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The Exclusion Process: A paradigm for non-equilibrium behaviour

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In these lectures, we shall present some remarkable results that have been obtained for systems far from equilibrium during the last two decades. We shall put a special emphasis on the concept of large deviation functions that provide us with a unified description of many physical situations. These functions are expected to play, for systems far from equilibrium, a role akin to that of the thermodynamic potentials. These concepts will be illustrated by exact solutions of the Asymmetric Exclusion Process, a paradigm for non-equilibrium statistical physics.

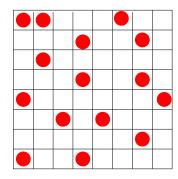
A system at mechanical and at thermal equilibrium obeys the principles of thermodynamics that are embodied in the laws of equilibrium statistical mechanics. The fundamental property is that a system, consisting of a huge number of microscopic degrees of freedom, can be described at equilibrium by only a few macroscopic parameters, called state variables. The values of these parameters can be determined by optimizing a potential function (such as the entropy, the free energy, the Gibbs free energy...) chosen according to the external constraints imposed upon the system. The connection between the macroscopic description and the microscopic scale is obtained through Boltzmann's formula (or one of its variants). Consider, for example, a system system at thermal equilibrium with a reservoir at temperature T. Its thermodynamical properties are encoded by Boltzmann-Gibbs canonical law:

$$P_{\rm eq}(\mathcal{C}) = \frac{{\rm e}^{-E(\mathcal{C})/kT}}{Z}$$

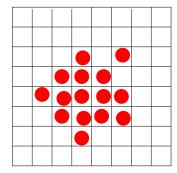
where the Partition Function Z is related to the thermodynamic Free Energy F via

$$F = -kTLog Z$$
.

This expression (which is a consequence of Boltzmann's formula $s = k \log \Omega$) shows that the determination of the thermodynamic potentials can be expressed as a combinatorial (or counting) problem, which of course, can be extremely complex. Nevertheless, equilibrium statistical physics provides us with a well-defined prescription to analyse thermodynamic systems: an explicit formula for the canonical law is given; this defines a probability measure on the configuration space of the system; statistical properties of observables (mean-values, fluctuations) can be calculated by performing averages with respect to this probability measure. The paradigm of equilibrium statistical physics is the Ising Model (see Figure 1). It was solved in two dimensions by L. Onsager (1944). We emphasize that equilibrium statistical mechanics predicts macroscopic fluctuations (typically Gaussian) that are out of reach of classical thermodynamics: the paradigm of such fluctuations is the Brownian Motion.



High Temperature



Low Temperature

FIG. 1: The 2d Ising Model: the 'SCORE' of a given configuration is defined as the number of particles without a neighbour. Then, the probability to observe a configuration defined to be proportional to $e^{-\beta SCORE}$, where β is proportional to the inverse temperature. This model displays a phase transition: At High Temperature, $\beta \to 0$, the system does not display any order, we have gas; at low Temperature, $\beta \to \infty$ a clustering occurs and the system is in a condensed phase. A phase transition occurs at a Critical Temperature β_c .

For systems far from equilibrium, a theory that would generalize the formalism of equilibrium statistical mechanics to time-dependent processes is not yet available. However, although the theory is far from being complete, substantial progress has been made, particularly during the last twenty years. One line of research consists in exploring structural properties of non-equilibrium systems: this endeavour has led to celebrated results such as Fluctuation Theorems that generalize Einstein's fluctuation relation and linear response theory. Another strategy, inspired from the research devoted to the Ising model, is to gain insight into non-equilibrium physics from analytical studies and from exact solutions of some special models. In the field of non-equilibrium statistical mechanics, the Asymmetric Simple Exclusion Process (ASEP) is reaching the status of a paradigm.

In these lecture notes, we shall first review equilibrium properties in Section I. Using Markov processes, we shall give a dynamical picture of equilibrium in Section IA. Then we shall introduce the detailed balance condition and explain how it is related to time reversal (Section IB). This will allow us to give a precise definition of the concept of 'equilibrium' from a dynamical point of view.

The study of non-equilibrium processes will begin in Section II. We shall use as a leitmotiv for non-equilibrium, the picture of rod (or pipe) in contact with two reservoirs at different temperatures, or at different electrical (chemical) potentials (see Figure 8). This simple picture will allow us to formulate some of the basic questions that have to be answered in order to understand non-equilibrium physics. The current theory of non-equilibrium processes requires the use of some mathematical tools, such as large-deviation functions, that are introduced, through various examples (Independent Bernoulli variables, random walk...), in Section II A; in particular, we explain how the thermodynamic Free Energy is connected to the large deviations of the density profile of a gas enclosed in a vessel. In Section II B, we show the relations between the large-deviation function and cumulants of a random variable. Section II C is devoted to the very important concept of generalized detailed balance, a fundamental remnant of the time-reversal invariance of physics, that prevails even in situations far from equilibrium. Then, in Section II D, the Fluctuation Theorem is derived for Markov system that obey generalized detailed balance.

From Section III on, these lectures focus on the Asymmetric Exclusion Process (ASEP) and on some of the techniques developed in the last twenty years to derive exact solutions for this model and its variants. After a brief presentation of the model and of some of its simple properties (Sections III A to III C), we apply the Mean-Field approximation to derive the hydrodynamic behaviour in Section III D; in particular, this technique is illustrated on the Lebowitz-Janowsky blockage model, a fascinating problem that has so far eluded an exact solution. Finally, in Section III E, the celebrated exact calculation of the steady state of the ASEP with open boundaries, using the Matrix Representation Method, is described.

Section IV contains a crash-course on the Bethe Ansatz. We believe that the ASEP on a periodic ring, is the simplest model to learn how to apply this very important method. We try to explain the various steps that lead to the Bethe Equations in Section IV A. These equations are analysed in the special TASEP case in Section IV B.

We are now ready to calculate large deviation functions for non-equilibrium problems: this is the goal of Section V. Our aim is to derive large deviations of the stationary current for the pipe picture, modelled by the ASEP. This is done first for the periodic case (ASEP on a ring) in Section VA, then for the open system in contact with two reservoirs (Section VB). The similarities between the two solutions are emphasized. Exact formulae for cumulants and for the large deviation functions are given. This Section is the most advanced part of the course and represents the synthesis of the concepts and techniques that were developed in earlier sections. Detailed calculations are not given and can be found in recent research papers.

The last section is devoted to concluding remarks and is followed by the Bibliography. We emphasize that these lecture notes are not intended to be a review paper. Therefore, the bibliography is rather succinct and is restricted to some of the books, review papers or articles that were used while preparing this course. More precise references can be found easily from these sources. Our major influences in preparing these lectures come from the review of B. Derrida [7] and from the book of P. L. Krapivsky, S. Redner and E. Ben-Naim [19].

I. DYNAMICAL PROPERTIES OF THE EQUILIBRIUM STATE

The average macroscopic properties of systems at thermodynamic equilibrium are independent of time. However, one should not think that thermodynamic equilibrium means absence of dynamical behaviour: at the microscopic scale, the system keeps on evolving from one micro-state to another. This never-ending motion manifests itself as fluctuations at the macroscopic scale, the most celebrated example being the Brownian Motion. However, one crucial feature of a system at thermodynamic equilibrium is the absence of currents in the system: there is no macroscopic transport of matter, charge, energy, momentum, spin or whatsoever within the system or between the system and its environment. This is a very fundamental property, first stated by Onsager, that stems from the time-reversal symmetry of the microscopic equations of motion. This property is true both for classical and quantum dynamics.

A. Markovian dynamical models

We want to describe the evolution of a complex system consisting of a very large number N of interacting degrees of freedom. In full rigour, one should write the N-body (quantum) Hamiltonian that incorporates the full evolution of the system under consideration. However, it is often useful to consider effective dynamical descriptions that are obtained, for example, by coarse-graining the phase-space of the system or by integrating-out fast modes. In the following, the models we shall study will follow classical Markovian dynamics and we shall give a short presentation of Markov systems. The interested reader can find more details, in particular about the underlying assumptions that lead to Markov dynamics, in e.g. the book by N. G. Van Kampen [29]. We also emphasize that many properties that we shall discuss here can be generalized to other dynamical systems.

The classical Markov processes that we shall study here will be fully specified by a (usually finite or numerable) set of microstates $\{C_1, C_2, \ldots\}$. At a given time t, the system can be found in one its microstates. The evolution of the system is specified by the following rule: Between t and t+dt, the system can jump from a configuration \mathcal{C} to a configuration \mathcal{C}' . It is assumed that the transition rate from \mathcal{C} to \mathcal{C}' does not depend on the previous history of the system: this is the crucial Markov hypothesis in which short time correlations are neglected. The rate of transition per unit time will be denoted by $M(\mathcal{C}',\mathcal{C})$ (or equivalently, by $M(\mathcal{C} \to \mathcal{C}')$). Note that this rate may vary with time and depend explicitly on t. This case will not be considered in the present lectures. To summarize, the Markov dynamics is specified by the following rules:

$$\mathcal{C} \to \mathcal{C}'$$
 with probability $M(\mathcal{C}', \mathcal{C})dt$

These dynamical rules can be illustrated by a network in the configuration space (see Figure 2): the nodes of the graph are the microstates and oriented-edges, weighted by the Markov rates $M(\mathcal{C}', \mathcal{C})$ represent possible transitions between configurations.

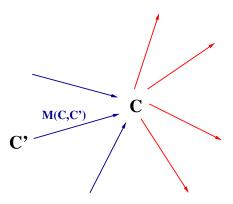


FIG. 2: Representation of a Markov process as a network.

For a system with Markov dynamics, one can define $P_t(\mathcal{C})$, the probability of being in the micro-state \mathcal{C} at time t. This probability measure varies with time: its evolution is governed by the Master equation, given by

$$\frac{\frac{d}{dt}P_t(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}, \mathcal{C}')P_t(\mathcal{C}') - \left\{ \sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}', \mathcal{C}) \right\} P_t(\mathcal{C}) }{(1)}$$

This equation is fundamental. To derive it, one must take into account all possible transitions between time t and t+dt that involve a given configuration \mathcal{C} . There are two types of moves: (i) transitions $into\ \mathcal{C}$ coming from a different configuration \mathcal{C}' ; (ii) transitions $out\ of\ \mathcal{C}$ towards a different configuration \mathcal{C}' . The moves (i) and (ii) contribute with a different sign to the change of the probability of occupying \mathcal{C} between time t and t+dt. Note that the Master equation can well be interpreted as a flux-balance equation on the network of Figure 2.

The way we have encoded the transition rates naturally suggests that the Master Equation can be rewritten in a Matrix form. Indeed, reinterpreting the rate $M(\mathcal{C}',\mathcal{C})$ as matrix-elements and defining the diagonal term

$$M(\mathcal{C}, \mathcal{C}) = -\sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}, \mathcal{C}'), \qquad (2)$$

allows us to rewrite Equation (1) as

$$\frac{dP_t}{dt} = M.P_t \tag{3}$$

We emphasize that the diagonal term $M(\mathcal{C}, \mathcal{C})$ is a negative number: it represents *minus* the rate of leaving the configuration \mathcal{C} . This leads to an important property: the sum of each column of M identically vanishes. This property guaranties, by simple algebra, that the total probability is conserved: $\sum_{\mathcal{C}} P_t(\mathcal{C}) = \sum_{\mathcal{C}} P_0(\mathcal{C}) = 1$ (the initial probability distribution being normalized).

Note that there is a formal analogy between Markov systems and quantum dynamics: the Markov operator M plays the role of a quantum Hamiltonian. However, M does not have to be a symmetric or Hermitian matrix (and is not, in general).

There are numerous examples of Markov processes in statistical physics. The paradigm is certainly the simple symmetric random walk on a discrete lattice (see Figure 3). Here, the configurations are the lattice sites and the transition rates are constant and uniform (i.e. translation-invariant). The corresponding Markov equation is the discrete Laplace equation on the lattice.

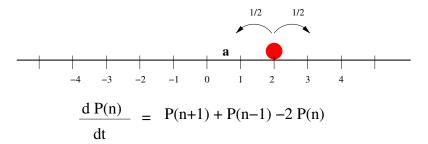


FIG. 3: The simple random walk is a Markov process.

Another important example is given by Langevin dynamics (see Figure 4). It was originally invented by Paul Langevin as mechanical model for the Brownian Motion but stochastic dynamics has become a widely studied subject, that allows for instance to model the effects of noise in mechanical and electric devices. The basic idea is to incorporate a random force that represents thermal noise into classical Newtonian dynamics:

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

Here $\xi(t)$ is a Gaussian white noise of amplitude Γ .

The state of a particle is a point in phase-space, i.e a configuration is specified by the position and the velocity (or momentum) of the particle (the set of possible configurations is continuous and non-enumerable). The corresponding Markov equation for the probability distribution function $P_t(x, v)$, of being at x with velocity v, is known as the Fokker-Planck equation:

$$\frac{dP_t}{dt} = -\frac{\partial}{\partial x} \left\{ v P_t \right\} + \frac{\partial}{\partial v} \left\{ \frac{\gamma v + \nabla U}{m} P_t \right\} + \frac{\Gamma}{m^2} \frac{\partial^2 P_t}{\partial v^2} = \mathcal{L}_{FP}.P_t \,.$$

The role of the Markov matrix is played by the Fokker-Planck operator \mathcal{L}_{FP} . There are many formal similarities between the Fokker-Planck equation and the discrete Markov dynamics given by (3); however, subtle mathematical issues can arise in the case of a continuous configuration space that require the use of functional analysis.

Both Markov and Fokker-Planck dynamics are mathematical models, that can be defined and studied without any specific reference to physical principles. However, to be physically relevant, these dynamics should be connected to the laws of thermodynamics and statistical physics. In particular, one can impose that the steady state of these equations is an equilibrium-state: in other words, the stationary probability distribution must be identical to the Boltzmann-Gibbs canonical law.

For a discrete Markov dynamics (3), this condition reads

$$\sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}, \mathcal{C}') e^{-E(\mathcal{C}')/kT} = e^{-E(\mathcal{C})/kT} \left\{ \sum_{\mathcal{C}' \neq \mathcal{C}} M(\mathcal{C}', \mathcal{C}) \right\}$$

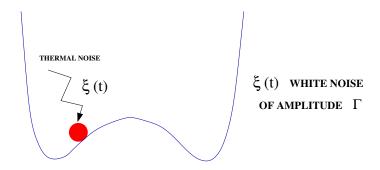


FIG. 4: Langevin dynamics in a double-well potential: this model leads to analytical calculations of reaction-rates and transition-times.

This is a set of global constraints on the rates, which is sometimes called the 'global balance' condition. Similarly, in the Langevin case, one imposes that the invariant measure of phase-space is given by

$$P_{\text{eq}}(x, v) = \frac{1}{Z} e^{-\frac{1/2mv^2 + \mathcal{U}(x)}{kT}}$$

Writing that this formula is the stationary solution of the Fokker-Planck equation, one observes that this fixes the the noise-amplitude Γ as a function of temperature

$$\Gamma = \gamma kT$$
.

This is in essence the reasoning followed by Langevin in his study of the Free Brownian Motion (for which the external potential vanishes $\mathcal{U}=0$). Substituting the value of Γ in the corresponding Fokker-Planck equation leads to

$$\frac{dP_t}{dt} = \frac{\gamma}{m} \frac{\partial}{\partial v} (vP_t) + \frac{\gamma kT}{m^2} \frac{\partial^2 P_t}{\partial v^2}$$

Multiplying both sides of this equation by x^2 and integrating over phase-space allows us to show that

$$\langle x^2 \rangle = 2Dt$$
 with $D = \frac{kT}{\gamma}$.

Using Stokes' formula $\gamma = 6\pi\eta a$ for the friction-coefficient (coefficient of the linearized force felt by a sphere of radius a, dragged at velocity v, in a liquid of viscosity η), leads to the celebrated formula of Einstein (1905) for the diffusion constant of the Brownian Motion, in terms of the Avogadro Number.

B. Time-reversal and Detailed Balance

We now discuss a fundamental characteristic of equilibrium dynamics that was first investigated by L. Onsager. Again, the property discovered by Onsager is a very general one. We shall present it here on Markov dynamics. The master equation (1) can be written in the following manner

$$\frac{d}{dt}P_t(\mathcal{C}) = \sum_{\mathcal{C}'} \left\{ M(\mathcal{C}, \mathcal{C}') P_t(\mathcal{C}') - M(\mathcal{C}', \mathcal{C}) P_t(\mathcal{C}) \right\} = \sum_{\mathcal{C}'} J_t(\mathcal{C}, \mathcal{C}'),$$

where we have introduced the local probability current $J_t(\mathcal{C}, \mathcal{C}')$ between \mathcal{C} and \mathcal{C}' (See Figure 5).

When the stationary state is reached, we know that the right-hand side of this equation must vanish. However, equilibrium is a very particular stationary state: at equilibrium the microscopic dynamics of the system is *time-reversible*. This symmetry property implies that all the *local* currents $J_t(\mathcal{C}, \mathcal{C}')$ vanish separately (Onsager):

$$M(\mathcal{C}, \mathcal{C}')P_{\text{eq}}(\mathcal{C}') = M(\mathcal{C}', \mathcal{C})P_{\text{eq}}(\mathcal{C})$$
(4)

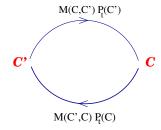


FIG. 5: A graphical representation of the local probability current $J_t(\mathcal{C}, \mathcal{C}')$.

This is the **detailed balance equation.** We emphasize that detailed balance is a very *strong property* goes beyond the laws of classical thermodynamics.

We shall now explain the mathematical relation between detailed balance and time-reversal. The main-idea is to use the transition rates to construct a probability measure on time-trajectories of the system.

The two important mathematical properties we shall use are the following:

1. Probability of remaining in C during a time interval τ :

$$\lim_{dt\to 0} \left(1 + M(\mathcal{C}, \mathcal{C})dt\right)^{\frac{\tau}{dt}} = e^{M(\mathcal{C}, \mathcal{C})\tau}$$

2. Probability of going from C to C during dt: M(C',C)dt

Relation 1 can be derived by calculating the probability of staying in the same configuration between t and t + dt and integrating over $0 \le t \le \tau$. Relation 2 is simply the definition of the transition rates in a Markov process.

Let us now consider a 'history' of the system between the initial time 0 and the final T. During this interval of time, the system follows a trajectory: it begins with a configuration C_0 , then at a date t_1 it jumps into configuration C_1 , stays there till t_2 and jumps to C_2 and so on. This special trajectory, denoted by C(t) is depicted in Figure 6.

TRAJECTORY C(t)

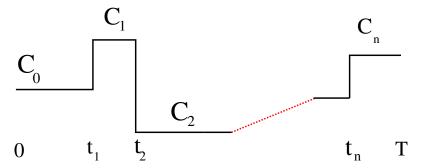


FIG. 6: A trajectory of a Markov process during the time interval [0, T].

Using the relations 1 and 2 above, we can calculate the weight of this specific trajectory C(t), i.e the probability $Pr\{C(t)\}$ of observing C(t), in the equilibrium state. The only extra ingredient we need to include is the fact that the initial condition C_0 at t=0 is chosen according to the equilibrium measure. We thus have

$$\Pr\{C(t)\} = e^{M(\mathcal{C}_n, \mathcal{C}_n)(T-t_n)} M(\mathcal{C}_n, \mathcal{C}_{n-1}) dt_n \ e^{M(\mathcal{C}_{n-1}, \mathcal{C}_{n-1})(t_n-t_{n-1})} \dots e^{M(\mathcal{C}_1, \mathcal{C}_1)(t_2-t_1)} M(\mathcal{C}_1, \mathcal{C}_0) dt_1 \ e^{M(\mathcal{C}_0, \mathcal{C}_0)t_1} P_{\text{eq}}(\mathcal{C}_0)$$

For any given trajectory C(t), a time-reversed trajectory can be defined as $\hat{C}(t) = C(T - t)$. This is a bona-fide history of the system (see Figure 7) and one can calculate the probability of observing it:

$$\Pr{\{\hat{C}(t)\}} = e^{M(\mathcal{C}_0, \mathcal{C}_0)t_1} \ M(\mathcal{C}_0, \mathcal{C}_1)dt_1 \ e^{M(\mathcal{C}_1, \mathcal{C}_1)(t_2 - t_1)} \ \dots e^{M(\mathcal{C}_{n-1}, \mathcal{C}_{n-1})(t_n - t_{n-1})} \ M(\mathcal{C}_{n-1}, \mathcal{C}_n)dt_n \ e^{M(\mathcal{C}_n, \mathcal{C}_n)(T - t_n)} P_{eq}(\mathcal{C}_n)$$

TIME-REVERSED TRAJECTORY C(T-t)

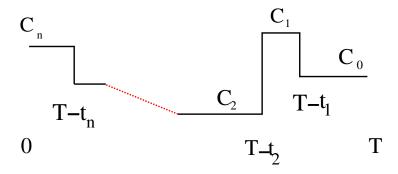


FIG. 7: Calculating the weight of the time-reversed trajectory.

If we now calculate the ratio of these two probabilities i.e. the ratio of the probability observing a given history $\hat{C}(t)$ by that of observing the reversed history $\hat{C}(t)$, we obtain the ratio between the probabilities of forward and backward trajectories:

$$\frac{\Pr\{\mathcal{C}(t)\}}{\Pr\{\hat{\mathcal{C}}(t)\}} = \frac{M(\mathcal{C}_n, \mathcal{C}_{n-1})M(\mathcal{C}_{n-1}, \mathcal{C}_{n-2})\dots M(\mathcal{C}_1, \mathcal{C}_0) P_{\text{eq}}(\mathcal{C}_0)}{M(\mathcal{C}_0, \mathcal{C}_1) M(\mathcal{C}_1, \mathcal{C}_2) \dots M(\mathcal{C}_{n-1}, \mathcal{C}_n) P_{\text{eq}}(\mathcal{C}_n)}$$
(5)

Using recursively the detailed balance condition:

$$M(\mathcal{C}_1, \mathcal{C}_0)P_{\text{eq}}(\mathcal{C}_0) = P_{\text{eq}}(\mathcal{C}_1)M(\mathcal{C}_0, \mathcal{C}_1)$$

and zipping it through the previous result leads us to the following remarkable identity

$$\frac{\Pr\{\mathcal{C}(t)\}}{\Pr\{\hat{\mathcal{C}}(t)\}} = 1$$

Hence, detailed balance implies that the dynamics is time reversible. The converse property is true: if we want that a dynamics to be time-reversal invariant, then the detailed balance relation must be satisfied (consider simply a history in which there occurs a single transition between two configurations \mathcal{C} and \mathcal{C}').

To conclude, the detailed balance relation is a profound property of the equilibrium state that reflects time-reversal invariance of the dynamics. This relation is now taken as a definition for the concept of equilibrium: a stationary state is an equilibrium state if and only if detailed balance is satisfied.

II. NONEQUILIBRIUM PROCESSES

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.

A basic example of a nonequilibrium process is a conductor, or a pipe, in contact with two reservoirs at different temperatures, or electrical or chemical potential. In the stationary state, a non-vanishing steady-state current will flow from the reservoir at higher potential towards the one at lower potential. This current clearly breaks time reversal invariance. In the vicinity of equilibrium, linear response theories allow us to predict the statistical behaviour of this current and to derive analytically the response coefficients (conductance, susceptibilities) from the knowledge of equilibrium fluctuations. However, one may wonder if a general microscopic theory, not obtained by a perturbative expansion in the vicinity of equilibrium, may be constructed. At present no such framework exists. However, in the last two decades, important progress and convincing proposals for a general description of non-equilibrium statistical mechanics have been made. We shall describe some of these theories in these lectures. Our main inspiration in this section is the two review papers by B. Derrida [7, 8].

For the moment being, we use the 'pipe model' (see Figure 8) as a paradigmatic illustration of stationary non-equilibrium behaviour and let us formulate some very basic questions:

- What are the *relevant macroscopic parameters*? How many macroscopic observables should we include to have a fair description of the system?
- Which functions describe the state of a system? Can the stationary state be derived by optimizing a potential?
- Do *Universal Laws* exist? Can one define Universality Classes for systems out of equilibrium? Are there some general equations of state?
- Can one postulate a general form for the *microscopic measure* that would generalize the Gibbs-Boltzmann canonical Law?
- What do the statistical properties of the current in the stationary state look like (In particular, are the current fluctuations Brownian-like)?

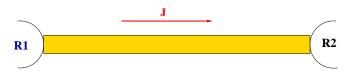


FIG. 8: A stationary driven system in contact with two reservoirs at different temperature and/or potential: In the steady state, a non-vanishing macroscopic current J flows. This pipe paradigm will be used as a leitmotiv throughout the text.

A. Large Deviations and Rare Events

Large Deviation Functions (LDFs) are important mathematical objects, used in probability theory, that are becoming widely used in statistical physics. Large deviation functions are used to quantify rare events that, typically, have exponentially vanishing probabilities. We shall introduce this concept through an elementary example. A very useful review on large deviations has recently been written by H. Touchette [28].

Let $\epsilon_1, \ldots, \epsilon_N$ be N independent binary variables, $\epsilon_k = \pm 1$, with probability p (resp. q = 1 - p). Their sum is denoted by $S_N = \sum_{1}^{N} \epsilon_k$. We know, from the Law of Large Numbers that $S_N/N \to p - q$ almost surely. Besides, the Central Limit Theorem tells us that the fluctuations of the sum S_N are of the order \sqrt{N} . More precisely, $[S_N - N(p-q)]/\sqrt{4pqN}$ converges towards a Normalized Gaussian Law.

One may ask a more refined question: how fast is the convergence implied by the Law of Large Numbers? In other words, what does the probability that S_N/N assumes a non-typical value look like when $N \to \infty$? For the example, we consider, elementary combinatorics shows that for -1 < r < 1, in the large N limit, we have

$$\Pr\left(\frac{S_N}{N} = r\right) \sim e^{-N \Phi(r)}$$

where the positive function $\Phi(r)$ vanishes for r = (p-q). This is an elementary example of a large deviation behaviour. The function $\Phi(r)$ is a called a rate function or a large deviation function. It encodes the probability of rare events. A simple application of Stirling's formula yields

$$\Phi(r) = \frac{1+r}{2} \ln\left(\frac{1+r}{2p}\right) + \frac{1-r}{2} \ln\left(\frac{1-r}{2q}\right)$$

We have discussed a very specific example but large deviations appear in many different contexts. We now consider an asymmetric random walker on a one-dimensional lattice with anisotropic hopping rates to neighbouring sites, given by p and q (see Figure 9). The average speed of the walker is given by p-q: If X_t is the (random) position of the walker at time t we have for $t \to \infty$

$$\frac{X_t}{t} \to p - q$$
 (almost surely)

We can define a large deviation function G(v) by the following relation:

Proba
$$\left(\frac{X_t}{t} = v\right) \sim e^{-t G(v)}$$

valid in the limit of large times.

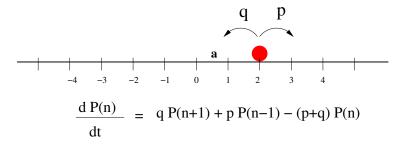


FIG. 9: An asymmetric random walker on a discrete line. The rates for right and left hopping are given by p and q respectively. The average speed of the walker is given by p-q.

This function can be calculated explicitly. It is given by:

$$G(v) = q + \frac{v}{2}\log\frac{q}{p} - \sqrt{v^2 + 4pq} - |v|\log\frac{2\sqrt{pq}}{|v| + \sqrt{v^2 + 4pq}}$$

Note that

- G(v) is a positive function that vanishes at v = p q.
- G(v) is convex.
- $G(v) G(-v) = v \log \frac{q}{p}$.
- Using the definition of the large deviation function, we observe that, in the long time limit, the previous identity implies

$$\frac{\operatorname{Proba}\left(\frac{X_t}{t} = v\right)}{\operatorname{Proba}\left(\frac{X_t}{t} = -v\right)} = e^{t \, v \log \frac{p}{q}}$$

Our third example is closer to physics. Let us consider a gas, at thermodynamic equilibrium at temperature T, consisting of N molecules enclosed in a vessel of total volume V. The average density is $\rho_0 = N/V$. We wish to probe local density fluctuations. We consider an imaginary volume v, containing a large number of molecules but remaining much smaller than the total volume, i.e. such that $\rho_0^{-1} \ll v \ll V$. Counting the number n of molecules in v will give us an empirical density $\rho = n/v$ (see Figure 10). Clearly, for v large enough the empirical density ρ will be very close to ρ_0 and typical fluctuations will scale as $\sqrt{v/V}$. What is the probability that ρ significantly deviates from ρ_0 ?

The probability of observing large fluctuations again satisfies a large deviation behaviour:

Proba
$$\left(\frac{n}{v} = \rho\right) \sim e^{-v \Phi(\rho)}$$
 with $\Phi(\rho_0) = 0$.

In order to determine $\Phi(\rho)$, we must count the fraction of the configurations of the gas in which there are $n = \rho v$ particles in the small volume v and N - n particles in the rest of the volume (V - v). Suppose that the interactions of the gas molecules are local. Then, neglecting surface effects, this number is given by

Proba
$$\left(\frac{n}{\mathbf{v}} = \rho\right) \simeq \frac{Z(\mathbf{v}, n, T)Z(V - \mathbf{v}, N - n, T)}{Z(V, N, T)}$$

Finally, we use that by definition, $Z(\mathbf{v}, n, T) = e^{-v\beta f(\rho, T)}$ where $\beta = 1/k_B T$ is the inverse temperature and $f(\rho, T)$ is the free energy per unit volume and perform an expansion for $1 \ll \mathbf{v} \ll V$. This leads to

$$\Phi(\rho) = \beta \left(f(\rho, T) - f(\rho_0, T) - (\rho - \rho_0) \frac{\partial f}{\partial \rho_0} \right).$$

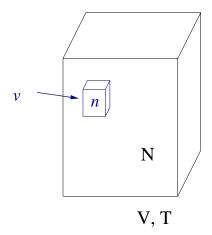


FIG. 10: Equilibrium Fluctuations of density in a gas vessel.

We emphasize that this large deviation function is very closely related to the thermodynamic Free Energy.

A more general question would be the large deviation of a density profile. Suppose we fully cover the large box with K = V/v small boxes. What is the probability of observing an empirical density ρ_1 in the first box, ρ_2 in the second box etc...? Here again, we can show that a large deviation principle is satisfied:

Proba
$$(\rho_1, \rho_2, \dots \rho_K) \simeq e^{-V \mathcal{F}(\rho_1, \rho_2, \dots \rho_K)}$$

where the large deviation function \mathcal{F} depends on K variables. A reasoning similar to the one above allows us to show that

Proba
$$(\rho_1, \rho_2, \dots \rho_K) \simeq \frac{\prod_k Z(n_k, v, T)}{Z(V, N, T)}$$

Taking the infinite volume limit, we obtain

$$\mathcal{F}(\rho_1, \rho_2, \dots \rho_K) = \frac{\beta}{K} \sum_{k=1}^K (f(\rho_i, T) - f(\rho_0, T))$$

If now, we let the number K of boxes go to infinity, then the question we are asking is the probability of observing a given density profile $\rho(x)$ in the big volume V. For $K \to \infty$, the large deviation function \mathcal{F} becomes a functional of the density profile:

$$\mathcal{F}[\rho(x)] = \beta \int dx \left(f(\rho(x), T) - f(\rho_0, T) \right)$$

 $f = -\log Z(\rho, T)$ being, as above, the *free energy per unit volume*. We conclude that the Free Energy of Thermodynamics could have been defined *ab initio* as a large deviation function. More generally, all thermodynamic potentials can be realized as large deviation functions.

However, the concept of large deviations does not pertain to equilibrium. Large deviation functions can be introduced for very general processes, even far from equilibrium. They are positive functions that attain their minimum for when their argument takes the typical stationary variable. These remarks suggest that these functions may be used as potentials in non-equilibrium statistical mechanics.

B. Large Deviations and Cumulants

Let X_t be a variable that satisfies a large deviation principle in the limit $t \to \infty$:

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

where the large deviation function $\Phi(j)$ is positive and vanishes at j = J.

Another way to encode the statistics of X_t is to study its moment-generating function, defined as the average value $\langle e^{\mu X_t} \rangle$. Expanding with respect of μ , we get

$$\log \left\langle e^{\mu X_t} \right\rangle = \sum_k \frac{\mu^k}{k!} \langle \langle X^k \rangle \rangle_c$$

where $\langle \langle X^k \rangle \rangle_c$ denotes the k-th cumulant of X_t .

From the large deviation principle, we can show the following behaviour:

$$\langle e^{\mu X_t} \rangle \simeq e^{E(\mu)t}$$
 when $t \to \infty$ (6)

This implies that all all cumulants of X_t grow linearly with time and their values are given by the successive derivatives of $E(\mu)$. Moreover, the cumulant generating function $E(\mu)$ and the large deviation function $\Phi(j)$ are related by Legendre transform. This can be seen by using the saddle-point method:

$$\langle e^{\mu X_t} \rangle = \int \Pr(X_t) e^{\mu X_t} dX_t = t \int \Pr\left(\frac{X_t}{t} = j\right) e^{\mu t j} dj \sim \int e^{\mu t j - t\Phi(j)}$$

From this relation we conclude that,

$$E(\mu) = \max_{j} (\mu j - \Phi(j))$$
(7)

In the following examples, we shall often calculate $E(\mu)$ first and then determine Φ by a Legendre transformation.

C. Generalized Detailed Balance

We have shown that detailed balance is a fingerprint of equilibrium. Conversely, out of equilibrium, time reversibility and detailed balance are broken. A priori, one could imagine that any arbitrary Markov operator could represent a physical system far from equilibrium. This is not the case: the fundamental laws of physics are time-reversible (leaving apart some aspects of weak-interaction). It is only after a coarse-graining procedure, when non-relevant degrees of freedom are integrated out, that the resulting effective dynamics appears to be irreversible for the restricted degrees of freedom we are interested in and for the space and time scales that we are considering. Nevertheless, whatever coarse-grained description is chosen at a macroscopic scale, a signature of this fundamental time-reversibility of physics must remain. In other words, in order to have a sound physical model, even very far from equilibrium, detailed balance can not be violated in an arbitrary manner: there is a 'natural way' of generalizing detailed balance. We shall investigate here what happens to detailed balance for a system connected to unbalanced reservoirs (as in the pipe paradigm).

We first reformulate the equilibrium detailed balance, to make generalizations more transparent.

The Equilibrium Case:

A system is a thermal equilibrium with a reservoir at T satisfies the detailed balance with respect to the Boltzmann weights. Equation (4) becomes

$$M(\mathcal{C}', \mathcal{C})e^{-\beta E(\mathcal{C})} = M(\mathcal{C}, \mathcal{C}') e^{-\beta E(\mathcal{C}')}$$
 (8)

Equivalently, defining $\Delta E = E(C') - E(C)$, which represents the energy exchanged between the system and the reservoir at a transition from C to C', the above equation becomes

$$M_{+\Delta E}(\mathcal{C} \to \mathcal{C}') = M_{-\Delta E}(\mathcal{C}' \to \mathcal{C}) e^{-\beta \Delta E}$$
 (9)

where we have added an index to keep track of the exchanges of energy.

The Non-Equilibrium Case:

Consider now a system S in contact with two reservoirs R_1 and R_2 at T_1 and T_2 . Suppose that during an elementary step of the process, the system can exchange energy (or matter...) ΔE_1 with the first reservoir and ΔE_2 with the second one. Then, generalized detailed balance is given by

$$M_{\Delta E_1, \Delta E_2}(\mathcal{C} \to \mathcal{C}') = M_{-\Delta E_1, -\Delta E_2}(\mathcal{C}' \to \mathcal{C}) e^{-\frac{\Delta E_1}{kT_1} - \frac{\Delta E_2}{kT_2}}$$

$$\tag{10}$$

where $\Delta E_i = E_i(\mathcal{C}') - E_i(\mathcal{C})$ for i = 1, 2. This equation can be obtained by the following physical reasoning. Consider the global system $S + R_1 + R_2$: this is an isolated system, its total energy $E(\mathcal{C}) + E_1 + E_2$ is conserved by the dynamics. Considered as a whole, the global system is governed by a reversible dynamics and in the infinite time limit it will reach the microcanonical measure. Besides, its dynamics must satisfy detailed balance with respect to this microcanonical measure. This condition is expressed as

$$e^{\frac{S_1(E_1) + S_2(E_2)}{k}} M(\{\mathcal{C}, E_1, E_2\} \to \{\mathcal{C}', E_1', E_2'\}) = M(\{\mathcal{C}', E_1', E_2'\} \to \{\mathcal{C}, E_1, E_2\}) e^{\frac{S_1(E_1') + S_2(E_2')}{k}}$$

where S_1 and S_2 are the entropies of the reservoirs (i.e. the logarithms of the phase-space volumes). Using the fact that the reservoirs are at well-defined temperatures and that energy exchanges with the system are small (i.e. $E'_i - E_i \ll E_i$), we can expand the entropy variations of each reservoir and this leads us to Equation (10).

We give now a more abstract formulation of generalized detailed balance in which energy exchanges with the reservoirs are replaced by the flux of an arbitrary quantity Y_t (it can be a mass, a charge, an entropy...). Let us suppose that during an elementary transition from \mathcal{C} to \mathcal{C}' between t and t+dt, the observable Y_t , is incremented by y:

$$\mathcal{C} \to \mathcal{C}'$$
 and $Y_t \to Y_t + y$ with probability $M_y(\mathcal{C}', \mathcal{C})dt$

We shall also assume that Y_t is odd with respect to time-reversal, i.e. by time reversal, the increment y changes its sign: $C' \to C$ and $Y_t \to Y_t - y$.

A generalized detailed balance relation with respect to Y_t will be satisfied if there exists a constant μ_0 such that the transition rates satisfy

$$M_{+y}(\mathcal{C}',\mathcal{C}) = M_{-y}(\mathcal{C},\mathcal{C}') e^{\mu_0 y}$$
(11)

This formula can be further extended by considering multiple exchanges of various quantities between different reservoirs: the statement of generalized detailed balance becomes

$$M_{y_1, y_2, \dots y_k}(\mathcal{C} \to \mathcal{C}') = M_{-y_1, -y_2, \dots -y_k}(\mathcal{C}' \to \mathcal{C}) e^{\mu_1^0 y_1 + \dots \mu_k^0 y_k}$$

D. The Fluctuation Theorem

We shall now discuss a very important property of systems out of equilibrium, known as the Fluctuation Theorem. This relation was derived by G. Gallavotti and E. D. G. Cohen [12]. Here, we follow the proof of the Fluctuation Theorem for valid for Markov processes that was given by Lebowitz and Spohn [22] A crucial emphasis is put on the generalized detailed balance relation.

The idea is to investigate how the generalized detailed balance equation (11) modifies the reasoning of in section IB, where we showed that detailed balance and time reversibility are equivalent.

As in section IB, we consider a trajectory (or history) of the system between time 0 and T. Now, for each jump between two configurations, we also keep track of the increment in the quantity Y_t for which the generalized detailed balance equation (11) is valid (see Figure 11).

As in section IB, we compute the ratio between the probabilities of forward and backward trajectories: equation (5) is not modified (it is true for any Markov process). But, now, we simplify this ratio by using the generalized detailed balance equation (11). We obtain

$$\frac{\Pr\{C(t)\}}{\Pr\{\hat{C}(t)\}} = e^{\mu_0 Y\{C(t)\}} \quad \frac{P_{\text{stat}}(\mathcal{C}_0)}{P_{\text{stat}}(\mathcal{C}_n)}$$
(12)

where $Y\{C(t)\}=y_1+y_2+\ldots y_n$ represents the total quantity of Y transferred when the system follows the trajectory C(t) between 0 and T.

Here, the ratio between the forward and backward probabilities is different from unity. The dynamics is not reversible anymore and the breaking of time-reversal is precisely quantified by the total flux of Y. Recall that Y is odd, under time reversal. Hence, we have

$$Y\{\hat{C}(t)\} = -Y\{C(t)\}$$

It is now useful to define the auxiliary quantity:

$$Z\{C(t)\} = Y\{C(t)\} + \frac{1}{\mu_0} \log \frac{P_{\text{stat}}(\mathcal{C}_0)}{P_{\text{stat}}(\mathcal{C}_n)}$$

TRAJECTORY C(t)

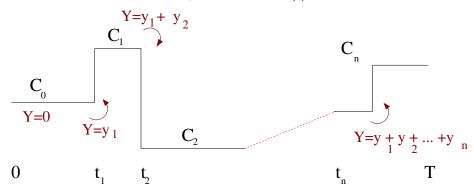


FIG. 11: A trajectory of the system for $0 \le t \le T$. At each transition, the observable Y is incremented by a quantity y.

The quantity $Z\{C(t)\}$ is again odd w.r.t. time-reversal and it satisfies

$$\frac{\Pr\{C(t)\}}{\Pr\{\hat{C}(t)\}} = e^{\mu_0 Z\{C(t)\}}$$

or, equivalently,

$$e^{(\mu-\mu_0)Z\{C(t)\}}\Pr\{C(t)\} = e^{\mu Z\{C(t)\}}\Pr\{\hat{C}(t)\} = e^{-\mu Z\{\hat{C}(t)\}}\Pr\{\hat{C}(t)\}$$
(13)

Summing over all possible histories between time 0 and t, leads us to

$$\sum_{\{C(t)\}} e^{(\mu - \mu_0)Z} \Pr\{C(t)\} = \sum_{\{\hat{C}(t)\}} e^{-\mu Z\{\hat{C}(t)\}} \Pr\{\hat{C}(t)\}$$

Interpreting both sides as average values, we obtain

$$\left\langle e^{(\mu-\mu_0)Z_t} \right\rangle = \left\langle e^{-\mu Z_t} \right\rangle$$
 (14)

This is the statement of the Fluctuation Theorem in Laplace space, for the auxiliary variable Z. The quantities Z_t and Y_t grow with time, linearly in general. Their difference remains, generically, bounded (beware: this could be untrue for some specific systems where 'condensation' in some specific configurations occurs. We assume here this does not happen). This implies that, in the long time limit, Z_t and Y_t have the same statistical behaviour and therefore

$$\left\langle e^{(\mu-\mu_0)Y_t} \right\rangle \simeq \left\langle e^{-\mu Y_t} \right\rangle \quad \text{when } t \to \infty$$

Inserting now the typical behaviour (6) derived in section IIB, $\langle e^{\mu Y_t} \rangle \simeq e^{E(\mu)t}$, we conclude that

$$E(\mu - \mu_0) = E(-\mu) \tag{15}$$

A Legendre transform yields the Gallavotti-Cohen Fluctuation Theorem for the large deviation function

$$\Phi(j) = \Phi(-j) - \mu_0 j \tag{16}$$

Using the large deviation principle, this identity implies

$$\frac{\Pr\left(\frac{Y_t}{t} = j\right)}{\Pr\left(\frac{Y_t}{t} = -j\right)} \simeq e^{\mu_0 j t} \tag{17}$$

This relation is the generic way of stating the Fluctuation Theorem. It compares the probability of occurrence of an event (for example, a total flux of charge, or energy or entropy) with that of the opposite event. This relation is

true far from equilibrium. It has been proved rigorously in various contexts (chaotic systems, Markov/Langevin dynamics...).

Remark: In the multiple variable case, we would obtain for the multi-cumulant generating function

$$E(\mu_1 - \mu_1^0, \dots, \mu_k - \mu_k^0) = E(-\mu_1, \dots, -\mu_k)$$

Or equivalently, for the large deviation function,

$$\Phi(j_1, \dots, j_k) = \Phi(-j_1, \dots, -j_k) - \sum_{i=1}^k \mu_i^0 j_i$$

III. THE EXCLUSION PROCESS

A fruitful strategy to gain insight into non-equilibrium physics is to extract as much information as possible from analytical studies and from exact solutions of some special models. Building a simple representation for complex phenomena is a common procedure in physics, leading to the emergence of paradigmatic systems: the harmonic oscillator, the random walker, the Ising model. All these 'beautiful models' often display wonderful mathematical structures [1].

In the field of non-equilibrium statistical mechanics, the Asymmetric Simple Exclusion Process (ASEP) is reaching the status of such a paradigm. The ASEP consists of particles on a lattice, that hop from a site to its immediate neighbours, and satisfy the exclusion condition (there is at most one particle per site). Therefore, a jump is allowed only if the target site is empty. Physically, the exclusion constraint mimics short-range interactions amongst particles. Besides, in order to drive this lattice gas out of equilibrium, non-vanishing currents must be established in the system. This can be achieved by various means: by starting from non-uniform initial conditions, by coupling the system to external reservoirs that drive currents through the system (transport of particles, energy, heat) or by introducing some intrinsic bias in the dynamics that favours motion in a privileged direction. Thus, each particle is an asymmetric random walker that interacts with the other and drifts steadily along the direction of an external driving force.

From Figure 12, it can be seen that the ASEP on a finite lattice, in contact with two reservoirs, is an idealization of the paradigmatic pipe picture of Figure 8 that we have been constantly discussing.

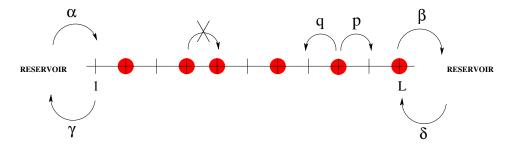


FIG. 12: The Asymmetric Exclusion Process with Open Boundaries.

To summarize, the ASEP is a minimal model to study non-equilibrium behaviour. It is simple enough to allow analytical studies, however it contains the necessary ingredients for the emergence of a non-trivial phenomenology:

- ASYMMETRIC: The external driving breaks detailed-balance and creates a stationary current in the system. The model exhibits a non-equilibrium stationary state.
- EXCLUSION: The hard core-interaction implies that there is at most 1 particle per site. The ASEP is a genuine N-body problem.
- PROCESS: The dynamics is stochastic and Markovian: there is no underlying Hamiltonian.

A. Definition of the Exclusion Process

The ASEP is a Markov process, consisting of particles located on a discrete lattice that evolves in continuous time. We shall consider only the case when the underlying lattice is one dimensional. The stochastic evolution rules are the following: at time t a particle located at a site i in the bulk of the system jumps, in the interval between t and t+dt, with probability p dt to the next neighbouring site i+1 if this site is empty (exclusion rule) and with probability p dt to the site i-1 if this site is empty. The scalars p and q are parameters of the system; by rescaling time, one often takes p=1 and q arbitrary. (Another commonly used rescaling is p+q=1). In the totally asymmetric exclusion process (TASEP) the jumps are totally biased in one direction (q=0 or p=0). On the other hand, the symmetric exclusion process (SEP) corresponds to the choice p=q. The physics and the phenomenology of the ASEP are extremely sensitive to the boundary conditions. We shall mainly discuss three types of boundary conditions (see Figure 13):

- (i) The periodic system: the exclusion process is defined on a one dimensional lattice with L sites (sites i and L+i are identical) and N particles. Note that the dynamics conserves the total number N of particles
- (ii) The finite one-dimensional lattice of L sites with open boundaries. Here, the site number 1 (entrance site) and site number L play a special role. Site 1 interacts with the left reservoir as follows: if site 1 is empty, a particle can enter with rate α whereas if it is occupied it can become vacant with rate γ . Similarly, the interactions with the right reservoir are as follows: if site L is empty, a particle can enter the system with rate δ and if L is occupied, the particle can leave the system with rate β . The entrance and exit rates represent the coupling of the finite system with infinite reservoirs which are at different potentials and are located at the boundaries. In the special TASEP case, $q = \gamma = \delta = 0$: particles are injected by the left reservoir, they hop in the right direction only and can leave the system from the site number L to the right reservoir.
- (iii) The ASEP can also be defined on the infinite one-dimensional lattice. Here, the boundaries are sent to $\pm \infty$. Boundary conditions are here of a different kind: the infinite system remains always sensitive to the configuration it started from. Therefore, when studying the ASEP on the infinite lattice one must carefully specify the initial configuration (or statistical set of configurations) the dynamics has begun with.

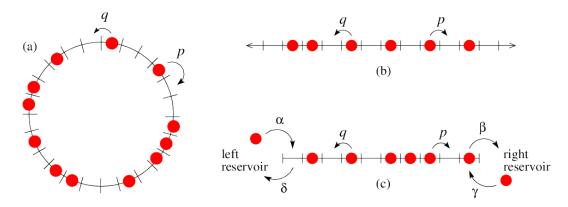


FIG. 13: Different types of boundary conditions: The ASEP can be studied on a periodic chain (a), on the infinite lattice (b) or on a finite lattice connected to two reservoirs (c).

B. Various Incarnations of the ASEP

Due to its simplicity, the ASEP has been introduced and used in various contexts. It was first proposed as a prototype to describe the dynamics of ribosomes along RNA [21] (see Figure 14). In the mathematical literature, Brownian processes with hard-core interactions were defined by Spitzer who coined the name exclusion process. The ASEP also describes transport in low-dimensional systems with strong geometrical constraints such as macromolecules transiting through capillary vessels, anisotropic conductors, or quantum dots where electrons hop to vacant locations and repel each other via Coulomb interaction. Very popular modern applications of the exclusion process include molecular motors that transport proteins along filaments inside the cells and, of course, ASEP and its variants are ubiquitous in discrete models of traffic flow [25]. More realistic models that are relevant for applications will not described further: we refer the reader to the review paper [6] that puts emphasis on biophysical applications.

Another feature of ASEP is its relation with growth processes and in particular to the Kardar-Parisi-Zhang equation in one-dimension (see Figure 15). A classic review on this subject is [16]. The relation between the exclusion process and KPZ has lead recently to superb mathematical developments: we refer the readers to recent reviews [20, 24] for details and references.

More generally, the ASEP belongs to the class of driven diffusive systems defined by Katz, Lebowitz and Spohn in 1984 [18] (see [26] for a review). We emphasize that the ASEP is defined through dynamical rules: there is no energy associated with a microscopic configuration. More generally, the kinetic point of view seems to be a promising and fruitful approach to non-equilibrium systems.

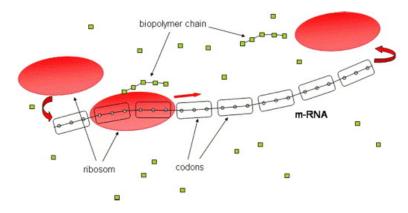


FIG. 14: The ASEP was first defined and studied as a model of biopolymerization on nucleic acid templates [5, 21, 25].

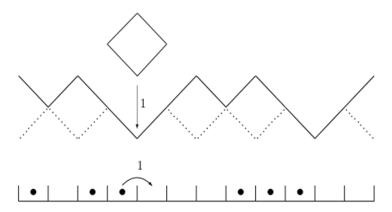


FIG. 15: The one-dimensional ASEP is a discrete version of the KPZ equation, satisfied by the height h(x,t) of a continuous interface: $\frac{\partial h}{\partial t} = \nu \frac{\partial^2 h}{\partial x^2} + \frac{\lambda}{2} \left(\frac{\partial h}{\partial x}\right)^2 + \xi(x,t)$ where $\xi(x,t)$ is a Gaussian white noise.

We emphasize that there are very many variants of the fundamental ASEP: the dynamical rules can be modified (discrete-time dynamics, sequential or parallel updates, shuffle updates); one can introduce local defects in the model by modifying the dynamics on some specific bonds; it is possible to consider different types of particles with different hopping rates; one can also consider quenched or dynamical disorder in the lattice; the lattice geometry itself can be changed (two-lane models, ASEP defined on a stripe, on a network etc...). All these alterations drastically modify the outcome of the dynamics and require specific methods to be investigated. Literally hundreds of works have been devoted to the ASEP and its variants during the last fifteen years. Here, we shall focus only on the homogeneous case with the three ideal types of boundary conditions discussed above and present some of the mathematical methods that have been developed for these three ideal cases.

C. Basis Properties of ASEP

The evolution of the ASEP is encoded in the Markov operator M. For a finite-size system, the Markov operator M is a matrix; for the infinite system M is an operator and its precise definition needs more elaborate mathematical tools [27]. Unless stated otherwise, we shall focus here on the technically simpler case of a finite configuration space of size L and the infinite system limit is obtained formally by taking $L \to \infty$. An important feature of the ASEP on a finite lattice is ergodicity: any configuration can evolve to any other one in a finite number of steps. This property insures that the Perron-Frobenius theorem holds true (see, for example [29]). This implies that the Markov matrix M contains the value 0 as a non-degenerate eigenvalue and that all other eigenvalues E have a strictly negative real part. The physical interpretation of the spectrum of E is the following: the right eigenvector associated with the eigenvalue 0 corresponds to the stationary state (or steady-state) of the dynamics. Because all non-zero eigenvalues E have a strictly negative real part, the corresponding eigenmodes of E are relaxation states: the relaxation time is given by E and the imaginary part of E leads to oscillations.

We emphasize that from the mathematical point of view, the operator M encodes all the required data of the dynamics and any 'physical' questions that one may ask about the system ultimately refers to some property of M. We shall now list some fundamental issues that may arise:

- Once the dynamics is properly defined, the basic question is to determine the steady-state P_{stat} of the system *i.e.*, the eigenvector of M with eigenvalue 0. Given a configuration C, the value of the component $P_{\text{stat}}(C)$ is the stationary weight (or measure) of C in the steady-state, *i.e.*, it represents the frequency of occurrence of C in the stationary state.
- The knowledge of the vector P_{stat} is similar to knowing the Gibbs-Boltzmann canonical law in equilibrium statistical mechanics. From P_{stat} , one can determine steady-state properties and all equal-time steady-state correlations. Some important questions are: what is the mean occupation ρ_i of a given site i? What does the most likely density profile, given by the function $i \to \rho_i$, look like? Can one calculate density-density correlation functions between different sites? What is the probability of occurrence of a density profile that differs significantly from the most likely one (this probability is called the large deviation of the density profile)?
- The ASEP, being a non-equilibrium system, carries a finite, non-zero, steady-state current J. The value of this current is an important physical observable of the model. The dependence of J on the external parameters of the system can allow to define different phases of the system.
- Fluctuations in the steady-state: the stationary state is a dynamical state in which the system constantly evolves from one micro-state to another. This microscopic evolution induces macroscopic fluctuations (which are the equivalent of the Gaussian Brownian fluctuations at equilibrium). How can one characterize steady-state fluctuations? Are they necessarily Gaussian? How are they related to the linear response of the system to small perturbations in the vicinity of the steady-state? These issues can be tackled by considering tagged-particle dynamics, anomalous diffusion, time-dependent perturbations of the dynamical rules etc...
- The existence of a current J in the stationary state corresponds to the physical transport of some extensive quantity Q (mass, charge, energy) through the system. The total quantity Q_t transported during a (long) period of time t in the steady-state is a random quantity. We know that the mean value of Q_t is given by Jt but there are fluctuations. More specifically, in the long time limit, the distribution of the random variable $(Q_t/t-J)$ represents exceptional fluctuations of the mean-current (known as large deviations): this is an important observable that quantifies the transport properties of the system.
- The way a system relaxes to its stationary state is also an important characteristic of the system. The typical relaxation time T of the ASEP scales with the size L of the system as $T \sim L^z$, where z is the dynamical exponent. The value of z is related to the spectral gap of the Markov matrix M, i.e., to the real-part of its largest non-vanishing eigenvalue. For a diffusive system, one has z=2. For the ASEP with periodic boundary condition, an exact calculation leads to z=3/2. More generally, the transitory state of the model can be probed using correlation functions at different times.
- The matrix M is generally a non-symmetric matrix and, therefore, its right eigenvectors differ from its left eigenvectors. For instance, a right eigenvector ψ_E corresponding to the eigenvalue E is defined as

$$M\psi_E = E\psi_E. (18)$$

Knowing the spectrum of M conveys a lot of information about the dynamics. There are analytical techniques, such as the Bethe Ansatz, that allow us to diagonalize M in some specific cases. Because M is a real matrix, its eigenvalues (and eigenvectors) are either real numbers or complex conjugate pairs.

• Solving analytically the master equation would allow us to calculate exactly the evolution of the system. A challenging goal is to determine the finite-time Green function (or transition probability) $P_t(\mathcal{C}|\mathcal{C}_0)$, the probability for the system to be in configuration \mathcal{C} at time t, knowing that the initial configuration at time t = 0 was \mathcal{C}_0 . The knowledge of the transition probability, together with the Markov property, allows us in principle to calculate all the correlation functions of the system.

The following sections are devoted to explaining some analytical techniques that have been developed to answer some of these issues for the ASEP.

D. Mean-Field analysis of the ASEP

Before discussing exact techniques to solve the dynamics of the ASEP, we want to explain the mean-field approach. In many physically important cases with inhomogeneities or more complex dynamical rules, mean-field calculations are the only available technique and they often lead to sound results that can be checked and compared with numerical experiments.

1. Burgers Equation in the Hydrodynamic Limit.

In the limit of large systems, it is natural to look for a continuous description of the model. Finding an accurate hydrodynamic model for interacting particle processes is a difficult and important problem. Here, we present a naive approach that reveals the relation between the ASEP and Burgers equation.

We recall that the binary variable $\tau_i = 0, 1$ characterizes if site i is empty or occupied. The average value $\langle \tau_i(t) \rangle$ satisfies the following equation:

$$\frac{d\langle \tau_i \rangle}{dt} = p[\langle \tau_{i-1}(1-\tau_i) \rangle - \langle \tau_i(1-\tau_{i+1}) \rangle] + q[\langle \tau_{i+1}(1-\tau_i) \rangle - \langle \tau_i(1-\tau_{i-1}) \rangle]
= p\langle \tau_{i-1} \rangle + q\langle \tau_{i+1} \rangle - (p+q)\langle \tau_i \rangle + (p-q)\langle \tau_i(\tau_{i+1}-\tau_{i-1}) \rangle$$

For $p \neq q$: 1-point averages couple to 2-points averages etc... A hierarchy of differential equations is generated (cf BBGKY). This set of coupled equations can not be solved in general. The mean-field approach can be viewed as a technique for closing the hierarchy. For the ASEP, the procedure is quite simple. We sketch it below:

- Define the continuous space variable $x = \frac{i}{L}$ and the limit $L \gg 1$.
- Define a smooth local density by $\langle \tau_i(t) \rangle = \rho(x,t)$.
- Rescale the rates: $p = 1 + \frac{\nu}{L}$ and $q = 1 \frac{\nu}{L}$
- Mean-field assumption: write the 2-points averages as products of 1-point averages.

After carrying out this program leads to, after a diffusive rescaling of time $t \to t/L^2$, to the following partial differential equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2} - 2\nu \frac{\partial \rho (1 - \rho)}{\partial x} \tag{19}$$

This is the Burgers equation with viscosity.

To resume, starting from the microscopic level, we have defined a local density $\rho(x,t)$ and a local current j(x,t) that depend on macroscopic space-time variables $x=i/L, t=s/L^2$ (diffusive scaling) in the limit of weak asymmetry $p-q=\nu/L$ (see Figure 16). Then, we have found that the typical evolution of the system is given by the hydrodynamic behaviour:

$$\partial_t \rho = \nabla^2 \rho - \nu \nabla \sigma(\rho)$$
 with $\sigma(\rho) = 2\rho(1-\rho)$

We have explained how to obtain this equation in a 'hand-waving' manner. However, the result is mathematically correct: it can be proved rigorously that the continuous limit of the weakly-asymmetric ASEP is described, on average, by this equation. The proof is a major mathematical achievement.

Had we kept a finite asymmetry: $p - q = \mathcal{O}(1)$, the same procedure (with ballistic time-rescaling) would have led us to the inviscid limit of Burgers equation:

$$\frac{\partial \rho}{\partial t} = \frac{1}{\mathbf{L}} \frac{\partial^2 \rho}{\partial x^2} - 2\nu \frac{\partial \rho (1 - \rho)}{\partial x}$$

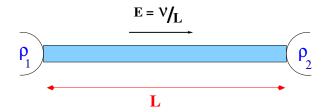


FIG. 16: Hydrodynamic description of the ASEP with open boundaries: the pipe model is retrieved. A weak asymmetry in the jumping rates can be interpreted as a weak bulk electric field, inversely proportional to the size of the system.

This equation is a textbook example of a PDF that generates shocks, even if the initial condition is smooth. A natural question that arises is whether these shocks an artefact of the hydrodynamic limit or do they genuinely exist at the microscopic level. The following model, invented by J. L. Lebowitz and S. A. Janowsky sheds light on this issue.

2. A worked-out example: The Lebowitz-Janowsky model

The Lebowitz-Janowsky model describes the formation of shocks at the microscopic scale [17]. This is very simple model, but it has not been solved exactly. It will provide us with a good illustration of mean-field methods.

The simplest version of Lebowitz-Janowsky model is a TASEP on a periodic ring with one defective bound: through that bound (say the bond between site L and site 1) the jump rate is given by r whereas through all the other bonds, the jump rates are equal to 1. For r < 1 (which is the most interesting case), we have a slow bond, i.e. a constriction, that may prevent the flow of particles through and generate a 'traffic-jam'. This is indeed what is going to happen: for any given density ρ , there is a critical value $r_c(\rho)$ such that for $r \le r_c$ a separation will occur between a dense phase before the slow bond and a sparse phase after that bond.

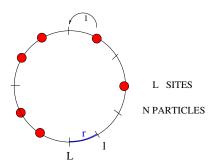


FIG. 17: The TASEP on a ring with an inhomogeneous bond with jump rate r.

The blockage model can be analysed by elementary mean-field considerations. Through a 'normal' bond (i, i + 1) the current is exactly given by $J_{i,i+1} = \langle \tau_i(1 - \tau_{i+1}) \rangle$. In the stationary state, this current is uniform $J_{i,i+1} = J$. Far from the blockage and from the shock region, the density is approximately uniform (as numerical simulations show, see Figure 17). Thus, using a mean-field assumption we can write

$$J = \rho_{low}(1 - \rho_{low}) = \rho_{high}(1 - \rho_{high})$$

where ρ_{low} and ρ_{high} are the values of the density plateaux on both sides of the slow bond. This relation leads to two possible solutions:

- Either the density is uniform everywhere, i.e., $\rho_{low} = \rho_{high} = \rho_0$
- Or we have different densities on the sides that make a shock. Then, necessarily: $\rho_{low} = 1 \rho_{high}$ To find the values of the density plateaux, we calculate the mean-field current right at the defective bond:

$$r\rho_L(1-\rho_1) = r\rho_{high}(1-\rho_{low}) = J$$

(This is a strong approximation that neglects correlations through the slow bond.) We now have enough equations to obtain

$$\rho_{low} = \frac{r}{1+r}$$
 $\rho_{high} = \frac{1}{1+r}$
and
 $J = \frac{r}{(1+r)^2}$

To conclude the analysis, we must find the condition for the existence of the shock: when do we have $\rho_{low} = \rho_{high}$ and when $\rho_{low} < \rho_{high}$? We must use the conservation of the number of particles. Let $1 \le S \le L$ be the position of the shock, then we have $N = S\rho_{low} + (L - S)\rho_{high}$ i.e., dividing by L:

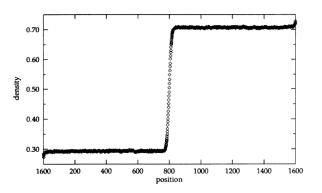
$$\rho_0 = \frac{s \, r + (1 - s)}{r + 1} \qquad \text{with} \qquad 0 \le s = \frac{S}{L} \le 1$$

This relation defines the phase boundary between the uniform and the shock phases. It can be rewritten in a more elegant manner as follows:

$$\left| \rho_0 - \frac{1}{2} \right| \le \frac{1-r}{2(r+1)}$$

From this equation, we observe, in particular, that a shock will always appear for $\rho_0 = 1/2$ as soon as r < 1. The full phase diagram of the system is drawn in Figure 18. Numerical simulations seem to support this phase diagram. However, no exact proof is available. Besides, using an improved mean field analysis, the form of the shock can be calculated. However, the results do not coincide with simulations.

The exact solution of the Lebowitz-Janowsky model is a celebrated open problem in this field (see [17] for references and some recent progress).



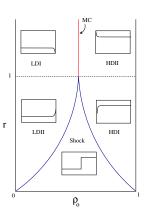


FIG. 18: Numerical simulations of the Lebowitz-Janowsky model in the shock phase. Picture of the phase diagram derived from the mean-field for all values of r and average density ρ_0 .

E. The Steady State of the open ASEP: The Matrix Ansatz

There does not exist a method to calculate the stationary measure for a non-equilibrium interacting model. After briefly describing the stationary state of the ASEP with periodic boundary conditions and of the ASEP on the infinite line, we shall focus on the ASEP with open boundaries.

For the ASEP on a ring the steady state is uniform: all configurations have the same probability. The proof is elementary: for any configuration \mathcal{C} the number of states it can reach to by an elementary move is equal to the total number of configurations that can evolve into it.

For the exclusion process on an infinite line, the stationary measures have been fully studied and classified [27]. There are two one-parameter families of invariant measures: one family, denoted by ν_{ρ} , is a product of local Bernoulli measures of constant density ρ , where each site is occupied with probability ρ ; the other family is discrete and is concentrated on a countable subset of configurations. For the TASEP, this second family corresponds to blocking measures, which are point-mass measures concentrated on step-like configurations (i.e., configurations where all sites to the left of a given site n are empty and all sites to the right of n are occupied).

We now consider the case of the ASEP on a finite and open lattice with open boundaries. For convenience, we rescale the time so that forward jumps occur with rate 1 and backward jumps with rate x = q/p. This scalar x is called the asymmetry parameter.

Here, the mean-field method gives a reasonably good approximation. However, it is not exact for a finite system. There are notable deviations in the density profile (i.e. the function $i \to \rho_i$ where ρ_i is the average density at site i). Moreover, fluctuations and rare events are not well accounted for by mean-field. We shall now explain a method to obtain the exact stationary measure for the ASEP with open boundaries. This technique, known as the Matrix Representation Method, was developed in [9]. Since that seminal paper, it has become a very important tool to investigate non-equilibrium models. The review written by R. A. Blythe and M. R. Evans allows one to learn the Matrix Representation Method for the ASEP and other models and also to find many references [3].

A configuration C can be represented by a string of length L, (τ_1, \ldots, τ_L) , where τ_i is the binary occupation variable of the site i (i.e. $\tau_i = 1$ or 0 if the site i is occupied or empty). The idea is to associate with each configuration C, the following matrix element:

$$P(\mathcal{C}) = \frac{1}{Z_L} \langle W | \prod_{i=1}^L \left(\tau_i D + (1 - \tau_i) E \right) | V \rangle.$$
 (20)

The operators D and E, the vectors $\langle W |$ and $|V \rangle$ satisfy

$$DE - xED = (1 - x)(D + E)$$

$$(\beta D - \delta E) |V\rangle = |V\rangle$$

$$\langle W|(\alpha E - \gamma D) = \langle W|$$
(21)

The claim is that if the algebraic relations (21) are satisfied then, the matrix element (20), duly normalized, is the stationary weight of the configuration C. Note that the normalization constant is $Z_L = \langle W | (D + E)^L | V \rangle = \langle W | C^L | V \rangle$ where C = D + E

This algebra encodes combinatorial recursion relations between systems of different sizes. Generically, the representations of this quadratic algebra are infinite dimensional (q-deformed oscillators).

$$D = \begin{pmatrix} 1 & \sqrt{1-x} & 0 & 0 & \dots \\ 0 & 1 & \sqrt{1-x^2} & 0 & \dots \\ 0 & 0 & 1 & \sqrt{1-x^3} & \dots \\ & & \ddots & \ddots \end{pmatrix} \quad \text{and} \quad E = D^{\dagger}$$

The matrix Ansatz allows one to calculate Stationary State Properties (currents, correlations, fluctuations) and to derive the Phase Diagram in the infinite size limit. There are three phases, determined by the values of ρ_a and ρ_b that represent effective densities of the left and the right reservoir, respectively. The precise formulae for these effective densities for the general ASEP model were found by T. Sasamoto:

$$\rho_{a} = \frac{1}{a_{+} + 1} \quad \text{where} \quad a_{\pm} = \frac{(1 - x - \alpha + \gamma) \pm \sqrt{(1 - x - \alpha + \gamma)^{2} + 4\alpha\gamma}}{2\alpha},$$

$$\rho_{b} = \frac{b_{+}}{b_{+} + 1} \quad \text{where} \quad b_{\pm} = \frac{(1 - x - \beta + \delta) \pm \sqrt{(1 - x - \beta + \delta)^{2} + 4\beta\delta}}{2\beta} \tag{22}$$

In the TASEP case $q = \gamma = \delta = 0$ and p = 1, the algebra simplifies and reduces to

$$DE = D + E$$

$$D|\beta\rangle = \frac{1}{\beta}|\beta\rangle$$

$$\langle\alpha|E = \frac{1}{\alpha}\langle\alpha|$$

For this case, many calculations can be performed in rather simple manner. In particular, the average stationary current is found to be

$$J = \langle \tau_i(1 - \tau_{i+1}) \rangle = \frac{\langle \alpha | C^{i-1} D E C^{L-i-1} | \beta \rangle}{\langle \alpha | C^L | \beta \rangle} = \frac{\langle \alpha | C^{L-1} | \beta \rangle}{\langle \alpha | C^L | \beta \rangle} = \frac{Z_{L-1}}{Z_L}$$

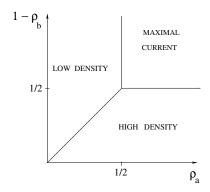


FIG. 19: The Phase Diagram of the open ASEP. The phase in which the system is found depends on the effective densities ρ_a and ρ_b .

In fact, the Matrix Ansatz gives access to all equal time correlations in the steady-state. For example, the density profile:

$$\rho_i = \langle \tau_i \rangle = \frac{\langle \alpha | C^{i-1} D C^{L-i} | \beta \rangle}{\langle \alpha | C^L | \beta \rangle}$$

or even Multi-body correlations:

$$\langle \tau_{i_1} \tau_{i_2} \dots \tau_{i_k} \rangle = \frac{\langle \alpha | C^{i_1 - 1} D C^{i_2 - i_1 - 1} D \dots D C^{L - i_k} | \beta \rangle}{\langle \alpha | C^L | \beta \rangle}$$

The expressions look formal but it is possible to derive explicit formulae: either by using purely combinatorial/algebraic techniques or via a specific representation (e.g., C can be chosen as a discrete Laplacian). For example, we have

$$\langle \alpha | C^L | \beta \rangle = \sum_{p=1}^L \frac{p (2L-1-p)!}{L! (L-p)!} \frac{\beta^{-p-1} - \alpha^{-p-1}}{\beta^{-1} - \alpha^{-1}}$$

The TASEP phase diagram is shown in Figure 20.

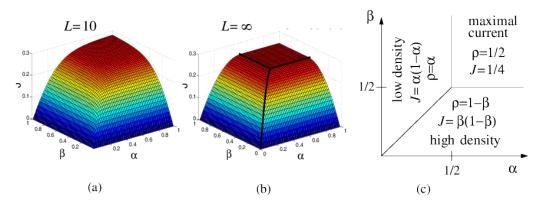


FIG. 20: The Phase Diagram of the open ASEP

For the general ASEP case, results can be derived through more elaborate methods involving orthogonal polynomials, as shown by T. Sasamoto (1999). More details and precise references can again be found in the review of R. Blythe and M. R. Evans [3].

The Matrix Ansatz is an efficient tool to investigate the stationary state. However, it does not allow us to access to time-depend properties: how does the system relax to its stationary state? Can we calculate fluctuations of history-dependent observables (such as the total number of particles exchanged between the two reservoirs during a certain amount of time)?

IV. THE BETHE ANSATZ FOR THE EXCLUSION PROCESS

In order to investigate the behaviour of the system which is not stationary, the spectrum of the Markov matrix is needed. For an arbitrary stochastic system, the evolution operator can not be diagonalized. However, the ASEP belongs to a very special class of models: it is *integrable* and it can be solved using the Bethe Ansatz as first noticed by D. Dhar in 1987. Indeed, the Markov matrix that encodes the stochastic dynamics of the ASEP can be rewritten in terms of Pauli matrices; in the absence of a driving field, the *symmetric* exclusion process can be mapped exactly into the Heisenberg spin chain. The asymmetry due to a non-zero external driving field breaks the left/right symmetry and the ASEP becomes equivalent to a non-Hermitian spin chain of the XXZ type with boundary terms that preserve the integrable character of the model. The ASEP can also be mapped into a six vertex model. These mappings suggest the use of the Bethe Ansatz to derive spectral information about the evolution operator, such as the spectral gap [13, 15] and large deviation function.

Let us apply the Bethe Ansatz to the ASEP on a ring. A configuration can be characterized by the positions of the N particles on the ring, (x_1, x_2, \ldots, x_N) with $1 \le x_1 < x_2 < \cdots < x_N \le L$. With this representation, the eigenvalue equation (18) becomes

$$E \psi_{E}(x_{1},...,x_{N}) = \sum_{i}' p \left[\psi_{E}(x_{1},...,x_{i-1}, x_{i}-1, x_{i+1},...,x_{N}) - \psi_{E}(x_{1},...,x_{n}) \right] + \sum_{j}' q \left[\psi_{E}(x_{1},...,x_{j-1}, x_{j}+1, x_{j+1},...,x_{N}) - \psi_{E}(x_{1},...,x_{N}) \right]$$

$$(23)$$

where the sum are restricted over the indexes i such that $x_{i-1} < x_i - 1$ and over the indexes j such that $x_j + 1 < x_{j+1}$; these conditions ensure that the corresponding jumps are allowed.

We observe that equation (23) is akin to a discrete Laplacian on a N-dimensional lattice: the major difference is that the terms corresponding to forbidden jumps are absent. Nevertheless, this suggests that a trial solution (Ansatz in German) in the form of plane waves may be useful. This is precisely the idea underlying the Bethe Ansatz. In the following we shall give an elementary introduction to this technique which is used in very many different areas of theoretical physics. Originally, H. Bethe developed it to study the Heisenberg spin chain model of quantum magnetism. The ASEP is the one of the simplest systems to learn the Bethe Ansatz.

A. Bethe Ansatz for ASEP: a crash-course

Our aim is to solve the linear eigenvalue problem (23) which corresponds to the relaxation modes of the ASEP with N particles on a ring of L sites. We shall study some special cases with small values of N in order to unveil the general structure of the solution.

The 1 particle case:

For N=1, equation (23) reads

$$E\psi_E(x) = p\psi_E(x-1) + q\psi_E(x+1) - (p+q)\psi_E(x), \qquad (24)$$

with $1 \le x \le L$ and where periodicity is assumed

$$\psi_E(x+L) = \psi_E(x). \tag{25}$$

Equation (24) is simply a linear recursion of order 2 that is solved as

$$\psi_E(x) = Az_+^x + Bz_-^x, (26)$$

where $r=z_{\pm}$ are the two roots of the characteristic equation

$$qr^{2} - (E+p+q)r + p = 0. (27)$$

The periodicity condition imposes that at least one of the two characteristic values is a L-th root of unity (Note that because $z_+z_-=p/q$ both of them can not be roots of unity as soon as $p \neq q$). The general solution is, finally,

$$\psi_E(x) = Az^x \qquad \text{with} \quad z^L = 1, \tag{28}$$

The solution is therefore a simple plane wave with momentum $2k\pi/L$ and with eigenvalue

$$E = \frac{p}{z} + qz - (p+q). (29)$$

The 2 particles case:

The case N=2 where two particles are present is more interesting because when the particles are located on adjacent sites the exclusion effect plays a role. Indeed, the general eigenvalue equation (23) can be split into two different cases:

• The Generic case: here x_1 and x_2 are separated by at least one empty site:

$$E\psi_E(x_1, x_2) = p\left[\psi_E(x_1 - 1, x_2) + \psi_E(x_1, x_2 - 1)\right] + q\left[\psi_E(x_1 + 1, x_2) + \psi_E(x_1, x_2 + 1)\right] -2(p + q)\psi_E(x_1, x_2).$$
(30)

• The (special) adjacency case: $x_2 = x_1 + 1$, some jumps are forbidden and the eigenvalue equation reduces to:

$$E\psi_E(x_1, x_1 + 1) = p\psi_E(x_1 - 1, x_1) + q\psi_E(x_1, x_1 + 2) - (p + q)\psi_E(x_1, x_1 + 1).$$
(31)

This equation differs from the generic equation (30) in which we substitute $x_2 = x_1 + 1$: there are missing terms. An equivalent way to take into account the adjacency case is to impose that the generic equation (30) is valid for all values of x_1 and x_2 and add to it the following cancellation boundary condition:

$$p\psi_E(x_1, x_1) + q\psi_E(x_1 + 1, x_1 + 1) - (p + q)\psi_E(x_1, x_1 + 1) = 0.$$
(32)

We now examine how these equations can be solved. In the generic case particles behave totally independently (i.e., they do not interact). The solution of the generic equation (30) can therefore be written as a product of plane waves $\psi_E(x_1, x_2) = Az_1^{x_1} z_2^{x_2}$, with the eigenvalue

$$E = p\left(\frac{1}{z_1} + \frac{1}{z_2}\right) + q(z_1 + z_2) - 2(p+q).$$
(33)

However, the simple product solution can not be the full answer: indeed the cancellation condition for the adjacency case (32) has to be satisfied also. The first crucial observation, following H. Bethe, is that the eigenvalue E, given in (33) is invariant by the permutation $z_1 \leftrightarrow z_2$. In other words, there are two plane waves $Az_1^{x_1}z_2^{x_2}$ and $Bz_2^{x_1}z_1^{x_2}$ with the same eigenvalue E which has a two-fold degeneracy; the full eigenfunction corresponding to E can thus be written as

$$\psi_E(x_1, x_2) = A_{12} z_1^{x_1} z_2^{x_2} + A_{21} z_2^{x_1} z_1^{x_2}, \tag{34}$$

where the amplitudes A_{12} and A_{21} are yet arbitrary. The second key step is to understand that these amplitudes can now be chosen to fulfil the adjacency cancellation condition: if we substitute the expression (34) in equation (32), we obtain the relation

$$\frac{A_{21}}{A_{12}} = -\frac{qz_1z_2 - (p+q)z_2 + p}{qz_1z_2 - (p+q)z_1 + p}.$$
(35)

The eigenfunction (34) is therefore determined, but for an overall multiplicative constant. We now implement the periodicity condition that takes into account the fact that the system is defined on a ring. This constraint can be written as follows for $1 \le x_1 < x_2 \le L$

$$\psi_E(x_1, x_2) = \psi_E(x_2, x_1 + L). \tag{36}$$

This relation plays the role of a quantification condition for the scalars z_1 and z_2 that we shall call hereafter the *Bethe roots*. Indeed, if we impose the condition that the expression (34) satisfies equation (36) for all generic values of the positions x_1 and x_2 we obtain new relations between the amplitudes:

$$\frac{A_{21}}{A_{12}} = z_2^L = \frac{1}{z_1^L} \,. \tag{37}$$

Comparing equations (35) and (37) leads to a set of algebraic equations obeyed by the Bethe roots z_1 and z_2 :

$$z_1^L = -\frac{qz_1z_2 - (p+q)z_1 + p}{qz_1z_2 - (p+q)z_2 + p}$$
(38)

$$z_2^L = -\frac{qz_1z_2 - (p+q)z_2 + p}{qz_1z_2 - (p+q)z_1 + p}$$
(39)

These equations are known as the *Bethe Ansatz Equations*. Finding the spectrum of the Matrix M for two particles on a ring of size L is reduced to solving these two coupled polynomial equations of degree of order L with unknowns z_1 and z_2 . Surely, this still remains a very challenging task but the Bethe equations are explicit and very symmetric. Besides, we emphasize that the size of the matrix M (and the degree of its characteristic polynomial) is of order L^2 .

The 3 particles case:

We are now ready to consider the case N=3. For a system containing three particles, located at $x_1 \le x_2 \le x_3$, the generic equation, valid when the particles are well separated, can readily be written using equation (23). But now, the special adjacency cases are more complicated:

(i) Two particles are next to each other and the third one is far apart; such a setting is called a 2-body collision and the boundary condition that results is identical to the one obtained for the case N=2. There are now two equations that correspond to the cases $x_1=x \le x_2=x+1 \ll x_3$ and $x_1 \ll x_2=x \le x_3=x+1$:

$$p\psi_E(x, x, x_3) + q\psi_E(x+1, x+1, x_3) - (p+q)\psi_E(x, x+1, x_3) = 0.$$
(40)

$$p\psi_E(x_1, x, x) + q\psi_E(x_1, x+1, x+1) - (p+q)\psi_E(x_1, x, x+1) = 0$$
(41)

We emphasize again that these equations are identical to equation (32) because the third particle, located far apart, is simply a spectator (x_3 is a spectator in the first equation; x_1 in the second one).

(ii) There can be 3-body collisions, in which the three particles are adjacent, with $x_1 = x, x_2 = x + 1, x_3 = x + 2$. The resulting boundary condition is then given by

$$p\{\psi_E(x,x,x+2) + \psi_E(x,x+1,x+1)\} + q\{\psi_E(x+1,x+1,x+2) + \psi_E(x,x+2,x+2)\} -2(p+q)\psi_E(x,x+1,x+2) = 0.$$
(42)

The fundamental remark is that 3-body collisions do not lead to an independent new constraint. Indeed, equation (42) is simply a linear combination of the constraints (40) and (41) imposed by the 2-body collisions. To be precise: equation (42) is the sum of equation (40), with the substitutions $x \to x$ and $x_3 \to x + 2$, and of equation (41) with $x_1 \to x$ and $x \to x + 1$. Therefore, it is sufficient to fulfil the 2-body constraints because then the 3-body conditions are automatically satisfied. The fact that 3-body collisions decompose or 'factorize' into 2-body collisions is the **crucial property** that lies at the very heart of the Bethe Ansatz. If it were not true, the ASEP would not be exactly solvable or 'integrable'.

For N=3, the plane wave $\psi_E(x_1,x_2,x_3)=Az_1^{x_1}z_2^{x_2}z_3^{x_3}$ is a solution of the generic equation with the eigenvalue

$$E = p\left(\frac{1}{z_1} + \frac{1}{z_2} + \frac{1}{z_3}\right) + q(z_1 + z_2 + z_3) - 3(p+q). \tag{43}$$

However, such a single plane wave does not satisfy the boundary conditions (40) and (41). Here again we note that the eigenvalue E is invariant under the permutations of z_1, z_2 and z_3 . There are 6 such permutations, that belong to Σ_3 the permutation group of 3 objects. The Bethe wave-function is therefore written as a sum of the 6 plane waves, corresponding to the same eigenvalue E, with unknown amplitudes:

$$\psi_E(x_1, x_2, x_3) = A_{123} z_1^{x_1} z_2^{x_2} z_3^{x_3} + A_{132} z_1^{x_1} z_3^{x_2} z_2^{x_3} + A_{213} z_2^{x_1} z_1^{x_2} z_3^{x_3} + A_{231} z_2^{x_1} z_3^{x_2} z_1^{x_3} + A_{312} z_3^{x_1} z_1^{x_2} z_2^{x_3} + A_{321} z_3^{x_1} z_2^{x_2} z_1^{x_3}$$

$$(44)$$

$$= \sum_{\sigma \in \Sigma_3} A_{\sigma} z_{\sigma(1)}^{x_1} z_{\sigma(2)}^{x_2} z_{\sigma(3)}^{x_3}. \tag{45}$$

The 6 amplitudes A_{σ} are uniquely and unambiguously determined (up to an overall multiplicative constant) by the 2-body collision constraints. It is therefore absolutely crucial that 3-body collisions do not bring additional independent constraints that the Bethe wave function could not satisfy. We strongly encourage the reader to perform the calculations (which are very similar to the N=2 case) of the amplitude-ratios.

Finally, the Bethe roots z_1 , z_2 and z_3 are quantized through the periodicity condition

$$\psi_E(x_1, x_2, x_3) = \psi_E(x_2, x_3, x_1 + L), \tag{46}$$

for $1 \le x_1 < x_2 < x_3 \le L$. This condition leads to the Bethe Ansatz equations (the equations for general N are given below).

The general case:

Finally, we briefly discuss the general case N > 3. Here one can have k-body collisions with k = 2, 3, ... N. However, all multi-body collisions 'factorize' into 2-body collisions and ASEP can be diagonalized using the Bethe Wave Function

$$\psi_E(x_1, x_2, \dots, x_N) = \sum_{\sigma \in \Sigma_N} A_{\sigma} z_{\sigma(1)}^{x_1} z_{\sigma(2)}^{x_2} \dots z_{\sigma(N)}^{x_N},$$
(47)

where Σ_N is the permutation group of N objects. The N! amplitudes A_{σ} are fixed (up to an overall multiplicative constant) by the 2-body collision constraints. The corresponding eigenvalue is given by

$$E = p \sum_{i=1}^{N} \frac{1}{z_i} + q \sum_{i=1}^{N} z_i - N(p+q).$$
(48)

The periodicity condition

$$\psi_E(x_1, x_2, \dots, x_N) = \psi_E(x_2, x_3, \dots, x_N, x_1 + L) \quad \text{with} \quad 1 \le x_1 < x_2 < \dots < x_N \le L,$$
(49)

leads to a set of algebraic equations satisfied by the Bethe roots z_1, z_2, \ldots, z_N . The Bethe Ansatz equations are given by

$$z_i^L = (-1)^{N-1} \prod_{j \neq i} \frac{q z_i z_j - (p+q) z_i + p}{q z_i z_j - (p+q) z_j + p} = (-1)^{N-1} \prod_{j \neq i} \frac{x z_i z_j - (1+x) z_i + 1}{x z_i z_j - (1+x) z_j + 1},$$
(50)

for i = 1, ... N. The last equation is obtained by using the asymmetry parameter x = q/p.

The Bethe Ansatz thus provides us with a set of N coupled algebraic equations of degree of order L (Recall that the size of the matrix M is of order 2^L , when $N \simeq L/2$). Although the Bethe equations are highly non-linear, a huge variety of methods have been developed to analyse them.

We remark that for p = q = 1 the Bethe equations are the same as the ones derived by H. Bethe in 1931. Indeed, the symmetric exclusion process is identical to the isotropic Heisenberg spin chain.

B. Analysis of the Bethe Equations for the TASEP

For TASEP, the Bethe equations take a simpler form: making the change of variable $\zeta_i = \frac{2}{z_i} - 1$, these equations become

$$(\mathbf{1} - \zeta_{\mathbf{i}})^{\mathbf{N}} (\mathbf{1} + \zeta_{\mathbf{i}})^{\mathbf{L} - \mathbf{N}} = -2^{\mathbf{L}} \prod_{i=1}^{\mathbf{N}} \frac{\zeta_{\mathbf{j}} - 1}{\zeta_{\mathbf{j}} + 1} \quad \text{for} \quad i = 1, \dots N$$

Note that the r.h.s. is a constant independent of i: There is an effective DECOUPLING. The corresponding eigenvalue is

$$E = \frac{1}{2}(-N + \sum_{j} \zeta_{j})$$

For a fixed value of the r.h.s. the roots ζ_i lie on curves that satisfy

$$|1 - \zeta|^{\rho} |1 + \zeta|^{1-\rho} = const$$

where $\rho = N/L$ is the density (see Figure 21).

The fact that the Bethe equations can be reduced to an effective single-variable polynomial suggests the following self-consistent procedure for solving them:

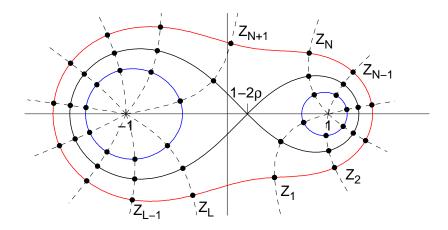


FIG. 21: The loci of the roots of the Bethe Equations for TASEP are remarkable curves known as the Cassini Ovals.

- For any given value of Y, SOLVE $(1-z_i)^N(1+z_i)^{L-N}=Y$. The roots are located on Cassini Ovals
- CHOOSE N roots $z_{c(1)}, \ldots z_{c(N)}$ amongst the L available roots, with a choice set $c: \{c(1), \ldots, c(N)\} \subset \{1, \ldots, L\}$.
- SOLVE the self-consistent equation $\mathbf{A_c}(\mathbf{Y}) = \mathbf{Y}$ where

$$A_c(Y) = -2^L \prod_{j=1}^N \frac{z_{c(j)} - 1}{z_{c(j)} + 1}.$$

• DEDUCE from the value of Y, the $z_{c(j)}$'s and the energy corresponding to the choice set c:

$$2E_c(Y) = -N + \sum_{j=1}^{N} z_{c(j)}.$$

This program can be carried through to calculate the spectral gap of the Markov matrix M, which amounts to calculating E_1 the eigenvalue with largest strictly negative real part. For a density $\rho = N/L$, one obtains for the TASEP

$$E_1 = -2\sqrt{\rho(1-\rho)} \frac{6.509189337...}{L^{3/2}} \pm \frac{2i\pi(2\rho-1)}{L}.$$
 (RELAXATION) (OSCILLATIONS)

The first excited state consists of a pair of conjugate complex numbers when ρ is different from 1/2. The real part of E_1 describes the relaxation towards the stationary state: we find that the largest relaxation time scales as $T \sim L^z$ with the dynamical exponent z = 3/2 [11, 15]. This value agrees with the dynamical exponent of the one-dimensional Kardar-Parisi-Zhang equation that belongs to the same universality class as ASEP (see the review of Halpin-Healy and Zhang 1995 [16] and [20, 24] for recent developments.). The imaginary part of E_1 represents the relaxation oscillations and scales as L^{-1} ; these oscillations correspond to a kinematic travelling wave that propagates with the group velocity $2\rho - 1$. For the partially asymmetric case ($x \neq 0$), the Bethe equations do not decouple and analytical results are much harder to obtain (see [13] for references).

V. LARGE DEVIATION FAR FROM EQUILIBRIUM

We now return to our basic picture of a conducting pipe between two unbalanced reservoirs (Figure 8) and formulate some questions involving the concept of large deviations. Using the ASEP as a paradigm, we shall explain how the tools developed above (Bethe Ansatz, Matrix Representation) can help us to give mathematically precise answers to these problems.

1. In the pipe model, a steady-state is reached with a non-vanishing constant current J and a stationary density profile $\rho(x)$. Typically, this density profile will be linear (as seen by using Fick's phenomenological law). We have seen above that for a system in equilibrium (i.e. when the two reservoirs are at the same potential) the large deviations of the density profile are determined by the free energy. A similar question can be raised in the non-equilibrium stationary state: What is the probability of observing an atypical density profile in the steady state (see Figure 22)? More precisely, assuming a large deviation behaviour,

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

what does the functional $\mathcal{F}(\{\rho(x)\})$ look like in this non-equilibrium system?



FIG. 22: Density Profiles in the pipe model: the average profile is linear. However, non-typical density distributions may occur.

For the ASEP, the answer to this question was given by B. Derrida, J. Lebowitz E. Speer in 2002. These authors calculated the probability of observing an atypical density profile in the steady state of the ASEP, starting from the exact microscopic solution of the exclusion process, with the help of the Matrix Ansatz. For the symmetric exclusion process (which corresponds to a discrete version of Fick's law), the large deviation functional 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

$$F(F'^2 + (1 - F)F'') = F'^2 \rho$$
 with $F(0) = \rho_1$ and $F(1) = \rho_2$.

It is important to note that this functional is non-local as soon as $\rho_1 \neq \rho_2$ and that it is is NOT identical to the one given by assuming local equilibrium.

2. A similar problem can be raised about the current fluctuations. Let us call Y_t the total charge (or time-integrated current) transported through the system between time 0 and time t, then

$$\frac{Y_t}{t} \to J$$
 when $t \to \infty$

where J is the average steady-state current. However, the observable Y_t is a random variable, that may take non-typical values. Its fluctuations obey a large deviation principle:

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

where $\Phi(j)$ is the large deviation function of the total current. Note that $\Phi(j)$ is positive, vanishes at j = J and is convex (in general). A natural question is to derive a mathematical formula $\Phi(j)$. We shall describe below the exact solution for the ASEP.

A. Current Fluctuations far from equilibrium on a periodic ring

We consider in this section the case of a periodic ring and study the statistics of the total displacement of all the particles in the system time 0 and time t. Because the system is finite, this total displacement is proportional to the time integrated current. The ASEP on a periodic ring is drawn again in Figure 23, For convenience, time has been rescaled so that forward jumps occur with rate 1, whereas backward jumps occur with rate x = q/p.

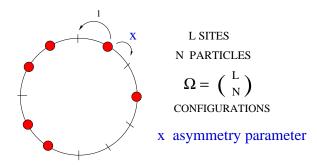


FIG. 23: The ASEP on a periodic ring. After a suitable rescaling of time, the asymmetry parameter is denoted by x.

Thus, here, Y_t will represent the total distance covered by all the particles between time 0 and time t and $P_t(\mathcal{C}, Y)$ is the joint probability of being in the configuration \mathcal{C} at time t and having $Y_t = Y$. The evolution equation of $P_t(\mathcal{C}, Y)$ is:

$$\frac{d}{dt}P_t(\mathcal{C},Y) = \sum_{\mathcal{C}'} \left(M_0(\mathcal{C},\mathcal{C}')P_t(\mathcal{C}',Y) + M_1(\mathcal{C},\mathcal{C}')P_t(\mathcal{C}',Y-1) + M_{-1}(\mathcal{C},\mathcal{C}')P_t(\mathcal{C}',Y+1) \right). \tag{51}$$

Using the generating function $F_t(\mathcal{C})$

$$F_t(\mathcal{C}) = \sum_{Y=0}^{\infty} e^{\mu Y} P_t(\mathcal{C}, Y), \qquad (52)$$

the evolution equation becomes

$$\frac{d}{dt}F_t(\mathcal{C}) = \sum_{\mathcal{C}'} \left(M_0(\mathcal{C}, \mathcal{C}') + e^{\mu} M_1(\mathcal{C}, \mathcal{C}') + e^{-\mu} M_{-1}(\mathcal{C}, \mathcal{C}') \right) F_t(\mathcal{C}') = \sum_{\mathcal{C}'} M(\mu)(\mathcal{C}, \mathcal{C}') F_t(\mathcal{C}'). \tag{53}$$

This equation is similar to the original Markov equation for the probability distribution but now the original Markov matrix M is deformed by a jump-counting fugacity μ into $M(\mu)$ (which is not a Markov matrix in general), given by

$$M(\mu) = M_0 + e^{\mu} M_1 + e^{-\mu} M_{-1}. \tag{54}$$

In the long time limit, $t \to \infty$, the behaviour of $F_t(\mathcal{C})$ is dominated by the largest eigenvalue $E(\mu)$ and one can write

$$\langle e^{\mu Y_t} \rangle \simeq e^{E(\mu)t}$$
 (55)

Thus, in the long time limit, the function $E(\mu)$ is the generating function of the cumulants of the total current Y_t . But $E(\mu)$ is also the dominant eigenvalue of the matrix $M(\mu)$. Therefore, the current statistics has been traded into an eigenvalue problem. Fortunately, the deformed matrix $M(\mu)$ can still be diagonalized by the Bethe Ansatz. In fact, a small modification of the calculations described in Section IV leads to the following Bethe Ansatz equations

$$z_i^L = (-1)^{N-1} \prod_{j=1}^N \frac{x e^{-\mu} z_i z_j - (1+x) z_i + e^{\mu}}{x e^{-\mu} z_i z_j - (1+x) z_j + e^{\mu}}.$$
 (56)

where the asymmetry parameter x = q/p is the ratio of the rates of backward to forward jumps. The eigenvalues of $M(\mu)$ are given by

$$E(\mu; z_1, z_2 \dots z_N) = e^{\mu} \sum_{i=1}^{N} \frac{1}{z_i} + x e^{-\mu} \sum_{i=1}^{N} z_i - N(1+x).$$
 (57)

The cumulant generating function corresponds to the largest eigenvalue.

1. The periodic TASEP Case

For the TASEP, x=0, and the Bethe equations (56) again decouple and can be studied by using the procedure outlined in Section IV B. This case was completely solved by B. Derrida and J. L. Lebowitz in 1998 [10]. These authors calculated $E(\mu)$ by Bethe Ansatz to all orders in μ . More precisely, they obtained the following representation of the function $E(\mu)$ in terms of an auxiliary parameter B:

$$E(\mu) = -N \sum_{k=1}^{\infty} {kL-1 \choose kN} \frac{B^k}{kL-1}, \qquad (58)$$

$$\mu = -\sum_{k=1}^{\infty} \binom{kL}{kN} \frac{B^k}{kL}. \tag{59}$$

These expressions allow to calculate the cumulants of Y_t , for example the mean-current J and the diffusion constant D:

$$J = \lim_{t \to \infty} \frac{\langle Y_t \rangle}{t} = \frac{\mathrm{d}E(\mu)}{\mathrm{d}\mu} \Big|_{\mu=0} = \frac{N(L-N)}{L-1}, \tag{60}$$

$$D = \lim_{t \to \infty} \frac{\langle Y_t^2 \rangle - \langle Y_t \rangle^2}{t} = \frac{\mathrm{d}^2 E(\mu)}{\mathrm{d}\mu^2} \Big|_{\mu=0} = \frac{N^2 (2L-3)! (N-1)!^2 (L-N)!^2}{(L-1)!^2 (2N-1)! (2L-2N-1)!}.$$
(61)

When $L \to \infty$, with a fixed density $\rho = L/N$ and $|j - L\rho(1 - \rho)| \ll L$, the large deviation function G(j) can be written in the following scaling form:

$$G(j) = \sqrt{\frac{\rho(1-\rho)}{\pi N^3}} H\left(\frac{j - L\rho(1-\rho)}{\rho(1-\rho)}\right)$$
(62)

with

$$H(y) \simeq -\frac{2\sqrt{3}}{5\sqrt{\pi}}y^{5/2} \quad \text{for} \quad y \to +\infty,$$
 (63)

$$H(y) \simeq -\frac{4\sqrt{\pi}}{3}|y|^{3/2}$$
 for $y \to -\infty$. (64)

This large deviation function is not a quadratic polynomial, even in the vicinity of the steady state. Moreover, the shape of this function is skew: it decays as the exponential of a power law with an exponent 5/2 for $y \to +\infty$ and with an exponent 3/2 for $y \to -\infty$.

2. The periodic ASEP: Functional Bethe Ansatz

In the general case $x \neq 0$, the Bethe Ansatz equations do not decouple and a procedure for solving them was lacking. For example, it did not even seem possible to extract from the Bethe equations (56) a formula for the mean stationary current (which can be obtained very easily by other means from the fact that the stationary measure is uniform). This problem was solved in a few steps and the complete solution was given by S. Prolhac in 2010 [23]

The periodic ASEP can be analysed by rewriting the Bethe Ansatz as a functional equation and restating it as a purely algebraic problem, as we shall now explain. First, we perform the following change of variables,

$$y_i = \frac{1 - e^{-\mu} z_i}{1 - x e^{-\mu} z_i} \,. \tag{65}$$

In terms of the variables y_i the Bethe equations read

$$e^{L\mu} \left(\frac{1 - y_i}{1 - xy_i} \right)^L = -\prod_{i=1}^N \frac{y_i - xy_j}{xy_i - y_j} \text{ for } i = 1 \dots N.$$
 (66)

Here again the equations do not decouple as soon as $x \neq 0$. However, these equations are now built from first order monomials in the y_i 's and they are symmetrical in these variables. This observation suggests to introduce an auxiliary

variable T that plays the same role with respect to all the y_i 's and allows to define the auxiliary equation:

$$e^{L\mu} \left(\frac{1 - \mathbf{T}}{1 - x\mathbf{T}} \right)^{L} = -\prod_{j=1}^{N} \frac{\mathbf{T} - xy_{j}}{x\mathbf{T} - y_{j}} \quad \text{for} \quad i = 1 \dots N.$$
 (67)

This equation, in which T is the unknown, and the y_i 's are parameters, can be rewritten as a polynomial equation:

$$P(T) = e^{L\mu} (1 - T)^{L} \prod_{i=1}^{N} (xT - y_i) + (1 - xT)^{L} \prod_{i=1}^{N} (T - xy_i) = 0.$$
 (68)

Because the Bethe equations (66) imply that $P(y_i) = 0$ for $i = 1 \dots N$, the polynomial Q(T), defined as

$$Q(T) = \prod_{i=1}^{N} (T - y_i),$$
(69)

must divide the polynomial P(T). Now, if we examine closely the expression of P(T), we observe that the factors that contain the y_i 's inside the products over i can be written in terms of Q(T). Therefore, we conclude that Q(T) DIVIDES $e^{L\mu}(1-T)^LQ(xT)+(1-xT)^Lx^NQ(T/x)$. Equivalently, there exists a polynomial R(T) such that

$$Q(T)R(T) = e^{L\mu}(1-T)^{L}Q(xT) + x^{N}(1-xT)^{L}Q(T/x).$$
(70)

This functional equation is equivalent to the Bethe Ansatz equations (it is also known as Baxter's TQ equation). It can be used to determine the polynomial Q(T) of degree N that vanishes at the Bethe roots. In the present case, equation (70) can be solved perturbatively w.r.t. μ to any desired order. Knowing Q(T) perturbatively an expansion of $E(\mu)$ is derived, leading to the cumulants of the current and to the large deviation function. For example, this method allows to calculate the following cumulants of the total current:

- Mean Current $J: J = (1-x)\frac{N(L-N)}{L-1} \sim (1-x)L\rho(1-\rho)$ for $L \to \infty$.
- Diffusion Constant D:

$$D = (1 - x) \frac{2L}{L - 1} \sum_{k>0} k^2 \frac{C_L^{N+k}}{C_L^N} \frac{C_L^{N-k}}{C_L^N} \left(\frac{1 + x^k}{1 - x^k}\right).$$

In the limit of a large system size, $L \to \infty$, with asymmetry parameter $x \to 1$ and with a fixed value of $\phi = \frac{(1-x)\sqrt{L\rho(1-\rho)}}{2}$, the diffusion constant assumes a simple expression

$$D \sim 4\phi L \rho (1 - \rho) \int_0^\infty du \frac{u^2}{\tanh \phi u} e^{-u^2}.$$

• Third cumulant: the Skewness measures the non-Gaussian character of the fluctuations. An exact combinatorial expression of the third moment, valid for any values of L, N and x, was calculated by S. Prolhac in 2008. It is given by

$$\begin{split} \frac{E_3}{6L^2} &= \frac{1-x}{L-1} \sum_{i>0} \sum_{j>0} \frac{C_L^{N+i} C_L^{N-i} C_L^{N+j} C_L^{N-j}}{(C_L^N)^4} (i^2+j^2) \frac{1+x^i}{1-x^i} \frac{1+x^j}{1-x^j} \\ &- \frac{1-x}{L-1} \sum_{i>0} \sum_{j>0} \frac{C_L^{N+i} C_L^{N+j} C_L^{N-i-j}}{(C_L^N)^3} \frac{i^2+ij+j^2}{2} \frac{1+x^i}{1-x^i} \frac{1+x^j}{1-x^j} \\ &- \frac{1-x}{L-1} \sum_{i>0} \sum_{j>0} \frac{C_L^{N-i} C_L^{N-j} C_L^{N+i+j}}{(C_L^N)^3} \frac{i^2+ij+j^2}{2} \frac{1+x^i}{1-x^i} \frac{1+x^j}{1-x^j} \\ &- \frac{1-x}{L-1} \sum_{i>0} \frac{C_L^{N+i} C_L^{N-i}}{(C_L^N)^2} \frac{i^2}{2} \left(\frac{1+x^i}{1-x^i}\right)^2 \\ &+ (1-x) \frac{N(L-N)}{4(L-1)(2L-1)} \frac{C_{2L}^{2N}}{(C_L^N)^2} \\ &- (1-x) \frac{N(L-N)}{6(L-1)(3L-1)} \frac{C_{3L}^{3N}}{(C_L^N)^3} \,. \end{split}$$

For $L \to \infty$, $x \to 1$ and keeping $\phi = \frac{(1-x)\sqrt{L\rho(1-\rho)}}{2}$ fixed, this formula becomes

$$\frac{E_3}{\phi(\rho(1-\rho))^{3/2}L^{5/2}} \simeq -\frac{4\pi}{3\sqrt{3}} + 12\int_0^\infty dudv \frac{(u^2+v^2)e^{-u^2-v^2} - (u^2+uv+v^2)e^{-u^2-uv-v^2}}{\tanh\phi u \tanh\phi v}.$$

This shows that the fluctuations display a non-Gaussian behaviour. We remark that for $\phi \to \infty$ the TASEP limit is recovered:

$$E_3 \simeq \left(\frac{3}{2} - \frac{8}{3\sqrt{3}}\right) \pi (\rho(1-\rho))^2 L^3$$
.

3. The weakly asymmetric limit

In this section, we make some remarks specific to the weakly asymmetric case, for which the asymmetry parameter scales as $x = 1 - \frac{\nu}{L}$ in the limit of large system sizes $L \to \infty$. In this case, we also need to rescale the fugacity parameter as μ/L and the following asymptotic formula for the cumulant generating function can be derived

$$\tilde{E}(\mu,\nu) \equiv E\left(\frac{\mu}{L}, 1 - \frac{\nu}{L}\right) \simeq \frac{\rho(1-\rho)(\mu^2 + \mu\nu)}{L} - \frac{\rho(1-\rho)\mu^2\nu}{2L^2} + \frac{1}{L^2}\phi[\rho(1-\rho)(\mu^2 + \mu\nu)], \tag{71}$$

with
$$\phi(z) = \sum_{k=1}^{\infty} \frac{B_{2k-2}}{k!(k-1)!} z^k$$
, (72)

and where the B_j 's are Bernoulli Numbers. We observe that the leading order (in 1/L) is quadratic in μ and describes Gaussian fluctuations. It is only in the subleading correction (in $1/L^2$) that the non-Gaussian character arises. We observe that the series that defines the function $\phi(z)$ has a finite radius of convergence and that $\phi(z)$ has a singularity for $z = -\pi^2$. Thus, non-analyticities appear in $\tilde{E}(\mu, \nu)$ as soon as

$$\nu \ge \nu_c = \frac{2\pi}{\sqrt{\rho(1-\rho)}} \,.$$

By Legendre transform, non-analyticities also occur in the large deviation function G(j). At half-filling, the singularity appears at $\nu_c = 4\pi$ as can be seen in Figure 24. For $\nu < \nu_c$ the leading behaviour of G(j) is quadratic (corresponding to Gaussian fluctuations) and is given by

$$G(j) = \frac{(j - \nu \rho (1 - \rho))^2}{4L\rho (1 - \rho)}.$$
 (73)

For $\nu > \nu_c$, the series expansions (71) and (72) break down and the large deviation function G(j) becomes nonquadratic even at leading order. This phase transition was predicted by T. Bodineau and B. Derrida using macroscopic fluctuation theory (see [4] for a general discussion). One can observe in Figure 24 that for $\nu \geq \nu_c$, the large deviation function G(j) becomes non-quadratic and develops a kink at a special value of the total current j.

4. The general structure of the solution

A systematic expansion procedure that completely solves the problem to all orders and yields exact expressions for all the cumulants of the current, for an arbitrary value of the asymmetry parameter x, was carried out by S. Prolhac in [23].

Using the functional Bethe Ansatz, S. Prolhac derived a parametric representation of the cumulant generating function $E(\mu)$ similar to the one given for the TASEP in equations (58) and (59),

$$\mu = -\sum_{k\geq 1} C_k \frac{B^k}{k}$$

$$E = -(1-x)\sum_{k\geq 1} D_k \frac{B^k}{k}$$
(74)

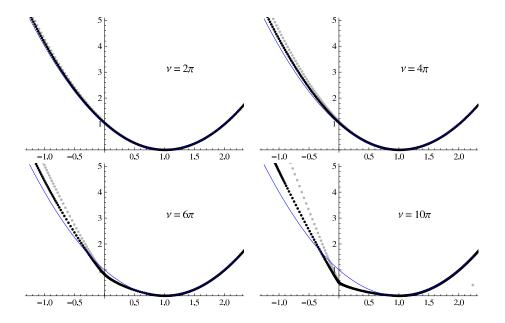


FIG. 24: Behaviour of the large deviation function as a function of the current $j/(\nu\rho(1-\rho))$ for different values of ν . The grey dots correspond to L=50, N=25 and the black dots correspond to L=100, N=50. They are obtained by solving numerically the functional Bethe Ansatz equation (70). The thin blue curve represents the leading Gaussian behaviour (73).

where C_k and D_k can be expressed as residues of a complex function $\phi_k(z)$:

$$C_k = \oint_{\mathcal{C}} \frac{dz}{2 i \pi} \frac{\phi_k(z)}{z}$$
 and $D_k = \oint_{\mathcal{C}} \frac{dz}{2 i \pi} \frac{\phi_k(z)}{(z+1)^2}$.

It can be shown that C_k and D_k are combinatorial factors that are enumerate to some tree structures. To find these numbers, we need the functions $\phi_k(z)$. These functions can be embodied into a generating function $W_B(z)$ defined as

$$W_B(z) = \sum_{k \ge 1} \phi_k(z) \frac{B^k}{k} \tag{75}$$

This function $W_B(z)$ encodes the full information about the statistics of the current: if we know how to determine it, the problem is solved.

It can be proved that $W_B(z)$ is the solution of the following functional Bethe equation:

$$W_B(z) = -\ln\left(1 - BF(z)e^{X[W_B](z)}\right) \quad \text{with} \quad F(z) = \frac{(1+z)^L}{z^N}$$
 (76)

and
$$X[W_B](z_1) = \oint_{\mathcal{C}} \frac{dz_2}{i2\pi z_2} W_B(z_2) K(z_1, z_2)$$
 (77)

where the kernel $K(z_1, z_2)$ is given by

$$K(z_1, z_2) = 2\sum_{k=1}^{\infty} \frac{x^k}{1 - x^k} \left\{ \left(\frac{z_1}{z_2}\right)^k + \left(\frac{z_2}{z_1}\right)^k \right\}$$
 (78)

Equations (76, 77 and 78) determine the unknown function $W_B(z)$. They are the core of the problem's solution. Using them, a closed expansion of $E(\mu)$ w.r.t. μ was derived. This expansion, valid for any finite values of L, N and x, can be used to study the large system size limit with various scalings of the asymmetry. Various regimes were found and the corresponding expressions for the cumulants were fully worked out:

• For $1-x \ll \frac{1}{L}$, the model falls into the Edward-Wilkinson universality class.

- The range $1-x \sim \frac{\nu}{L}$, where ν is a finite number, defines the weakly asymmetric regime (to be discussed below).
- The intermediate regime, corresponding to $\frac{1}{L} \ll 1 x \ll \frac{1}{\sqrt{L}}$, exhibits a specific scaling behaviour that, to our knowledge, can not be represented by a continuous stochastic equation.
- For $1-x \sim \frac{\Phi}{\sqrt{\rho(1-\rho)L}}$ the system is in the strongly asymmetric regime.
- The range $1-x\gg \frac{1}{\sqrt{L}}$ corresponds to the KPZ universality class, which contains the TASEP.

B. Open System with reservoirs

Finally, we can explain how to calculate the large deviation of the current in the open ASEP in contact with two reservoirs [14]. Now, the observable Y_t counts the total number of particles exchanged between the system and the left reservoir between times 0 and t. During a time interval dt, Y_t increases by 1 if a particle enters at site 1 (at rate α), it decreases by if a particle exits from 1 (at rate γ) and is unchanged if no particle exchange with the left reservoir has occurred during dt.

We know that $\frac{\langle Y_t \rangle}{t}$ converges towards the average current $J(x, \alpha, \beta, \gamma, \delta, L)$ when $t \to \infty$. We wish to determine the large deviation function associated with Y_t or, equivalently, its cumulant generating function, that we recall is defined by

$$\langle e^{\mu Y_t} \rangle \simeq e^{E(\mu)t}$$
 for $t \to \infty$

The function $E(\mu)$ can be calculated by the Matrix Ansatz method. The solution obtained has structure very similar to the one obtained in Equations (76, 77 and 78) for the periodic case. For arbitrary values of x and $(\alpha, \beta, \gamma, \delta)$, and for any system size L the parametric representation of $E(\mu)$ is given by

$$\mu = -\sum_{k=1}^{\infty} C_k(x; \alpha, \beta, \gamma, \delta, L) \frac{B^k}{2k}$$

$$E = -\sum_{k=1}^{\infty} D_k(x; \alpha, \beta, \gamma, \delta, L) \frac{B^k}{2k}$$

The coefficients C_k and D_k are given by contour integrals in the complex plane:

$$C_k = \oint_{\mathcal{C}} \frac{dz}{2 i \pi} \frac{\phi_k(z)}{z}$$
 and $D_k = \oint_{\mathcal{C}} \frac{dz}{2 i \pi} \frac{\phi_k(z)}{(z+1)^2}$

where the complex contour \mathcal{C} encircles 0, $x^k a_+, x^k a_-, x^k b_+, x^k b_-$ for $k \geq 0$ $[a_{\pm}, b_{\pm}]$ were defined in equation (22)]. Here again, there exists an auxiliary function $W_B(z) = \sum_{k \geq 1} \phi_k(z) \frac{B^k}{k}$ that contains the full information about the statistics of the current. The functional equation for $W_B(z)$ is given by

$$W_B(z) = -2\ln\left(1 - BF(z)e^{X[W_B](z)}\right)$$
 (79)

 $X[W_B]$ being the same operator defined in equations (77) and (78). But the function F(z) is now given by

$$F(z) = \frac{(1+z)^L (1+z^{-1})^L (z^2)_{\infty} (z^{-2})_{\infty}}{(a+z)_{\infty} (a+z^{-1})_{\infty} (a-z)_{\infty} (a-z^{-1})_{\infty} (b+z)_{\infty} (b+z^{-1})_{\infty} (b-z)_{\infty} (b-z^{-1})_{\infty}}$$

where we use the notation $(A)_{\infty} = \prod_{k=0}^{\infty} (1 - x^k A)$. This function, related to Askey-Wilson polynomials, was used by T. Sasamoto in his study of the stationary state of the ASEP with open boundaries (see [3] for references).

If we specialize these formulae to the special TASEP case $x = \gamma = \delta = 0$ with non-zero rates equal to unity $\alpha = \beta = 1$, the expression becomes rather explicit. The parametric representation of the cumulant generating

function $E(\mu)$ is given by

$$\begin{split} \mu \; &=\; -\sum_{k=1}^{\infty} \frac{(2k)!}{k!} \frac{[2k(L+1)]!}{[k(L+1)]! [k(L+2)]!} \frac{B^k}{2k} \; , \\ E \; &=\; -\sum_{k=1}^{\infty} \frac{(2k)!}{k!} \frac{[2k(L+1)-2]!}{[k(L+1)-1]! [k(L+2)-1]!} \frac{B^k}{2k} \; . \end{split}$$

By eliminating recursively B in terms of μ in second equation and substituting in the first one, we can calculate the first few cumulants of the current:

• Mean Value : $J = \frac{L+2}{2(2L+1)}$

• Variance : $\Delta = \frac{3}{2} \frac{(4L+1)![L!(L+2)!]^2}{[(2L+1)!]^3(2L+3)!}$

• Skewness : $E_3 = 12 \frac{[(L+1)!]^2[(L+2)!]^4}{(2L+1)[(2L+2)!]^3} \left\{ 9 \frac{(L+1)!(L+2)!(4L+2)!(4L+4)!}{(2L+1)![(2L+2)!]^2[(2L+4)!]^2} - 20 \frac{(6L+4)!}{(3L+2)!(3L+6)!} \right\}$

For large systems: $E_3 \to \frac{2187 - 1280\sqrt{3}}{10368} \pi \sim -0.0090978...$

More generally, in the limit of large system sizes, the asymptotic behaviour of $E(\mu)$ can be carried out, for the general ASEP, in the different phases. In the Low Density (and High Density) Phases, the large deviation function, obtained after a Legendre transform, takes a particularly simple form:

$$\Phi(j) = (1 - q) \left\{ \rho_a - r + r(1 - r) \ln \left(\frac{1 - \rho_a}{\rho_a} \frac{r}{1 - r} \right) \right\}$$

where the current j is parametrized as j = (1 - q)r(1 - r).

The exact expressions can also be compared with numerical results obtained by the Density Matrix Renormalization Group technique.

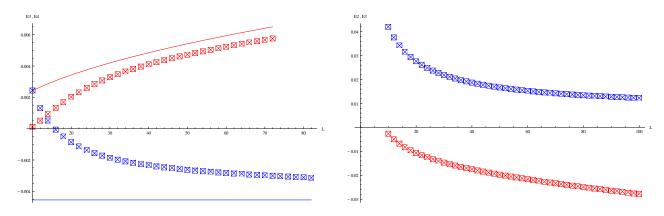


FIG. 25: Left: Third and Fourth cumulants plotted against the system size in the Maximal Current phase with x = 0.5, $a_+ = b_+ = 0.65$, $a_- = b_- = 0.6$. Right: Second and Third cumulants in the High Density phase with x = 0.5, $a_+ = 0.28$, $b_+ = 1.15$, $a_- = -0.48$ and $b_- = -0.27$. The crosses and the squares compare numerical with analytical results. The continuous curves correspond to asymptotic behaviours [14].

VI. CONCLUDING REMARKS: TOWARDS A FLUCTUATING HYDRODYNAMICS DESCRIPTION

In these lectures, we have explained that non-equilibrium processes can be explored by studying the large deviations of some physical observable such as the total current transported through a wire or the density profile. Indeed, large deviation functions appear to be to right generalization of the thermodynamic potentials to non-equilibrium systems. They exhibit remarkable properties such as the Fluctuation Theorem that is valid far away from equilibrium. Large deviation functions are likely to play a key-role in the future of non-equilibrium statistical mechanics.

The asymmetric exclusion process is a paradigm for non-equilibrium behaviour in low dimensions. Just as the Ising model for phase transitions, the ASEP is the simplest non-trivial model that embodies the minimal ingredients to study mathematically statistical physics far from equilibrium.

For the specific case of the ASEP, we have shown how large deviation function can be calculated exactly by using techniques borrowed from the theory of integrable systems, such as the Bethe Ansatz or the Matrix Representation method. The results obtained are exact and mathematically appealing, but the calculations required are rather involved and can only be applied to very specific models. It would be highly desirable to have at our disposal a more physical picture and a a set of tools more versatile that would allow us to study very general non-equilibrium systems.

It seems that such a theory has been emerging in the recent years. This approach is based upon a fluctuating hydrodynamic description. As a conclusion of these lectures, we shall briefly describe this theory and its relation to the problems studied here.

We consider again a diffusive system in contact with two reservoirs and we adopt the hydrodynamic description of Figure 16 consider the case with no applied field ($\nu = 0$). On average, the evolution of the profile and the current is governed by Burgers equation (19). But, what if we are interested in stochastic properties of the profile and the current? Suppose we want to know the probability to observe an *atypical* current j(x,t) and the corresponding density profile $\rho(x,t)$ during $0 \le s \le L^2 T$? For many systems, this probability will follow a large deviation behaviour:

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

(This is highly non-trivial. We simply assume it here). The functional $\mathcal{I}(j,\rho)$ is the large deviation functional.

For driven diffusive systems, G. Jona-Lasinio and coworkers have developed a formalism to calculate $\mathcal{I}(j,\rho)$, known as the Macroscopic Fluctuation Theory (MFT) (see [2, 4, 7] for reviews). The goal is to replace the deterministic Burgers equation by a stochastic equation that describes correctly the fluctuations of the system in the diffusive scaling limit of large systems and long times. We shall formulate the MFT using once again the pipe model language: Consider Y_t the total number of particles transferred from the left reservoir to the right reservoir during time t. Then one has

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

where the two 'phenomenological' coefficients encode the value of the average current and its quadratic fluctuations. For the symmetric exclusion process, they are given by

$$D(\rho) = 1$$
 and $\sigma(\rho) = 2\rho(1-\rho)$.

The stochastic equation of motion is obtained as

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

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

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

If we discard the noise term, we recover the Burgers equation (19). The important fact is that in the Macroscopic limit, fluctuations are accurately described by a *multiplicative* Gaussian white noise, the amplitude of this noise being proportional to the conductivity σ . Besides, the fact that this noise is vanishing small (its amplitude has a 1/L factor) will allow us to use saddle point/WKB methods.

Indeed, the equation of fluctuating hydrodynamics allows us to express the large-deviation functional as a pathintegral. Since 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 be written as

Proba
$$(\rho(x,t), j(x,t)|\rho_0(x), j_0(x)) =$$

$$\int_{\substack{\rho_0 \to \rho_t \\ j_0 \to 1t}} \mathcal{D}\rho \mathcal{D}j \prod_{\substack{0 \le x \le 1 \\ 0 \le t' \le t}} \delta\left(\frac{\partial \rho}{\partial t'} + \frac{\partial j}{\partial x}\right) \exp\left(-\frac{L}{2} \int_0^t dt' \int_0^1 dx \frac{(j + D(\rho)\frac{\partial \rho}{\partial x} - \nu \sigma(\rho))^2}{\sigma(\rho)}\right)$$

In the large L limit, the integral will be dominated by the optimal value of the exponent (saddle-point). Hence, the large deviation functional can be written as the solution of an optimal path problem:

$$\mathcal{I}(j,\rho) = \min_{\rho,j} \left\{ \int_0^T dt \int_0^1 dx \frac{(j - \nu \sigma(\rho) + D(\rho) \nabla \rho)^2}{2\sigma(\rho)} \right\}$$
(80)

with the constraint: $\partial_t \rho = -\nabla . j$. Then, knowing $\mathcal{I}(j,\rho)$ one can deduce (by the contraction principle [28]) the LDF of the current or the profile. For example, for the current: $\Phi(j) = \min_{\rho} \{\mathcal{I}(j,\rho)\}$.

This variational problem (80) has a Hamiltonian structure and can be expressed by using a pair of conjugate variables (p,q). Mathematically, one has to solve the corresponding Euler-Lagrange equations. After some transformations, a set of coupled non-linear PDEs is obtained:

$$\partial_t q = \partial_x [D(q)\partial_x q] - \partial_x [\sigma(q)\partial_x p]$$

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

where q(x,t) is the density-field and p(x,t) is a conjugate field. These equations have to be completed by suitable boundary conditions. We emphasize that this formalism can be applied to general diffusive systems: Physics is embodied in the transport coefficients D and σ that carry the information of the microscopic dynamics relevant at the macroscopic scale.

In principle, the MFT provides us with a general framework but the non-linear PDEs obtained are very difficult to solve in general. If we can solve them, we should be able to calculate large deviation functions directly at the macroscopic level, without having to cope with the intricate combinatorics at the microscopic scale. For the moment being, very few solutions of these equations exist. The exact results we have described in these lectures can be used as benchmarks for the analysis of this new set of hydrodynamic equations, a field of research that has just opened.

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