Macroscopic Fluctuations in Non-Equilibrium Systems

K. Mallick

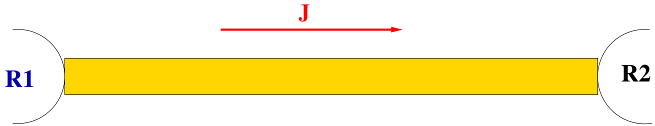
Institut de Physique Théorique Saclay (France)

LPTMC, October 8th 2024

Outline

Systems at equilibrium

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

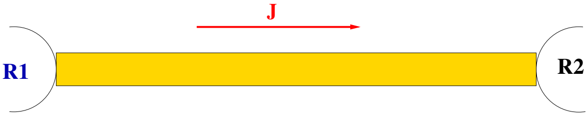


- If $T_1 = T_2$: Equilibrium Statistical Mechanics. The state of the system, characterized by very few parameters, is determined by optimizing the relevant thermodynamic potential and leads to an equation of state.

  This allows us to study phase transitions, universality classes, statistical fluctuations (generically Gaussian).

Systems *near* equilibrium

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



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

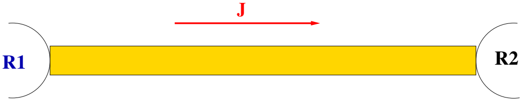
This flow of the current implies that entropy is continuously generated and keeps on increasing with time.

The average value of the flux is given by a linear formula (Ohm's Law) and conductivity is 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) from the point of view of Statistical Physics?

Static Equilibrium (Thermodynamic) Fluctuations

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

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

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

Expanding the entropy around its maximum value leads to a definite negative quadratic form. Fluctuations of the thermodynamic variables $\mathbf{x}$ at a given time are Gaussian, governed by the Hessian matrix – 2nd derivatives– of the entropy (cf. H. B. Callen's book).

Dynamical near-equilibrium fluctuations

We are now interested in correlations at at different times between thermodynamic variables. The analysis of the time-series $\mathbf{x}(t)$ requires the knowledge of *constitutive relations, e.g.*, Fourier's Law: $j_E = -\lambda \nabla T$, where λ is the thermal conductivity.

More generally, near equilibrium, currents (or fluxes) can be written as linear combinations of the gradients of the thermodynamic variables, through *a linear response* matrix L.

In 1931, Onsager proved, using microscopic reversibility, that L is (anti-)symmetric (Reciprocity relations).

Then, Onsager and Machlup (1953) showed that fluctuations in the vicinity of equilibrium can be described by the following linear Ornstein-Uhlenbeck dynamics:

$$\dot{\mathbf{x}} = LA\mathbf{x} + \xi$$

with

$$\langle \xi(t)\xi(t') \rangle = 2L\delta(t - t')$$

Here, $\mathbf{x}(t)$ is the vector of thermodynamic variables, A the Hessian of the Entropy and L Onsager's matrix.

The Onsager-Machlup Principle

Thanks to this stochastic Langevin dynamics, the statistics of the time series of the thermodynamic observables $\mathbf{x}(t)$ can be probed near equilibrium and multiple-time equilibrium correlations can be, in principle, calculated.

More precisely, this yields a probability distribution for all possible time evolutions of these observables *in the linear response regime*.

Indeed, Onsager and Machlup showed that the linear Ornstein-Uhlenbeck dynamics satisfied by near equilibrium fluctuations is equivalent to the following path-integral representation

$$\boxed{\mathrm{Proba}\left(\mathbf{x}(t)\right) = \exp\left(-\frac{1}{4}\int_0^T \left[\dot{\mathbf{x}} - LA\mathbf{x}\right]^T L^{-1}\left[\dot{\mathbf{x}} - LA\mathbf{x}\right]\mathrm{d}t\right)\mathcal{D}\mathbf{x}(t)}$$

Here $\mathbf{x}(t)$ is a vector of thermodynamic variables, A the Hessian of the Entropy and L Onsager's matrix.

As we shall see, the Macroscopic Fluctuation Theory can be viewed as a non-linear generalization, far from equilibrium, of Onsager and Machlup's principle.

Large deviations and

Macroscopic Fluctuation Theory

In Nature, many systems are far from thermodynamic equilibrium and keep on exchanging matter, energy, information with their surroundings. There is no general conceptual framework to study such systems.

Density Fluctuations

Consider a gas in a room, at **thermal equilibrium.** The probability of observing a density profile $\rho(x)$ takes the form:

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

What is $\mathcal{F}(\{\rho(x)\}$?

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

Equilibrium Free Energy can be seen as a Large Deviation Function.

Density Fluctuations

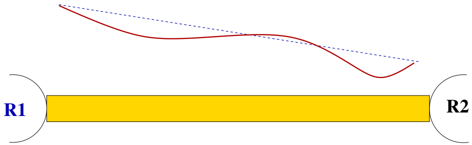
Consider a gas in a room, at **thermal equilibrium.** The probability of observing a density profile $\rho(x)$ takes the form:

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

What is $\mathcal{F}(\{\rho(x)\}$?

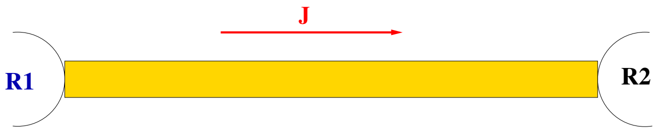
$$\mathcal{F}(\{\rho(x)\}) = \int_0^1 \left(f(\rho(x), T) - f(\bar{\rho}, T)\right) d^3x$$

Equilibrium Free Energy can be seen as a Large Deviation Function.



What is the probability of observing an atypical density profile in the steady state? What does the functional $\mathcal{F}(\{\rho(x)\})$ look like for such a non-equilibrium system?

Large Deviations of the Total Current



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

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

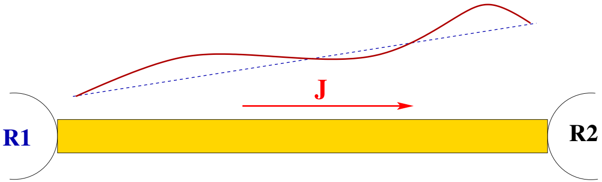
The fluctuations of Q_t obey a Large Deviation Principle:

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

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

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

The General Large Deviations Problem



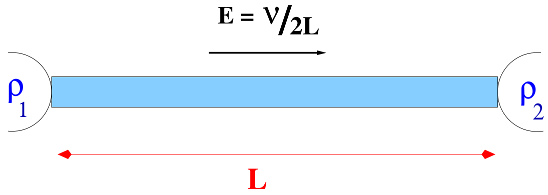
The Probability to observe an atypical local current $j(x,t)$ and the density profile $\rho(x,t)$ during $0 \leq s \leq L^2\, T$ (L being the size of the system) assumes a Large Deviation behaviour

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

Knowing $\mathcal{I}(j,\rho)$, one could deduce the large deviations of the current and of the density profile. For instance, $\Phi(j) = \min_\rho\{\mathcal{I}(j,\rho)\}$.

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

Hydrodynamic description of driven diffusive systems



Starting from the microscopic level, local density $\rho(x,t)$ and current $j(x,t)$ are defined for macroscopic space-time variables $x = i/L, t = s/L^2$ (diffusive scaling). The typical, average, evolution of many diffusive processes is described at hydrodynamic scale by

$$\partial_t \rho(x,t) = -\nabla . j(x,t) = -\nabla . (-D(\rho)\nabla\rho + \sigma(\rho)\nu\ )$$

(De Masi, Ferrari, Kipnis, Lebowitz, Olla, Presutti, Spohn, Varadhan...)

The transport coefficients $D(\rho)$ and $\sigma(\rho)$ have to be extracted from microscopic calculations.

Note that these equations are deterministic: there are no fluctuations.

The MFT Principle

For such diffusive systems, 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

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

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

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.

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

Heuristics: MFT from Fluctuating Hydrodynamics

Heuristically, this action S_{MFT} results from the Langevin PDE

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

The transport coefficients, $D(\rho)$ (bulk diffusivity) and $\sigma(\rho)$ (conductivity) must be determined at the level of microscopic physics.

Hereafter, there will be no external bias: $\nu = 0$.

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

The MFT can be seen as a generalization far from equilibrium, for driven diffusive systems, of the Onsager-Machlup functional.

The MFT Equations

The optimal Euler-Lagrange equations give, by a Legendre transform, a Hamiltonian structure, by using a pair variables (ρ, H), conjugate to (ρ, j), where $\rho(x,t)$ is the density-field and $H(x,t)$ is a conjugate ('momentum') field.

In terms of these variables, the optimal equations are:

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

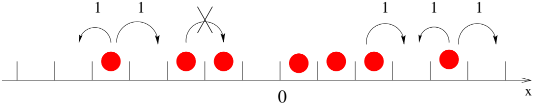
with Hamiltonian $\mathcal{H} = \sigma(\rho)(\partial_x H)^2/2 - D(\rho)\partial_x \rho \partial_x H.$

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.

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

Diffusivity and Conductivity of some lattices gases

- Independent particles: $D = 1$, $\sigma = 2\rho$
- Simple Exclusion Process: $D_{\mathrm{SEP}} = 1$, $\sigma_{\mathrm{SEP}} = 2\rho(1-\rho)$



- Kipnis-Marchioro-Presutti model: $D_{\mathrm{KMP}} = 1$, $\sigma_{\mathrm{KMP}} = 2\rho^2$
- Repulsion Process (P. Krapivsky, 2015): Hops increasing the number of nearest neighbour pairs are forbidden:

$$D_{\mathrm{RP}} = \begin{cases} \frac{1}{(1-\rho)^2} & \text{if } 0 < \rho < \frac{1}{2} \\ \frac{1}{\rho^2} & \text{if } \frac{1}{2} < \rho < 1 \end{cases} \quad \sigma_{\mathrm{RP}} = \begin{cases} \frac{2\rho(1-2\rho)}{1-\rho} & \text{if } 0 < \rho < \frac{1}{2} \\ \frac{2(1-\rho)(2\rho-1)}{\rho} & \text{if } \frac{1}{2} < \rho < 1 \end{cases}$$

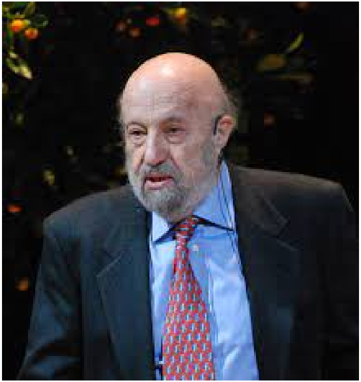
• The MFT equations describe the non-equilibrium behaviour of many diffusive interacting particle systems (dynamical transitions).

• Mathematical/Numerical difficulties: well-posedness; non-local boundary conditions.

• Time-dependent equations were solved only in non-interacting case. For many years, no analytic time-dependent solutions for the interacting case were known.

• The only known exact results were obtained by using integrability techniques (Bethe Ansatz) at the microscopic level.

• Recently, several solutions for closely related problems involving PDE's of optimal fluctuation paths were found: Krajenbrink and Le Doussal (weak-noise KPZ), Grabsch, Poncet, Rizkallah, Illien and Bénichou (Single File Systems), Bettelheim, Smith and Meerson (KMP), and Moriya-M-Sasamoto (SEP).



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

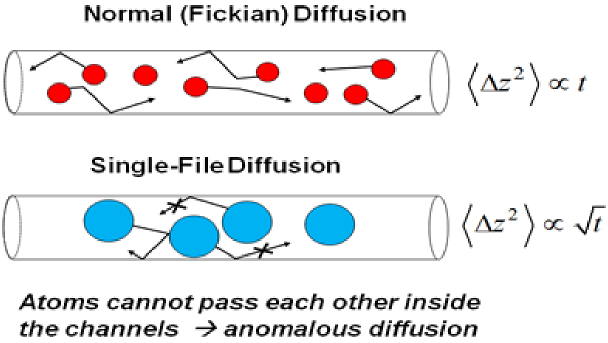
Unfortunately, solving these equations was not a straightforward task. Exact results were first obtained at the microscopic level and, then, coarse-grained.

INTERACTING PARTICLE

SYSTEMS

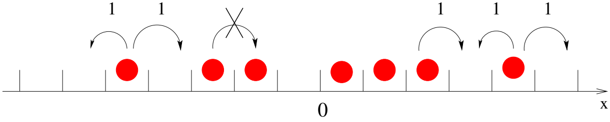
Single-file diffusion

Single-file diffusion is an important phenomena soft-condensed matter (for example, transport through cell membranes).



The exclusion process

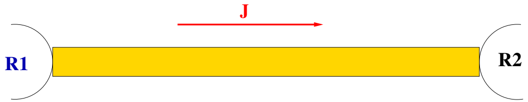
A pristine model for single-file diffusion is the Symmetric Exclusion Process, in which particles perform continuous-time random walks with hard-core (classical) exclusion interaction



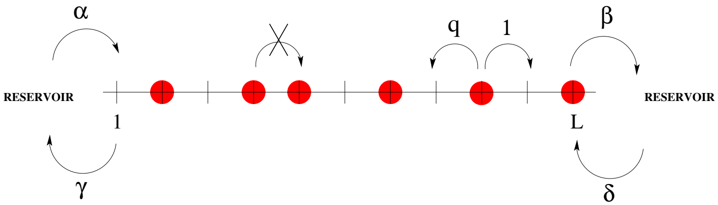
This minimal model appears as a building block in many realistic studies of 1d transport and studied extensively in biophysics, condensed matter, polymer reptation, growth processes (KPZ equation), combinatorics, probability and even traffic flow.

The exclusion process: Classical Transport in 1d

A picture of a non-equilibrium system



A paradigm: the simple exclusion process



A building block in many realistic models of 1d transport and studied extensively in probability, combinatorics, condensed matter physics...
Thousands of articles devoted to this model in the last 20 years.

A solvable model: Integrability

One of the reasons that makes the exclusion process (and some variants) so attractive and popular is that it is **integrable**.

A key observation was made Shlomo Alexander and, independently, by Deepak Dhar in the eighties. The Markov matrix of the exclusion process is **identical** to the Heisenberg Spin chain Hamiltonian:

$$M = \sum_{l=1}^{L} \left(\mathbf{S}_l^+ \mathbf{S}_{l+1}^- + q \mathbf{S}_l^- \mathbf{S}_{l+1}^+ + \frac{1+q}{4} \mathbf{S}_l^z \mathbf{S}_{l+1}^z - \frac{1+q}{4} \right)$$

where $\mathbf{S} = (S_x, S_y, S_z)$ are the Pauli matrices (and q represents the asymmetry of the jumps; $q = 1$ for symmetric walks).

Thus, the exclusion process can be solved using (quantum) integrability methods (Bethe Ansatz).

The microscopic analysis of this interacting, non-equilibrium, N-body process, can be carried out to extreme precision (B. Derrida, M. Evans, J. Lebowitz, V. Hakim, D. Mukamel, G. Schütz, E. Speer, H. Spohn...).

A more physical approach, based on hydrodynamics, would be appealing.

The Symmetric Exclusion Process (SEP) on Z.

Consider the Symmetric Exclusion Process, $(p = q = 1)$ on $\mathbb{Z}$ with a uniform finite density ρ of particles.

Suppose that we tag and observe a particle that was initially located at site 0 and monitor its position X_t with time.

On the average $\langle X_t \rangle = 0$ but how large are its fluctuations?

- If the particles were non-interacting (no exclusion constraint), each particle would diffuse normally $\langle X_t^2 \rangle = Dt$.
- Because of the exclusion condition, a particle displays an anomalous diffusive behaviour: when $t \to \infty$, we have

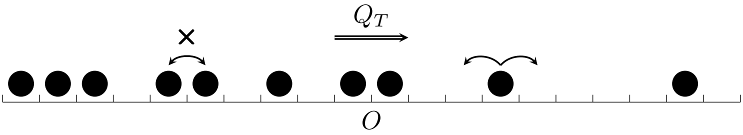
$$\langle X_t^2 \rangle \simeq 2\frac{1-\rho}{\rho}\sqrt{\frac{Dt}{\pi}} \qquad \text{(Arratia, 1983)}$$

The exact probability distribution of X_t remained unknown for almost 40 years.

Large deviations of the total current in SEP

We now study the symmetric exclusion process, $p = q = 1$, on the infinite line $\mathbb{Z}$ and start with 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 $(0, T)$.



- LDP for large T: $\mathrm{Prob}\left(\frac{Q_T}{\sqrt{T}} = q\right) \simeq \exp[-\sqrt{T}\Phi(q)]$.
- Cumulant Generating Function (Legendre Tr.): $\langle e^{\lambda Q_T} \rangle \simeq e^{\sqrt{T}\mu(\lambda)}$
- In the continuous limit: $Q_T = \int_0^\infty [\rho(x, T) - \rho(x, 0)]dx$

GOAL: Determine $\mu(\lambda)$ [or $\Phi(q)$] + the associated profile ρ and the conditioning momentum field H.

The MFT equations for single-file diffusion

For the Simple Exclusion Process, $D_{\mathrm{SEP}} = 1$, $\sigma_{\mathrm{SEP}} = 2\rho(1-\rho)$. Hence, in the MFT language, we must solve the coupled PDE's

$$\begin{aligned} \partial_t \rho &= \partial_x \left[\partial_x \rho - 2\rho(1-\rho)\partial_x H\right] \\ \partial_t H &= -\partial_{xx} H - (1-2\rho)(\partial_x H)^2 \end{aligned}$$

With non-local boundary condition:

$$H(x, T) = \lambda\theta(x)$$

$$H(x, 0) = \lambda\theta(x) + \log \frac{\rho(x,0)(1-\bar{\rho}(x))}{\bar{\rho}(x)(1-\rho(x,0))}$$

where $\bar{\rho}(x) = \rho_-\theta(-x) + \rho_+\theta(x)$ is the mean-initial step profile.

From the optimal profile ρ^* solving of this system, the CGF (and the rate function) are obtained from

$$\frac{d\mu}{d\lambda} = \frac{Q_T}{\sqrt{T}} = \int_0^\infty \left[\rho^*(x,T) - \rho^*(x,0)\right] \frac{dx}{\sqrt{T}}$$

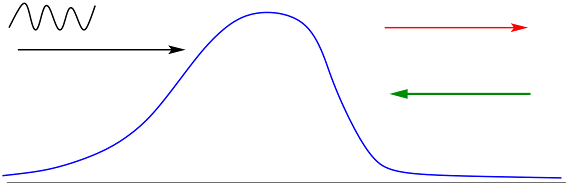
MACROSCOPIC FLUCTUATION THEORY

AND

INVERSE SCATTERING

Quantum Mechanical Scattering

Consider, in Quantum Mechanics, a localized potential $U(x)$ on which a plane wave is scattered.



One solves the Schrödinger equation, with plane wave asymptotic states. The scattering process can be characterized by the scattering amplitudes (proportional to the reflection and transmission coefficients). They are denoted by $a(k), b(k), \bar{a}(k)$ and $\bar{b}(k)$.

Reconstruction by Inverse Scattering

The scattering amplitudes encode information about the potential $U(x)$. Ideally knowing $a(k), b(k), \bar{a}(k)$ and $\bar{b}(k)$ (and information about bound states if there are any) should allow us to reconstruct $U(x)$.

This is the Inverse Scattering Problem: the potential is retrieved by solving a linear integral equation, with kernels constructed from (the Fourier-Transform of) the reflexion and transmission coefficients. Such equations are known as the Gelfand-Levitan-Marchenko equations.

$* * *$

Inverse Scattering for Non-Linear Waves

Consider, *as an example* the KdV equation, a non-linear, dispersive, wave equation:

$$\partial_t u - 6u\partial_x u + \partial_{xxx} u = 0$$

with the initial condition $u(x, 0) = U(x)$. This equation has an infinite number of independent conserved quantities and solitary waves that scatter in a 'nice' way. But it is a non-linear PDE!!

How can we determine $u(x, t)$ the solution of such a non-linear wave equation?

The Inverse Scattering Method (ISM) is the following:

1. Take the initial condition $u(x,0) = U(x)$ as a potential in the Schrödinger equation. Solve the associated quantum-mechanical scattering problem by determining the initial scattering amplitudes $a_0(k), b_0(k), \bar{a}_0(k)$ and $\bar{b}_0(k)$.

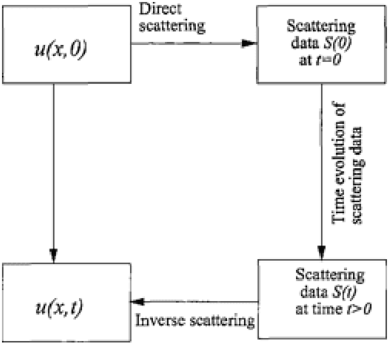
2. Now, consider the Schrödinger equation with potential $u(x,t)$, where $u(x,t)$ is the (unknown) solution of KdV at a given, frozen, time t.

• Just by using the fact that $u(x,t)$ satisfies KdV, one can prove, *without solving KdV*, that the scattering amplitudes for the Schrödinger equation with potential $u(x,t)$ are related to the initial $t = 0$ scattering amplitudes in a very simple manner:

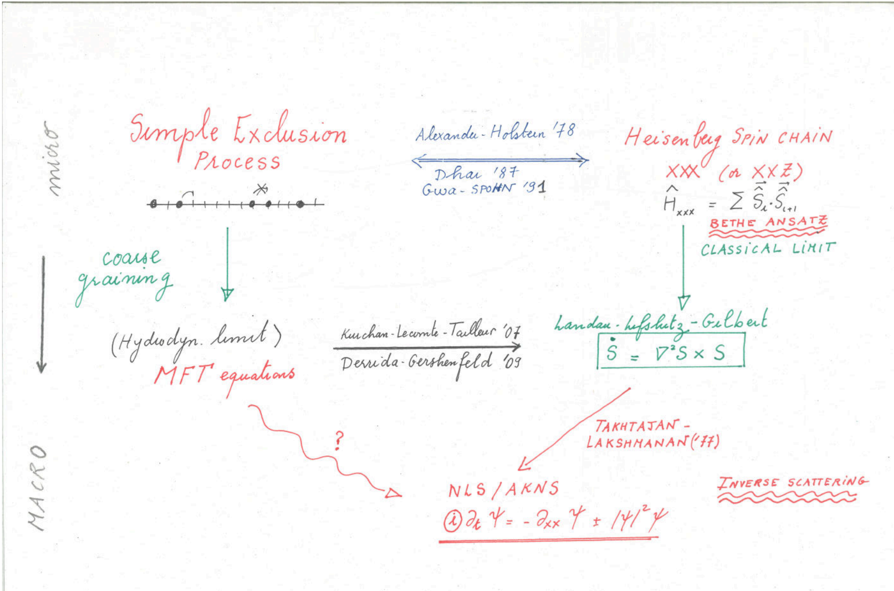
$$a(k,t) = a_0(k) \qquad \text{and} \qquad b(k,t) = b_0(k)\mathrm{e}^{8ik^3 t}$$

• The knowledge of the scattering amplitudes at any time t, allows you to reconstruct $u(x,t)$ by Inverse Scattering by solving a linear problem.

ISM as a non-linear Fourier Transform



SOLVING MFT BY ISM: A chart of models



A generalization of the Cole-Hopf mapping

The following novel non-local transformation

$$u(x,t) = \left(\frac{\partial \rho}{\partial x} - \rho(1-\rho)\frac{\partial H}{\partial x}\right) \exp\left[-\int_{-\infty}^{x} dy(1-2\rho)\partial_y H\right],$$
$$v(x,t) = -\frac{\partial H}{\partial x} \exp\left[\int_{-\infty}^{x} dy(1-2\rho)\partial_y H\right]$$

maps the MFT to the *Ablowitz-Kaup-Newell-Segur (AKNS) system:*

$$\boxed{\begin{aligned} \partial_t u(x,t) &= \partial_{xx} u(x,t) - 2u(x,t)^2 v(x,t) \\ \partial_t v(x,t) &= -\partial_{xx} v(x,t) + 2u(x,t) v(x,t)^2 \end{aligned}}$$

The boundary conditions transform also well (still non-local in time):

$$u(x,0) = \omega\delta(x) \qquad \text{and} \qquad v(x,T) = \delta(x)$$

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

Integrability of AKNS

The AKNS equations have an infinite number of conserved quantities in involution. They are classically integrable in the sense of Liouville.

The AKNS equations can be solved by using the Inverse Scattering Theory.

The Linear Scattering Problem associated to AKNS is a two-component wave equation in which the unknown functions $u(x,t)$ and $v(x,t)$ play the role of the scattering potentials:

$$\begin{cases} \frac{\partial}{\partial x}\psi_1(x,t) & = -ik\psi_1 + v(x,t)\psi_2 \\ \frac{\partial}{\partial x}\psi_2(x,t) & = u(x,t)\psi_1 + ik\psi_2 \end{cases}$$

where ψ_1 and ψ_2 behave as plane waves at $x = \pm\infty$. (Here, t is simply a parameter).

Remark: The AKNS equations are related to the NLS equation in imaginary time ($u \to \psi$ and $v \to \psi^*$).

Solving MFT by Inverse Scattering

We wish to apply ISM to Simple Exclusion (MFT). However, we have non-local boundary conditions (*not* Cauchy initial conditions):

$$u(x,0) = \omega\delta(x) \qquad \text{but} \qquad v(x,0) \text{ is unknown}$$
$$v(x,T) = \delta(x) \qquad \text{but} \qquad u(x,T) \text{ is unknown}$$

Then, integrability allows you match the scattering data at initial and final times and 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:

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

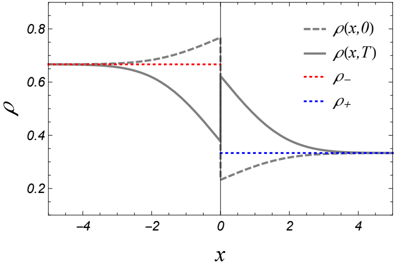
where $1 + \hat{u}_{\pm}$ is analytic on the upper (respectively lower) complex plane, with a given product along $\mathbb{R}$. This is exactly the same equation that was constructed by Grabsch, Poncet, Rizkallah, Illien and Bénichou.

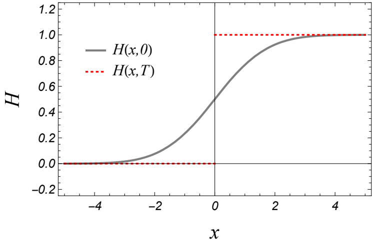
Optimal Profiles and Control Fields

The Riemann–Hilbert problem is solved by Cauchy Transform:

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

Gathering all the pieces and going back to variables (ρ^*, H^*), solves the MFT equations and explicit formulas for the optimal fields are obtained.





Optimal profiles of ρ (left) and H (right) at $t = 0$ and at $t = T$, with $\rho_+ = 1/3$, $\rho_- = 2/3$, $\lambda = 1$ and $T = 1$.

Cumulant Generating Function 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

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

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

The CGF has been previously calculated at microscopic level using combinatorial techniques (Derrida and Gershenfeld 2007, Imamura, M. and Sasamoto 2017 and 2021). Microscopic and macroscopic approach match perfectly.

Optimal profiles describing the dynamical evolution that generates a given fluctuation – or a rare event – appear to be out of reach at microscopic level but are found by solving the MFT.

Conclusions

A major challenge in non-equilibrium physics is to determine the large deviations, considered to be the relevant generalizations of the thermodynamic potentials (Free Energy) far from equilibrium.

Interacting particle processes (such as the exclusion process) are ideal toy-models to investigate these questions with a large variety of methods:

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

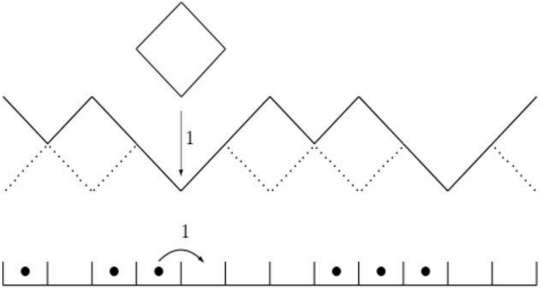
• Coarse-grained level: hydrodynamic limits, fluctuating hydrodynamics (SPDE), Macroscopic Fluctuation Theory for optimal paths (PDE)...

Finding explicit time-dependent solutions of the MFT has been a challenge since this theory was proposed (2001).

These exact results are based on the Inverse Scattering Method, originally developed to study for solitons and non-linear dispersive hydrodynamics.

Applications of the MFT framework to other fields (population dynamics, turbulence) are very promising.

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 Exclusion Process is a discrete version of the KPZ equation in one-dimension.

Finite time distribution of the tracer

The distribution function of the tracer X_t is given, at all times, in terms of a Fredholm determinant:

$$\boxed{\mathbb{P}[X_t \leq x] = \int_{C_0} \frac{dz}{1-z} \det(1 + \omega K_{x,t})_{L_2(C_0)} W_0(z)}$$

where

$$\omega(z) = \rho_+(z^{-1} - 1) + \rho_-(z-1) + \rho_+\rho_-(z^{-1} - 1)(z-1)$$

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

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

The ω variable expresses fundamental symmetries of the model : parity and time-reversal. (It appears recurrently in calculations for SEP).

The Kernel $K_{t,x}$ originates from the Bethe Ansatz.

The function W_0 carries 'Poisson-like' boundary conditions.

C_0 is a small enough complex contour around 0 (poles from the denominator of the kernel are excluded).

Fredholm determinant (aparte)

Let $K = (K_{ij})$ be a finite matrix. Then, the following expansion holds:

$$\det(I + \omega K) =$$

$$1 + \omega \sum_i K_{ii} + \frac{\omega^2}{2!} \sum_{i_1, i_2} \begin{vmatrix} K_{i_1 i_1} & K_{i_1 i_2} \\ K_{i_2 i_1} & K_{i_2 i_2} \end{vmatrix} + \frac{\omega^3}{3!} \sum_{i_1, i_2, i_3} \begin{vmatrix} K_{i_1 i_1} & K_{i_1 i_2} & K_{i_1 i_3} \\ K_{i_2 i_1} & K_{i_2 i_2} & K_{i_2 i_3} \\ K_{i_3 i_1} & K_{i_3 i_2} & K_{i_3 i_3} \end{vmatrix} + \ldots$$

For a compact trace-class operator with kernel $K(x, y)$, we do the following replacement (i.e. discretize)

$$\sum_i K_{ii} \to \int dx\, K(x, x)$$

$$\sum_{i_1, i_2} \begin{vmatrix} K_{i_1 i_1} & K_{i_1 i_2} \\ K_{i_2 i_1} & K_{i_2 i_2} \end{vmatrix} \to \int \int dxdy \begin{vmatrix} K(x, x) & K(x, y) \\ K(y, x) & K(y, y) \end{vmatrix} \quad \text{etc...}$$

Classical Integrability I: Lax Pair

The AKNS equations can be solved by using **the Inverse Scattering Theory,** a method developed to study solitons and non-linear dispersive equations (KdV, NLS, Sine-Gordon, LLE...).
Consider the following auxiliary linear problem ('Lax pair'):

$$\begin{cases} \frac{\partial}{\partial x}\Psi(x,t) & = U(x,t;k)\Psi(x,t) \\ \frac{\partial}{\partial t}\Psi(x,t) & = V(x,t;k)\Psi(x,t) \end{cases}$$

with $\Psi^T(x,t) = (\psi_1(x,t), \psi_2(x,t))$; $U(x,t)$ and $V(x,t)$ are the matrices:

$$U = \begin{pmatrix} -ik & v(x,t) \\ u(x,t) & ik \end{pmatrix} \quad \text{and} \quad V = \begin{pmatrix} 2k^2 + uv & 2ik\, v - \partial_x v \\ 2ik\, u + \partial_x u & -2k^2 - uv \end{pmatrix}$$

The compatibility of these equations, $\partial_t \partial_x \Psi = \partial_x \partial_t \Psi$, is ensured by the zero curvature condition:

$$\boxed{\frac{\partial U}{\partial t} - \frac{\partial V}{\partial x} + [U, V] = 0}$$

This will be ensured if the functions u and v satisfy the AKNS system.

Classical Integrability II: Scattering

We focus on the first equation of the pair. In components, it reads:

$$\begin{cases} \frac{\partial}{\partial x}\psi_1(x,t) &= -ik\psi_1 + v(x,t)\psi_2 \\ \frac{\partial}{\partial x}\psi_2(x,t) &= u(x,t)\psi_1 + ik\psi_2 \end{cases}$$

This is nothing but a linear scattering problem on $\mathbb{R}$, for any given value of the time parameter t, in which the unknown functions $u(x,t)$ and $v(x,t)$ (that solve AKNS) appear as potentials.

Because these potentials vanish at infinity, asymptotic states are well-defined, and ψ_1 and ψ_2 behave as plane waves at $x = \pm\infty$.

Henceforth, incoming/outgoing plane waves from $x \to -\infty$

$$\phi(x;k) \sim \begin{pmatrix} e^{-ikx} \\ 0 \end{pmatrix} \qquad \text{and} \qquad \bar{\phi}(x;k) \sim -\begin{pmatrix} 0 \\ e^{ikx} \end{pmatrix}$$

will scatter at $x \to +\infty$ as follows

$$\phi(x;k) \sim \begin{pmatrix} a(k,t)e^{-ikx} \\ b(k,t)e^{ikx} \end{pmatrix} \quad \text{and} \quad \bar{\phi}(x;k) \sim \begin{pmatrix} \bar{b}(k,t)e^{-ikx} \\ -\bar{a}(k,t)e^{ikx} \end{pmatrix}$$

The functions $a, \bar{a}, b, \bar{b}$ are the scattering amplitudes associated to this scattering process.

Classical Integrability III: Diagonalization

Using the second equation of the Lax pair, which describes the time dynamics of Ψ and the asymptotic plane-wave expressions, the time evolution of the scattering amplitudes is obtained explicitly:

$$\boxed{\begin{array}{ll} a(k,t) = a(k,0), & b(k,t) = b(k,0)e^{-4k^2 t} \\ \bar{a}(k,t) = \bar{a}(k,0), & \bar{b}(k,t) = \bar{b}(k,0)e^{4k^2 t} \end{array}}$$

Key feature: **The dynamics drastically simplifies in terms of the scattering amplitudes.**

The scattering amplitudes are the action-angle variables of the dynamics.

If we know the scattering amplitudes at initial time, they can be determined at all times. Then, the potentials $u(x,t)$ and $v(x,t)$ can be reconstructed at any time by the inverse-scattering procedure (Gelfand-Levitan-Marchenko).

The Inverse Scattering Method can be viewed as a Non-Linear Fourier Transform.