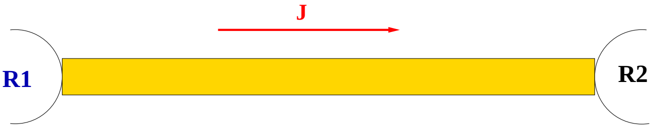
Macroscopic Fluctuation Theory

Annecy, April 20-24, 2015

Large Deviations of the Total Current



Let Y_t be the total charge transported through the system (total current) between time 0 and time t.

In the stationary state: a non-vanishing mean-current $\frac{Y_t}{t} \to J$

The fluctuations of Y_t obey a Large Deviation Principle:

$$P\left(\frac{Y_t}{t} = j\right) \sim e^{-t\Phi(j)}$$

$\Phi(j)$ being the *large deviation function* of the total current.

Note that $\Phi(j)$ is positive, vanishes at $j = J$ and is convex (in general).

Density Fluctuations in the open ASEP

Recall that Density Fluctuations in a gas at thermal equilibrium were obtained as

$$\Pr\{\rho(x)\} \sim \mathrm{e}^{-\beta V \mathcal{F}(\{\rho(x)\}}$$

where the Large-Deviation Functional is local and is given by

$$\mathcal{F}(\{\rho(x)\} = \int_0^1 (f(\rho(x), T) - f(\bar{\rho}, T))\, d^3x$$

What do the Density Fluctuations in the ASEP look like?

The probability of observing an **atypical density profile in the steady state of the ASEP** was calculated starting from the exact microscopic solution of the exclusion process, with the help of the Matrix Ansatz (B. Derrida, J. Lebowitz E. Speer, 2002).

Large Deviations of the Density Profile in ASEP

The Large Deviation Functional for the symmetric case $q = 0$ is given by

$$\mathcal{F}(\{\rho(x)\}) = \int_0^1 dx \left(B(\rho(x), F(x)) + \log \frac{F'(x)}{\rho_2 - \rho_1} \right)$$

where $B(u, v) = (1 - u) \log \frac{1-u}{1-v} + u \log \frac{u}{v}$ and $F(x)$ satisfies

$$F \left(F'^2 + (1 - F)F'' \right) = F'^2 \rho \quad \text{with} \quad F(0) = \rho_1 \text{ and } F(1) = \rho_2 \,.$$

This functional is non-local as soon as $\rho_1 \neq \rho_2$.

This functional is NOT identical to the one given by local equilibrium.

Note that in the case of equilibrium, for $\rho_1 = \rho_2 = \bar{\rho}$, we recover

$$\mathcal{F}(\{\rho(x)\}) = \int_0^1 dx \left\{ (1 - \rho(x)) \log \frac{1 - \rho(x)}{1 - \bar{\rho}} + \rho(x) \log \frac{\rho(x)}{\bar{\rho}} \right\}$$

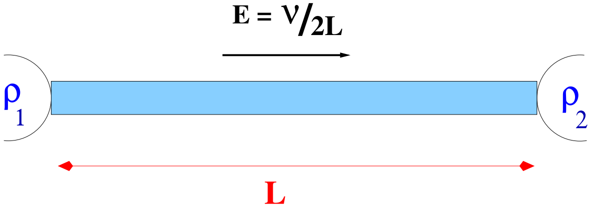
The General Large Deviations Problem

More generally, the probability to observe an atypical current $j(x,t)$ and the corresponding density profile $\rho(x,t)$ during $0 \le s \le L^2\, T$ (L being the size of the system) is given by

$$\Pr\{j(x,t), \rho(x,t)\} \sim \mathrm{e}^{-L\, \mathcal{I}(j,\rho)}$$

Is there a Principle which gives this large deviation functional for systems out of equilibrium?

The Hydrodynamic Limit: Diffusive case



Starting from the microscopic level, define local density $\rho(x,t)$ and current $j(x,t)$ with macroscopic space-time variables $x = i/L, t = s/L^2$ (diffusive scaling).
The typical evolution of the system is given by the hydrodynamic behaviour (Burgers-type equation):

$$\partial_t \rho = \nabla\left(D(\rho)\nabla\rho\right) - \nu\nabla\sigma(\rho) \quad \text{with} \quad D(\rho) = 1 \text{ and } \sigma(\rho) = 2\rho(1-\rho)$$

(Lebowitz, Spohn, Varadhan)

How can Fluctuations be taken into account?

Fluctuating Hydrodynamics

Consider Y_t the total number of particles transfered from the left reservoir to the right reservoir during time t.

- $\lim_{t\to\infty} \frac{\langle Y_t \rangle}{t} = D(\rho)\frac{\rho_1-\rho_2}{L} + \sigma(\rho)\frac{\nu}{L}$ for $(\rho_1 - \rho_2)$ small
- $\lim_{t\to\infty} \frac{\langle Y_t^2 \rangle}{t} = \frac{\sigma(\rho)}{L}$ for $\rho_1 = \rho_2 = \rho$ and $\nu = 0$.

Then, the equation of motion is obtained as:

$$\partial_t \rho = -\partial_x j \quad \text{with} \quad j = -D(\rho)\nabla\rho + \nu\sigma(\rho) + \sqrt{\sigma(\rho)}\xi(x,t)$$

where $\xi(x,t)$ is a Gaussian white noise with variance

$$\langle \xi(x',t')\xi(x,t) \rangle = \frac{1}{L}\delta(x-x')\delta(t-t')$$

For the symmetric exclusion process, the 'phenomenological' coefficients are given by

$$D(\rho) = 1 \quad \text{and} \quad \sigma(\rho) = 2\rho(1-\rho)$$

Large Deviations at the Hydrodynamic Level

What is the probability to observe an atypical current $j(x,t)$ and the corresponding density profile $\rho(x,t)$ during $0 \leq s \leq L^2\,T$?

$$\Pr\{j(x,t), \rho(x,t)\} \sim \mathrm{e}^{-L\,\mathcal{I}(j,\rho)}$$

Use fluctuating hydrodynamics to write the Large-Deviation Functional as a path-integral: the current and the density evolve $(\rho(x,t), j(x,t))$ according to a stochastic dynamics. The weight of a trajectory between 0 and t can written as:

$$\text{Weight}\left(\{\rho(x,t'), j(x,t')\}_{\substack{0\leq x\leq 1\\ 0\leq t'\leq t}}\right) =$$

$$\int \mathcal{D}\xi(x,t')\ \exp\left(-\frac{L}{2}\int_0^t dt' \int_0^1 dx\,\xi^2(x,t)\right)$$

$$\prod_{\substack{0\leq x\leq 1\\ 0\leq t'\leq t}} \delta\left(\frac{\partial\rho}{\partial t'} + \frac{\partial j}{\partial x}\right) \prod_{\substack{0\leq x\leq 1\\ 0\leq t'\leq t}} \delta\left(j + D(\rho)\frac{\partial\rho}{\partial x} - \nu\sigma(\rho) + \sqrt{\sigma(\rho)}\xi\right)$$

This formula is analogous to the one used to change variables in probability theory:
If X is a random variable distributed according to $P(X)$ and if $Y = F(X)$ (F being known function) then the distribution of Y is given by

$$\mathrm{Prob}(Y) = \int dX\, P(X)\, \delta(Y - F(X))$$

Now the probability of observing $\rho(x,t)$ and $j(x,t)$ at time t knowing that we started with $\rho_0(x), j_0(x)$ is given by the sum of the weights of all possible trajectories beginning with $\rho_0(x), j_0(x)$ and ending up at $\rho(x,t)$ and $j(x,t)$:

$$\text{Proba}\,(\rho(x,t), j(x,t)|\rho_0(x), j_0(x)) = \int_{\substack{\rho_0 \to \rho_t \\ j_0 \to \jmath_t}} \mathcal{D}\rho(x,t')\,\mathcal{D}j(x,t')\,\text{Weight}\left(\{\rho(x,t'), j(x,t')\}_{\substack{0 \le x \le 1 \\ 0 \le t' \le t}}\right)$$

Using the previous expression for the Trajectory Weight and performing the integral over the noise ξ, we obtain:

$$\text{Proba}\,(\rho(x,t), j(x,t)|\rho_0(x), j_0(x)) = \int_{\substack{\rho_0 \to \rho_t \\ j_0 \to j_t}} \mathcal{D}\rho \mathcal{D}j \prod_{\substack{0 \leq x \leq 1 \\ 0 \leq t' \leq t}} \delta\left(\frac{\partial \rho}{\partial t'} + \frac{\partial j}{\partial x}\right)$$

$$\exp\left(-\frac{L}{2}\int_0^t dt' \int_0^1 dx \frac{(j + D(\rho)\frac{\partial \rho}{\partial x} - \nu\sigma(\rho))^2}{\sigma(\rho)}\right)$$

We are interested in the large L limit: the integral will be dominated by the optimal value of the exponent (saddle-point).

The value at the saddle-point will provide us with the large deviation functional.

Macroscopic Fluctuation Theory

The large deviation functional can be written as the solution of an optimal path problem (G. Jona-Lasinio et al.)

$$\mathcal{I}(j,\rho) = \min_{\rho,j} \left\{ \int_0^T dt \int_0^1 dx \frac{(j - \nu\sigma(\rho) + D(\rho)\nabla\rho)^2}{2\sigma(\rho)} \right\}$$

with the constraint: $\partial_t \rho = -\nabla . j$
Knowing $\mathcal{I}(j,\rho)$ one can deduce (by contraction) the LDF of the current or the profile.
For example

$$\Phi(j) = \min_{\rho} \{\mathcal{I}(j,\rho)\}$$

This variational problem has a Hamiltonian structure and can be expressed by using a pair of conjugate variables (p, q).

MFT Formalism

Mathematically, one has to solve the corresponding Euler-Lagrange equations. After some transformations, one obtains a set of coupled PDE's (here, we take $\nu = 0$):

$$
\begin{aligned}
\partial_t q &= \partial_x [D(q)\partial_x q] - \partial_x [\sigma(q)\partial_x p] \\
\partial_t p &= -D(q)\partial_{xx} p - \frac{1}{2}\sigma'(q)(\partial_x p)^2
\end{aligned}
$$

where $q(x,t)$ is the density-field and $p(x,t)$ is a conjugate field.
The physical content is encoded in the 'transport coefficients' $D(q)(= 1)$ and $\sigma(q)(= 2q(1-q))$ that contain the information of the microscopic dynamics relevant at the macroscopic scale.
Do note that these equations have a Hamiltonian structure.

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- A general framework but these non-linear MFT equations are very difficult to solve in general. By using them one can in principle calculate large deviation functions directly at the macroscopic level.
- The analysis of this new set of 'hydrodynamic equations' has just begun!

Conclusions

The asymmetric exclusion process is a paradigm for the behaviour of systems far from equilibrium in low dimensions. The ASEP is important for the Theory and for its multiple Applications (especially in biophysics).

Large deviation functions (LDF) appear as a generalization of the thermodynamic potentials for non-equilibrium systems. They exhibit remarkable properties such as the Fluctuation Theorem, valid far away from equilibrium. The LDF's are very likely to play a key-role in the future of non-equilibrium statistical mechanics.

Current fluctuations are a signature of non-equilibrium behaviour. The exact results we derived can be used to calibrate the more general framework of fluctuating hydrodynamics (MFT), which is currently being developed.