Large deviations of the current in collisional dynamics

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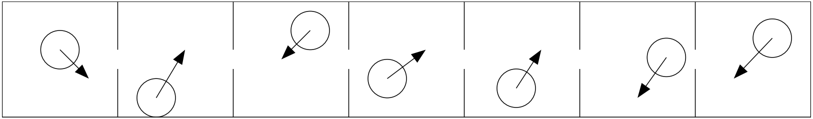
Collaborations

- 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

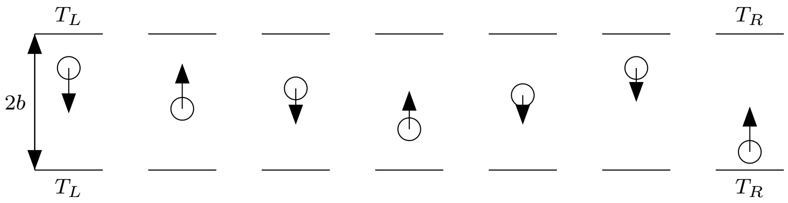
Aerogels

Local collision dynamics.



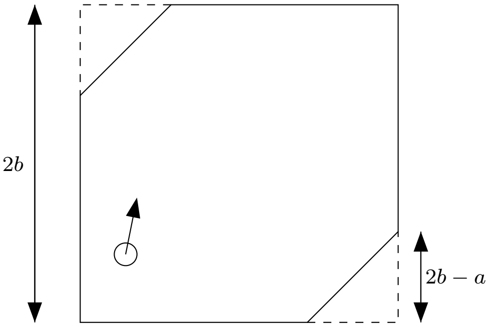
Local collisions dynamics

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 $|q_i - q_{i+1}| = a$ $(p_i = v, p_{i+1} = v') \to (p_i = v', p_{i+1} = v)$

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.

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

$$T_N(x,t) = \frac{1}{\varepsilon N} \sum_{i \in B_\varepsilon(x)} E(i, N^2 t), \quad B_\varepsilon(x) = \{i : |\frac{i}{N} - x| \le \varepsilon\}$$

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

Want to show :

Fourier law

When $N \to \infty$, $\Delta t \to 0$, $\varepsilon \to 0$, $(T_N, \mathcal{J}_N)$ 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 $\kappa(T) \sim (T)^{\frac{1}{2}}$ and suitable b.c.

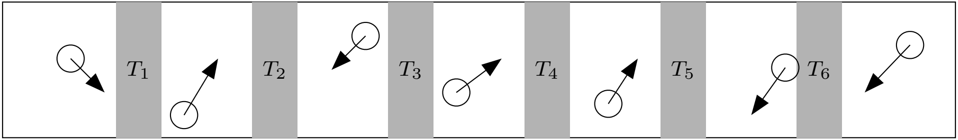
Much too hard!

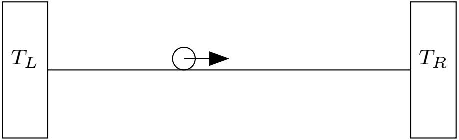
Evolution of energy :

$$E(n, s + \Delta s) - E(n, s) = J(n, [s, s + \Delta s]) - J(n - 1, [s, s + \Delta s])$$

Replace by stochastic model :

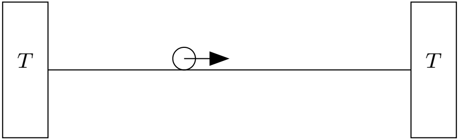
1. Thermal baths having temperatures $T(n, s)$, piecewise constant in time
2. Tracer particles carrying energy current $J(n, [s, s + \Delta s])$ and interacting randomly with the heat baths





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

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



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

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

Renewal process

- Waiting times distributed with ($\beta_\pm = T_\pm^{-1}$)

$$\psi_-(\tau) := \frac{\beta_-}{\tau^3} \exp(-\frac{\beta_-}{2\tau^2}) \quad \text{and} \quad \psi_+(\tau) := \frac{\beta_+}{\tau^3} \exp(-\frac{\beta_+}{2\tau^2}).$$

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

$$S_k^\pm := S_0^\pm + \sum_{i=1}^k (\tau_i^\pm + \tau_i^\mp), \quad \tau_i^\pm \sim \psi_\pm$$

- Renewal processes :

$$N_t^\pm = \sup\{k : S_k^\pm \le t\}$$

  with waiting times distributed with $\psi^+ * \psi^-$.

Let

$$S_k = \sum_{n=1}^{k} \tau_n$$

and

$$N_t = \sup\{k \geq 1 : S_k \leq t\}$$

Strong law of large numbers and renewal theorem

$$\lim_{t\to\infty} \frac{N_t}{t} = \frac{1}{\mathbb{E}(\tau)}, \quad a.s.$$

$$\lim_{t\to\infty} \frac{\mathbb{E}N_t}{t} = \frac{1}{\mathbb{E}(\tau)}$$

Average current

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

where $v_k^\pm \sim \varphi^\pm(v) = \beta_\pm v e^{-\beta_\pm \frac{v^2}{2}}$.

Proposition

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

where T_L and T_R are the left and right temperatures.

Proof :

$$\lim_{t\to\infty} \frac{N_t^\pm}{t} = \frac{1}{\mathbb{E}(\tau^+ + \tau^-)} = \frac{1}{(\frac{\pi}{2T_L})^{\frac{1}{2}} + (\frac{\pi}{2T_R})^{\frac{1}{2}}} := \kappa, \quad \text{a.s.}$$

$$\mathbb{E}(\frac{(v_1^\pm)^2}{2}) = T_\pm$$

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,

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

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

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

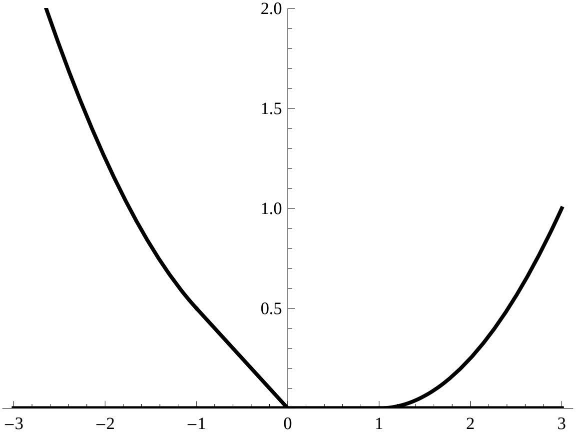


Figure: Plot of $\mathcal{G}$ as a function of j for $\kappa\tau = \kappa T^2 = 1$

Gallavotti-Cohen symmetry:

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

Origin:

1. Current :

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

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

$$\psi(\tau) \sim \frac{1}{\tau^\gamma}, \quad \text{as} \quad \tau \to \infty, \quad \gamma > 2.$$

Flat part

Take a i.i.d sequence $(\tau_i)_{i\geq 1}$ distributed with density $\psi(\tau)$ and compute

$$\varphi(\lambda) = \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}(\exp \lambda N_t)$$

$$\mathbb{E}(\exp \lambda N_t) = \sum_{n=0}^{\infty} \mathbb{P}(N_t = n) \exp(\lambda n)$$

Note first that

$$\mathbb{E}(\exp \lambda N_t) \geq \mathbb{P}(N_t = 0) = \mathbb{P}(\tau_1 > t) \sim \frac{1}{t^{\gamma-1}}, \quad \text{as} \quad t \to \infty$$

so that

$$\varphi(\lambda) \geq \lim\inf_{t\to\infty} \frac{1}{t} \log \mathbb{E}(\exp \lambda N_t) \geq \lim_{t\to\infty} -\frac{1}{t} \log t^{\gamma-1} = 0$$

But for $\lambda \leq 0$, one has $\varphi(\lambda) \leq 0$. For $\lambda > 0$, $\varphi(\lambda)$ is the unique solution of the implicit equation for $x \in \mathbb{R}$:

$$\exp \lambda \int_0^{\infty} e^{-x\tau} \psi(\tau) d\tau = 1$$

which is strictly positive.

Fix $\Delta t > 0$, $t_k = k\Delta t$, $s_k = N^2 t_k$, $k \in \mathbb{N}$,

1. $$T(n,s) = T(n,s_k), \quad s_k \le s < s_{k+1}, \quad k \in \mathbb{N}$$

2. Total energy exchanged (stochastic) between the wall n and $n+1$ at fixed temperatures over the time interval $[s_k, s_{k+1}]$

   $$J(n,[s_k,s_{k+1}]) = \dots$$

   $J(n,[s_k,s_{k+1}])$ is computed with $\{T(n,s_k), T(n+1,s_k)\}$.

3. Evolution of temperatures

   $$T(n,s_{k+1}) - T(n,s_k) = J(n,[s_k,s_{k+1}]) - J(n-1,[s_k,s_{k+1}]), \quad k \in \mathbb{N}$$

Diffusive scaling

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

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

We can show :

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.

Large deviations : thermodynamic potentials in equilibrium

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

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

$I(m,\beta)$ 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 T_N and $\mathcal{J}_N$ are related to microscopic energy and current by a diffusive scaling):

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

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

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

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

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

Local billard dynamics might be different!

Want to look at :

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

At finite N, and for each $(x,t) \in [0,1] \times [0,1]$, $\mathcal{J}_N(x,t)$ is a random variable (and so is $T_N(x,t)$).

"Independence" over small space-time windows :

$$\mathbb{P}\left(\{T_N \simeq \hat{T}, \mathcal{J}_N \simeq j\} \text{ on}[0,1] \times [0,1]\right) = \prod_{k,l} \mathbb{P}[\frac{J(l,[s_k,s_{k+1}])}{N^2\Delta t} = \frac{j(x_l,t_k)}{N}]$$

Current computed with temperatures $\{\hat{T}(x_l,t_k), \hat{T}(x_{l+1},t_k)\}$ and "compatibility conditions" for temperatures.

Compute :

$$\begin{aligned} & \log \mathbb{P}\left(\{T_N \simeq \hat{T}, \mathcal{J}_N \simeq j\} \text{ on}[0,1] \times [0,1]\right) \\ = \quad & \Delta t \cdot N^2 \sum_{k,l} \frac{1}{N^2\Delta t} \log \mathbb{P}[\frac{J(l,[s_k,s_{k+1}])}{N^2\Delta t} = \frac{j(x_l,t_k)}{N}] \end{aligned}$$

.

Remember : the theorem allows to compute:

$$\begin{aligned} & \lim_{\varepsilon\to 0} \lim_{s\to\infty} \frac{1}{\varepsilon^2}\frac{1}{s} \log \mathbb{P}[\frac{J(l,[s_k,s_k+s]}{s} = \varepsilon j(x_l,t_k)] \\ = \quad & \mathcal{G}(j(x_l,t_k), \partial_x \hat{T}(x_l,t_k), \hat{T}(x_l,t_k)) \end{aligned}$$

if $\hat{T}(x_l,t_k) - \hat{T}(x_{l+1},t_k) = \varepsilon \partial_x \hat{T}(x_l,t_k)$.

Putting everything together :

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

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

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

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

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

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

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.
- Applications to continuous time random walk