsilon\to 0} \lim_{s\to\infty} \frac{1}{\varepsilon^2}\frac{1}{s} \log \mathbb{P}[\frac{J([Nx],[0,s])}{s} = \varepsilon j(x,t)] \\ = \quad & \mathcal{G}(j(x,t), \partial_x T(x,t), T(x,t)) \end{aligned}$$

Putting everything together :

$$\mathbb{P}\left(\{T_N \simeq T, j_N \simeq j\}\right) \sim \exp[-N\,\hat{\mathcal{I}}(j,T)]$$

where $\hat{\mathcal{I}}(j,T)$ is given by

$$\hat{\mathcal{I}}(j,T) = \int_0^S dt \int_0^1 dx\, \mathcal{G}(j(x,t), \partial_x T(x,t), T(x,t))$$

if j and T satisfy $\partial_s T(x,s) = -\partial_x j(x,s)$, and $\hat{\mathcal{I}} = +\infty$ otherwise.

$$\mathcal{G}(j,\tau,T) = \begin{cases} \frac{(j-\kappa\tau)^2}{4\kappa T^2} \text{ if } j\tau > \kappa\tau^2 \\ 0 \text{ if } j\tau \in [0,\kappa\tau^2] \\ -\frac{j\tau}{2T^2} \text{ if } j\tau \in [-\kappa\tau^2, 0] \\ \frac{j^2+\kappa^2\tau^2}{4\kappa T^2} \text{ if } j\tau < -\kappa\tau^2, \end{cases}$$

$$\mathcal{G}(j,\tau,T) \neq \frac{(j-\kappa\tau)^2}{4\kappa T^2}!$$

Conclusions.

- Argument based on the fact that under (local) equilibrium distributions there are slow particles with sufficiently large probability.
- Apply to “tracer models” introduced by Larralde, Mejia-Monasterio, Leyvraz
- Draw experimental consequences and observe them in numerical simulations.