Rare events and fluctuations in systems far from equilibrium

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Static Equilibrium Fluctuations

A system, at the molecular scale, keeps on evolving through various microscopic configurations and a probabilistic description is required. Thermodynamic observables $\mathbf{x}$ fluctuate around their average values.

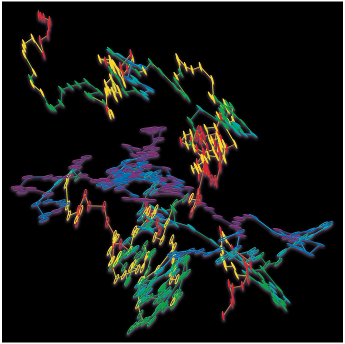
Equilibrium fluctuations can be precisely quantified by **inverting** Boltzmann formula (Einstein, 1906)

$$\boldsymbol{\Omega} \sim e^{\frac{S(x)}{k_B}}$$

Expanding the entropy around its maximum value leads to a definite negative quadratic form. Small static fluctuations of the thermodynamic variables $\mathbf{x}$ at a given time are Gaussian, governed by the 2nd derivatives (Hessian) of the entropy.

Dynamical Fluctuations: Brownian Motion

The macroscopic observable of a system at thermal equilibrium are stationary. But, at molecular scale things constantly change: the system keeps on evolving through various microscopic configurations.



Robert Brown (1773-1858)

Langevin Dynamics

Paul Langevin understood that thermal fluctuations can be accounted for by adding a random force to the dynamics:

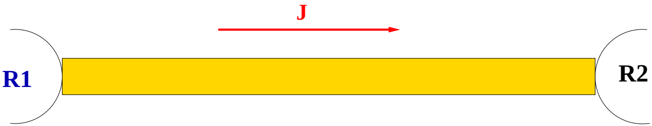
$$m\frac{d^2x}{dt^2} = -\gamma\frac{dx}{dt} - \nabla\mathcal{U}(x) + \xi(t)$$

where $\xi(t)$ is a white noise of amplitude $\Gamma = \gamma kT$

Paul Langevin (1872-1946)

Near equilibrium

Consider a Stationary System in contact with two reservoirs at temperatures T_1 and T_2 (or chemical, or electric, potentials μ_1, μ_2).



When $|T_1 - T_2| \ll T_1$ (slightly unbalanced reservoirs): A stationary current, breaking time reversal invariance, sets in, proportional to the temperature gradient.

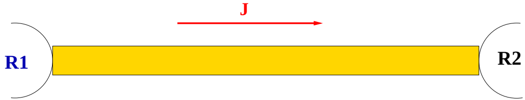
This flow of the current implies that entropy is continuously generated and keeps on increasing with time.

Conductivity determined by quadratic correlations *at equilibrium* (Einstein-Kubo linear response theory): mobility = diffusivity/kT

Minimal Entropy Production Rate (Prigogine): an elegant way to reformulate linear response theory.

Systems far from equilibrium

Consider now a Stationary Driven System in contact with reservoirs at different potentials: no microscopic theory is yet available.



- What are the relevant macroscopic parameters?
- Which functions describe the state of a system?
- Do Universal Laws exist? Can one define Universality Classes?
- Can one postulate a general form for the microscopic measure?
- What do the fluctuations look like ('non-gaussianity')?

In the steady state, a non-vanishing macroscopic current J flows.

What can we say about the non-equilibrium properties of observables (e.g., current, temperature or density fields) from the point of view of Statistical Physics?

Density Fluctuations

For a gas in a room, at thermal equilibrium, the probability of observing an arbitrary density profile $\rho(x)$ takes a large-deviation form (rare events are exponentially suppressed)

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

where the large deviation functional $\mathcal{F}(\{\rho(x))\}$ is given by

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

Equilibrium free energy $f(\rho, T)$ is viewed as a large deviation function.

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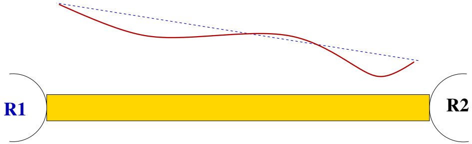
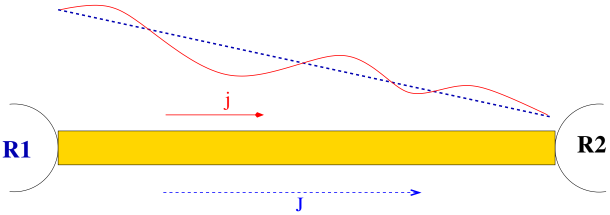
Out of equilibrium, what is the probability of observing an atypical density profile in the steady state? What does the functional $\mathcal{F}(\{\rho(x)\})$ look like?



Importance of Large Deviations

- Equilibrium Thermodynamic potentials (Entropy, Free Energy) can be constructed as large deviation functions.
- Large deviations are defined far from equilibrium and are good candidates for being non-equilibrium potentials.
- Large deviation functions obey remarkable identities, valid far from equilibrium (Gallavotti-Cohen Fluctuation Theorem; Jarzynski and Crooks Relations).
- These identities imply, in the vicinity of equilibrium, the fluctuation dissipation relation (Einstein), Onsager's relations and linear response theory (Kubo).

The General Large Deviations Problem



Assume the probability to observe an atypical local current $j(x, t)$ and density profile $\rho(x, t)$ during $0 \leq s \leq L^2\, T$ (i.e. diffusive scaling, L is the size of the system) satisfies a Large Deviation Principle:

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

Thus, knowing $\mathcal{I}(j, \rho)$, one could deduce the large deviations of the current and of the density profile (by contraction).

Macroscopic fluctuations

For a weakly-driven diffusive system, the large deviation form of the probability to observe a current $j(x,t)$ and a density profile $\rho(x,t)$ during a time T, is given by

$$\Pr\{j(x,t),\rho(x,t)\} \sim \mathrm{e}^{-\,S_{MFT}(j,\rho)}\,,$$

with

$$S_{MFT}(j,\rho) = \int_0^T dt \int_{-\infty}^{+\infty} \frac{(j + D(\rho)\nabla\rho)^2\,dx}{2\sigma(\rho)}$$

under the constraint $\partial_t \rho = -\nabla . j$

The relevant information at macroscopic scale from the microscopic dynamics is contained in the transport coefficients D and σ. Other microscopic details are 'blurred' in this description.

This is the MACROSCOPIC FLUCTUATION THEORY (MFT), developed by L. Bertini, D. Gabrielli, A. De Sole, G. Jona-Lasinio and C. Landim, from 2000's on.

The MFT Equations

In the large time limit, $T \to \infty$, the MFT action will be dominated by its saddle-points (instantons), found by optimizing it under (problem-dependent) constraints.

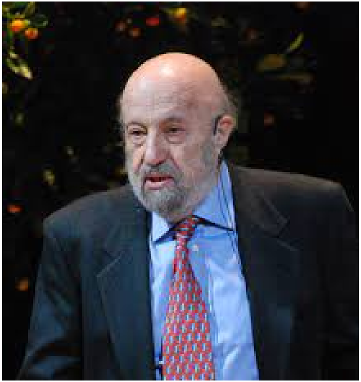
The optimal equations, in Hamiltonian form, where $\rho(x,t)$ is the density-field and $H(x,t)$ is a conjugate ('momentum') field, are given by

$$\partial_t \rho = \partial_x[D(\rho)\partial_x \rho] - \partial_x[\sigma(\rho)\partial_x H]$$

$$\partial_t H = -D(\rho)\partial_{xx} H - \frac{1}{2}\sigma'(\rho)(\partial_x H)^2$$

with Hamiltonian $\mathcal{H} = \sigma(\rho)(\partial_x H)^2/2 - D(\rho)\partial_x \rho \partial_x H$.

In principle, large deviations can be calculated at the macroscopic level by solving the full, time-dependent, MFT equations.



The macroscopic fluctuation theory generalizes the linear response fluctuation theory of Onsager and Machlup (1953)

Unfortunately, solving these equations was not a straightforward task. Exact results were first obtained at the microscopic level and, then, coarse-grained.

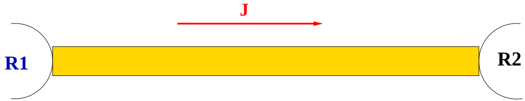
Driven lattice gases

Exact solutions of specific models (Ising, 6-vertex) have played a key role in equilibrium statistical mechanics to understand phase transitions and benchmarks for testing general theories or more versatile approximation methods.

Driven lattice gases (**Yves Pomeau**, Katz-Lebowitz-Spohn, Henri Cornille) are very useful systems to explore phenomena far from equilibrium.

Microscopic approach to classical Transport in 1d

A picture of a non-equilibrium system



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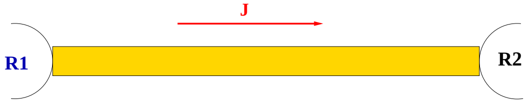
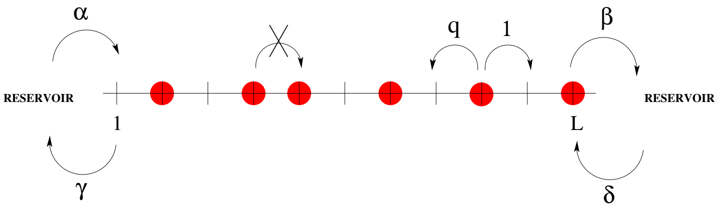
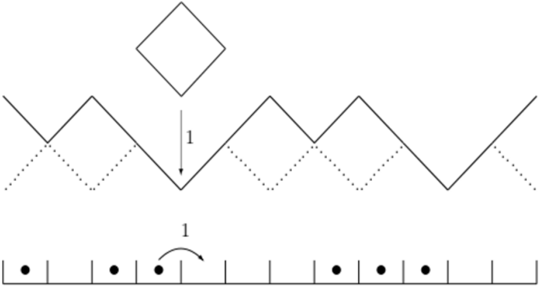


A paradigm: the asymmetric exclusion model with open boundaries



A building block in many realistic models of 1d transport and studied extensively in probability, combinatorics, condensed matter physics...

The Kardar-Parisi-Zhang equation in 1d



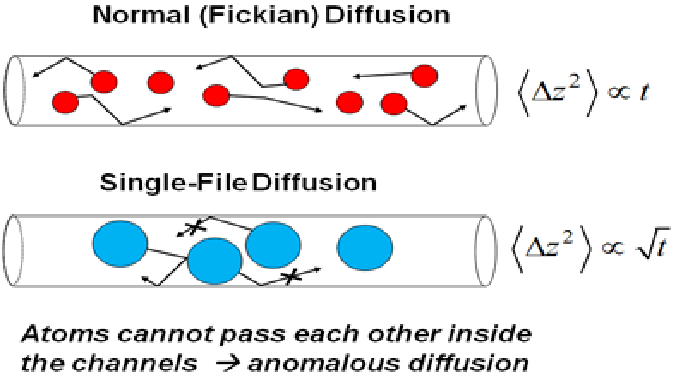
The height of an interface $h(x, t)$ satisfies the generic KPZ equation

$$\frac{\partial h}{\partial t} = \nu \frac{\partial^2 h}{\partial x^2} + \frac{\lambda}{2} \left(\frac{\partial h}{\partial x} \right)^2 + \xi(x, t)$$

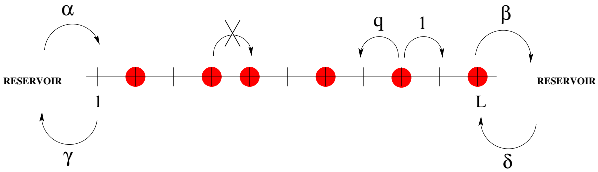
The ASEP is a discrete version of the KPZ equation in one-dimension.

Single-file diffusion

SEP is a pristine model for single-file diffusion, an important phenomena soft-condensed matter (for example, transport in chanels through cell membranes).



Stationary state of the open ASEP (DEHP, 1993)



The stationary probability of a configuration $\mathcal{C}$ is given by (Derrida, Evans, Hakim and Pasquier, 1993)

$$P(\mathcal{C}) = \frac{1}{Z_L} \langle W | \prod_{i=1}^{L} \left(\tau_i D + (1 - \tau_i) E \right) | V \rangle$$

where $\tau_i = 1$ (or 0) if the site i is occupied (or empty). The operators D and E, the vectors $\langle W|$ and $|V\rangle$ satisfy a quadratic algebra

$$\begin{aligned} D\,E - qE\,D &= (1-q)\,(D + E) \\ (\beta\, D - \delta\, E)\,|V\rangle &= |V\rangle \\ \langle W|(\alpha\, E - \gamma\, D) &= \langle W| \end{aligned}$$

Interacting particle processes are complex enough to exhibit a rich phenomenology that *captures* the physics involved.

On the other hand, some of these models have intricate mathematical properties, in particular some (deformed) algebraic symmetries, that allows us to solve them exactly: they are *quantum* **integrable.**

Some techniques involved:

- Bethe Ansatz (coordinate, algebraic, functional).
- Combinatorics (Young tableaux, RSK and special polynomials)
- Integrable probabilities and determinantal processes.

From microphysics...

During the last decades many groups of people have explored stochastic lattices gases from various sides and scales and a huge amount of knowledge has been acquired.

At the IPhT, with Olivier Golinelli, we learned apply the Bethe Ansatz to the ASEP and derived some exact combinatorial finite-size formulas that allowed us to classify states and degeneracies of the relaxation spectrum.

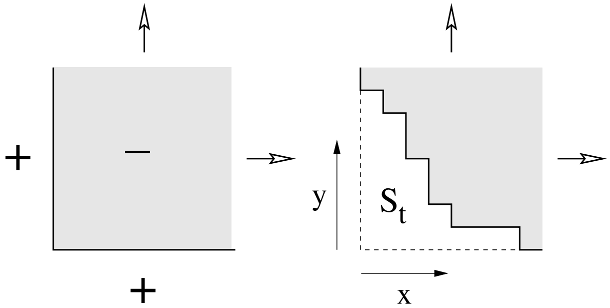
Then, the full large deviation function of the current in a periodic model was obtained by Sylvain Prolhac, inspired by an IPhT Lecture by Olivier Babelon.

Multicolor exclusion processes could be solved by using an (infinite) tensor product extension of the Matrix Ansatz (P. Ferrari, M. Evans, S. Prolhac, A. Ayyer, N. Rajewsky, S. Mallick, C. Boutillier, P. Francois, C. Arita, E. Ragoucy, N. Crampé, M. Vanicat).

These tensor algebras yielded the full large deviation function of the current in the open system with reservoirs (Alexandre Lazarescu and Vincent Pasquier).

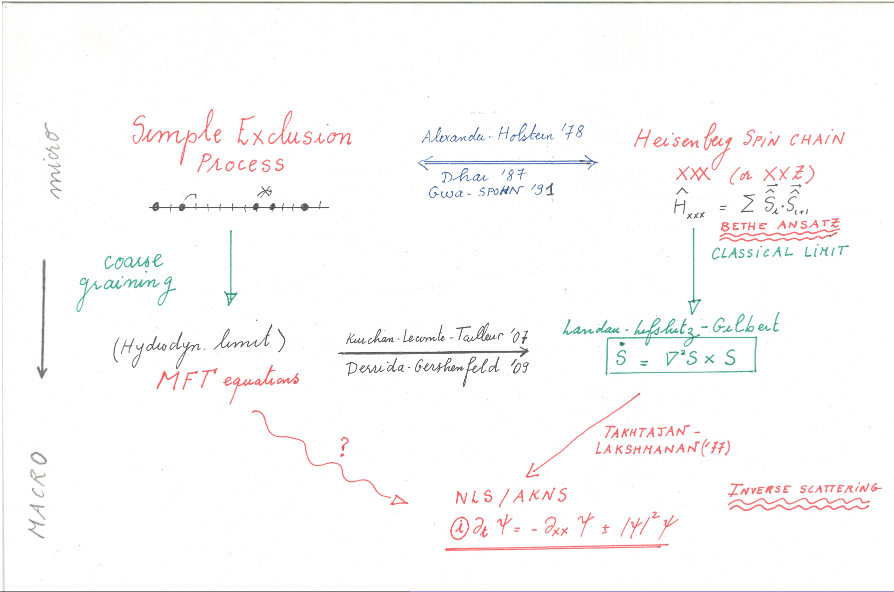
...To macrophysics

With Paul (Krapivsky), we used the MFT to do some concrete calculations building on some earlier work he had done with Baruch Meerson. In particular, we could compute perturbatively some simple quantities both at microscopic and macroscopic scale. The calculations look totally different but the results agree.



Perturbative calculations at higher and higher orders are more and more cumbersome but seem to remain possible, hinting towards some classically integrable structure in the MFT.

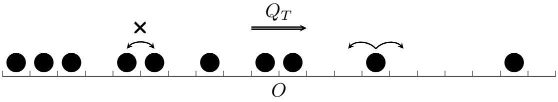
A chart of models



Current fluctuations in the SEP on Z

Consider the Symmetric Exclusion Process on $\mathbb{Z}$ with two-sided Bernoulli initial conditions ρ_- on the left, ρ_+ on the right at $t = 0$.

Time integrated current Q_T = total number of particles that have jumped from 0 to 1 *minus* the total number of particles that have jumped from 1 to 0 during the time interval $(0, T)$.



An exact microscopic combinatorial solution of the problem is possible: it yields the distribution of current and that of a tagged particle at any position and at any finite time. This involves the technology of Integrable Probabilities (Imamura, M. and Sasamoto, PRL 2017 and CMP 2021)).

The characteristic function of the current $N(x,t)$ is given by Fredholm determinant, this is the exact statistics, at any finite-time:

$$\boxed{\langle e^{\lambda N(x,t)} \rangle = \det(1 + \omega K_{t,x}) W_0(\lambda)}$$

where

$$K_{t,x}(\xi_1, \xi_2) = \frac{\xi_1^{|x|} e^{\epsilon(\xi_1) t}}{\xi_1 \xi_2 + 1 - 2\xi_2} \quad \text{with} \quad \epsilon(\xi) = \xi + \xi^{-1} - 2$$

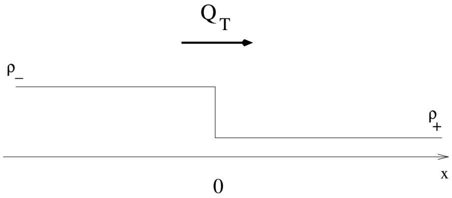
$$W_0(\lambda) = \left(1 + \rho_\pm (e^{\pm\lambda} - 1)\right)^{|x|} \text{ with } \pm = \text{sgn}(x)$$

and $\omega = \rho_+(e^{\lambda} - 1) + \rho_-(e^{-\lambda} - 1) + \rho_+\rho_-(e^{\lambda} - 1)(e^{-\lambda} - 1).$

Asymptotic analysis of these Fredholm determinants leads to exact expressions for all the moments of $N(x,t)$ to the large deviation function of the current at any position and of the position of a tagged particle.

A macroscopic hydrodynamic picture, based on the MFT, would be welcome.

Current fluctuations at macroscopic scale



In the continuous limit: $Q_T = \int_0^\infty [\rho(x, T) - \rho(x, 0)] dx$. And for large T, we have (LDP):

$$\langle e^{\lambda Q_T} \rangle \simeq e^{\sqrt{T}\mu(\lambda)}$$

How can we determine $\mu(\lambda)$, the cumulant generating function (CGF) using a purely macroscopic approach (MFT)?

For SEP, we have $D(\rho) = 1$ and $\sigma(\rho) = 2\rho(1 - \rho)$

From MFT to NLS

With H. Moriya and T. Sasamoto (2022), we observed that MFT equations for SEP can be mapped to the *Ablowitz-Kaup-Newell-Segur (AKNS) system:*

$$\partial_t u(x,t) = \partial_{xx} u(x,t) - 2u(x,t)^2 v(x,t)$$
$$\partial_t v(x,t) = -\partial_{xx} v(x,t) + 2u(x,t) v(x,t)^2$$

These AKNS equations are an imaginary time version of the Non-Linear Schrödinger equation.

The AKNS system is classically integrable by **inverse scattering theory**, an extension of the Fourier transform, useful to study non-linear dispersive wave equations.

Formula for the density profile

Inverse scattering allows us to show that the half-Fourier transform of the final profile

$$\hat{u}_\pm(k) = \int_{\mathbb{R}_\mp} u(x, T) e^{-2ikx} dx$$

satisfies a scalar Riemann–Hilbert factorization problem:

$$\boxed{(\hat{u}_+(k) + 1)(\hat{u}_-(k) + 1) = 1 + \omega e^{-4k^2 T}}$$

where $1 + \hat{u}_\pm$ is analytic on the upper (respectively lower) complex plane, with a given product along $\mathbb{R}$.

This Riemann–Hilbert problem is solved by using the Cauchy Formula (after taking logarithms) and we obtain:

$$\hat{u}_\pm(k) + 1 = \exp\left[-\frac{1}{2} \sum_{n=1}^{\infty} \frac{(-\omega e^{-4k^2 T})^n}{n} \mathrm{erfc}(\mp i\sqrt{4nT}k) \right]$$

Fluctuations of the current

Calculating the total current Q_T from the optimal profiles at $t = 0$ and $t = T$ yields the Cumulant Generating Function (CGF) of the current. In the long time limit, $\langle e^{\lambda Q_T} \rangle \simeq e^{\sqrt{T}\mu(\lambda)}$, with

$$\mu(\lambda) = \frac{1}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}\omega^n}{n^{3/2}}$$

where $\omega = (e^{\lambda} - 1)\rho_-(1 - \rho_+) + (e^{-\lambda} - 1)\rho_+(1 - \rho_-)$

This formula for the CGF is identical to the one obtained in the microscopic calculation: the MFT framework yields exact results and provides us with a classical field theory for non-linear macroscopic fluctuations far from equilibrium.

Conclusions

Large deviations are considered to be relevant generalizations of the thermodynamic potentials (Free Energy) far from equilibrium.

Interacting particle processes are ideal toy-models to investigate these problems with a large variety of methods:

• Microscopic scale: Combinatorics, Matrix representation, Bethe Ansatz, Integrable Probabilities.

• Coarse-grained level: fluctuating Langevin hydrodynamics, Macroscopic Fluctuation Theory for optimal paths: Exact results are based on the Inverse Scattering Method, originally developed to study non-linear dispersive hydrodynamics.

The relation between microscopic and macroscopic scales (continuous, or hydrodynamic, limit) and quantum vs classical integrability is very intriguing.

Extensions of the MFT framework to non-equilibrium systems with long range interactions, signal processing, turbulence, active matter, living matter and (of course) quantum systems are largely open and very promising.

Le monde commença à lui apparaître sous un jour nouveau. Comme une vaste entreprise dynamique, en fluctuation perpétuelle, modelée et remodelée sans cesse, et non ainsi qu'elle l'avait cru inconsciemment pendant des années, comme l'entité stable dans laquelle on pouvait piocher sans effort.

Tarun J. TEJPAL (Loin de Chandigarh)