Macroscopic fluctuation theory of local collisional dynamics

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Abstract
We review why the macroscopic fluctuations of deterministic local collision dynamics should be characterized by a non-strictly convex functional.

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The study of thermal conduction properties of extended lattice Hamiltonian systems has received recently a lot of attention by theoretical and mathematical physicists alike. The first issue is simply the derivation of the Fourier law, or equivalently the heat equation. On the other hand, an impressive amount of rigorous results concerning stochastic interacting particles system has been obtained over the last decades. The diffusion equation has been derived in the hydrodynamic limit and the behaviour of the fluctuations of the macroscopic observables of the system under a space–time diffusive scaling has been derived rigorously. In particular, the shape of the large deviations functional of the current and density of particles profile has been determined [1–7, 14]. This object may be seen as the out-of-equilibrium analogue of the equilibrium thermodynamic potentials.

The first example of local collision dynamics has been introduced in [8]. In that model, particles are locked in cells having a particular shape ensuring strong chaotic properties for the dynamics of each particle within its own cell. The cells are arranged so as to tile the plane and have a small opening so that particles in neighbouring cells may interact through elastic collisions. This model was taken up in [9] as a model for heat conduction when its boundaries are connected to heat baths. The authors argue that in a weakly interacting regime and after a suitable time rescaling, the energy exchange between neighbouring cells is described by a stochastic dynamics analogous to the ones encountered in stochastic interacting particles. This raised the hope of using the rigorous results obtained for those systems to derive Fourier law for deterministic dynamics. Unfortunately, the stochastic dynamics describing the exchange of energy does not satisfy the so-called ‘gradient’ condition (see for instance [16]) and is therefore difficult to analyse. In this paper, we want to review briefly how another approach to local collision dynamics allows to conjecture important features regarding the fluctuations (large deviations) of its macroscopic observables [10–13]. Consider \( N \) particles of unit mass with positions and momenta \( (q_i, p_i) \) \( i \leq N \), with \( q_i, p_i \in \mathbb{R}^d \). The positions are measured with respect to \( N \) fixed centres located on a one-dimensional (1D) lattice. The Hamiltonian \( H \) takes the form

\[
H(p, q) = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2} + V(q_i) + U(q_i - q_{i+1}) \right],
\]

where the interaction potential \( U \) is equal to zero inside a region \( \Omega_U \subset \mathbb{R}^d \) with smooth boundary \( \Lambda \) of dimension \( d - 1 \), and equal to infinity outside. Likewise, the pinning potential \( V \) is assumed to be zero inside a bounded region \( \Omega_V \) and infinity outside, implying that the motion of a single particle remains confined for all times. The regions \( \Omega_U \) and \( \Omega_V \) being specified, the dynamics is equivalent to a billiard in high dimension. A typical example of the dynamics we wish to consider is given by figure 1. The circles move freely within their square cells and collide with each other when they both get sufficiently close to the hole located in the wall separating two adjacent cells.

Physically, those models describe aerogels, i.e. gels whose liquid components have been removed and replaced by atoms of gases. One of the simplest example of this type of dynamics is the complete exchange model introduced in [15]. Although it is expected to display anomalous thermal conduction properties, it has nice aspects that underline the general important features of local collision dynamics. In the definition of the Hamiltonian (1), take \( d = 1 \) and the potentials
where \( n \).

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Figure 1. Simplified 1D aerogel dynamics.

\[ V(x) = \begin{cases} +\infty & \text{if } |x| > b, \\ 0 & \text{if } |x| \leq b, \end{cases} \quad U(x) = \begin{cases} +\infty & \text{if } |x| > a, \\ 0 & \text{if } |x| \leq a. \end{cases} \]

Each particle on the lattice moves freely on a 1D cell of size 2\( b \), changing directions at the boundaries. The interaction between a pair of particles acts when the difference between the positions of the two particles reaches the value \( a \), at which point they exchange their velocities.

The motion of a given pair of particles at sites \( i, i+1 \) is described as the motion of a point particle on a two-dimensional billiard table (figure 2) described by

\[ \Omega = \{(x_1, x_2) \in \mathbb{R}^2, \ |x_1| \leq b, \ |x_2| \leq b, \ |x_1 - x_2| \leq a \}. \]

It is straightforward to see that the energy of the particle \( n \) at time \( t \) is given by

\[ E(n, t) - E(n, 0) = J(n - 1, [0, t]) - J(n, (0, t]), \]

where \( J(n - 1, [0, t]) \) is the time-integrated current:

\[ J(n, [0, t]) = -\frac{1}{2} \sum_{k=1}^{C_n(t)} [p_n^2(\tau_k^+ - \tau_k^-)]. \]

\((\tau_k^\pm)\) is the sequence of collision times between particles \( n \) and \( n+1 \) and \( C_n(t) \) is the number of collisions up to time \( t \). For more general local collision dynamics, the current keeps this ‘gradient’-like expression with a prefactor in front of the difference of kinetic energy, see [10] for a detailed expression. This a fundamental difference with the expression in (2).

The motion of a given pair of particles at sites \( i, i+1 \) is described by

\[ \frac{\partial}{\partial \tau} = e^{\beta v c - \beta E}, \quad \beta \pm = T \pm. \]

One may associate to the motion of the particle the time-integrated current:

\[ J[0, t] = \sum_{k=1}^{N^+} \left( v^+ k \right)^2 - \sum_{k=1}^{N^-} \left( v^- k \right)^2, \]

where \( v_k^\pm \sim \varphi^\pm(v) = \beta \pm v e^{-\beta \pm \frac{v^2}{2}} \) and \( N^\pm \) counts the number of visits to the \( \pm \)-side of the interval. Regarding this current,
one can show the following:
\[
\lim_{t \to \infty} \frac{J[0, t]}{t} = \frac{T_+ - T_-}{\left(\frac{\pi}{2T}\right)^2 + \left(\frac{\pi}{2T}\right)^2}, \quad \text{a.s.,}
\]
where \(T_-\) and \(T_+\) are the left and right temperatures. But one can go one step further and study the fluctuations of the lhs before the limit is taken. Namely, one may compute the large deviations functional of the current \(I(j, \tau, T)\) roughly defined as
\[
P_{\tau, T} \left( \frac{J[0, t]}{t} = j \right) \sim e^{-\mathcal{G}(j, \tau, T)}, \quad t \to \infty.
\]
\(P_{\tau, T}\) is the stochastic dynamics with a fixed temperature difference \(\tau = T_+ - T_-\) and average temperature \(T = \frac{T_+ + T_-}{2}\).

If \(\tau \neq 0\) then one gets the following scaling result:
\[
\lim_{\varepsilon \downarrow 0} \varepsilon^{-2} I(\varepsilon j, \kappa \tau, T) = \mathcal{G}(j, \tau, T)
\]
where \(\kappa = \left(\frac{T}{2T}\right)^2\). The reason for the affine part of the functional is the fact that the particle will get a small velocity with a not so small probability and this will make the occurrence of small values of \(N_\varepsilon\) (and thus of \(J[(0, t)]\)) quite likely. This explains the fact that the functional vanishes between 0 and the average value \(\kappa \tau\) (figure 5): it is not exponentially unlikely to observe values of the current smaller than its average. The scaling expressed in the relation above turns out to be exactly what we need to conjecture the shape of the large deviations functional in the original billiard dynamics. Indeed, we want to mimic the slow variation of the local temperatures in the deterministic model, i.e. it is expected to change by a significant amount at a speed \(\sim 1/N^2\) at the microscopic time scale. In order to do so, we let the temperatures \(\{T(n, t)\}_{0 \leq n \leq N}\) of the scatterers in figure 3 evolve such that they satisfy the equation
\[
T(n, t + N^2 \Delta t) - T(n, t) = J(n, [t, t + N^2 \Delta t]) - J(n - 1, [t, t + N^2 \Delta t]),
\]
where the currents entering the equation are the ones on the lhs and rhs of the scatterer \(n\). Define \(T_N : [0, 1] \times \mathbb{R}^* \to \mathbb{R}^*\) and \(J_N : [0, 1] \times \mathbb{R}^* \to \mathbb{R}\):
\[
T_N(x, t) = T([Nx], N^2 t),
\]
\[
J_N(x, t) = \frac{1}{N^2 \Delta t} J(n, [N^2 t, N^2 (t + \Delta t)]).
\]
Then, one can show\(^1\) when \(N \to \infty, \Delta t \to 0\), \((T_N, J_N)\) converge in \(L^2\) to the unique solution \((\hat{T}, \hat{J})\) of
\[
\begin{align*}
\partial_t \hat{T}(x, t) & = \hat{\kappa} \partial_x \hat{J}(x, t), \\
\partial_t \hat{J}(x, t) & = -\kappa \hat{T}(x, t) \partial_x \hat{T}(x, t)
\end{align*}
\]
with \(\kappa(T) = (\frac{T}{2T})^2\) and suitable boundary conditions.

At finite \(N\), and for each \((x, t) \in [0, 1] \times [0, 1], J_N(x, t)\) and \(T_N(x, t)\) are random variables and the object one is really interested in is the large deviations functional \(\hat{G}\) appearing in
\[
P \left( (T_N \approx \hat{T}, J_N \approx \hat{J}) \right) \sim \exp[-N \hat{G}(j, \hat{T})],
\]
and one can show that
\[
\hat{G}(j, \hat{T}) = \int_0^1 dt \int_0^1 dx \hat{G}(j(x, t), \partial_x \hat{T}(x, t), \hat{T}(x, t))
\]
\(^1\) Precise statements as well as rigorous proofs of the results below will be the subject of an upcoming publication.
if $j$ and $\hat{T}$ satisfy $\partial_s \hat{T}(x, s) = -\partial_x j(x, s)$, and $\hat{T} = +\infty$ otherwise. The integrand $G$ is given by

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

And therefore

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

which shows that local billiard dynamics should have macroscopic fluctuations properties very different from the ones observed in the usual stochastic interacting particles such as the exclusion process. The large deviation functional is not a strictly convex function of the current. This aspect should translate into some interesting phase transitions–like effects.

The stochastic dynamics that is introduced is a very crude approximation of the deterministic dynamics. However, one should note that it is not the fact that we replaced the deterministic collisions by stochastic ones that is responsible for the special behaviour of $G$. This is caused by what is left of the deterministic dynamics, namely the ballistic motion of the particle and the fact that one assumes the particles to be in local equilibrium. Therefore, one should expect this feature to be robust and independent of the approximations that were made for the collisional part of the dynamics.

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