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Non-equilibrium steady states: fluctuations and large deviations of the density and of the current

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Abstract. These lecture notes give a short review of methods such as the matrix ansatz, the additivity principle or the macroscopic fluctuation theory, developed recently in the theory of non-equilibrium phenomena. They show how these methods allow us to calculate the fluctuations and large deviations of the density and the current in non-equilibrium steady states of systems like exclusion processes. The properties of these fluctuations and large deviation functions in non-equilibrium steady states (for example, non-Gaussian fluctuations of density or non-convexity of the large deviation function which generalizes the notion of free energy) are compared with those of systems at equilibrium.

Keywords: driven diffusive systems (theory), stationary states, current fluctuations, large deviations in non-equilibrium systems

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1. Introduction

The goal of these lectures, delivered at the Newton Institute in Cambridge for the workshop ‘Non-Equilibrium Dynamics of Interacting Particle Systems’ in March–April 2006, is to try to introduce some methods used to study non-equilibrium steady states for systems with stochastic dynamics and to review some results obtained recently on the fluctuations and the large deviations of the density and the current for such systems.

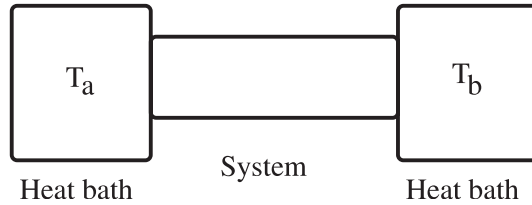


Figure 1. A system in contact with two heat baths at temperatures T_a and T_b .

Let us start with a few examples of non-equilibrium steady states:

- (1) *A system in contact with two heat baths at temperatures T_a and T_b .*

At equilibrium, i.e. when the two heat baths are at the same temperature ($T_a = T_b = T$), the probability $P(C)$ of finding the system in a certain microscopic configuration C is given by the usual Boltzmann–Gibbs weight

$$P_{\text{equilibrium}}(C) = Z^{-1} \exp\left[-\frac{E(C)}{kT}\right] \quad (1)$$

where $E(C)$ is the internal energy of the system in configuration C . Then the task of equilibrium statistical mechanics is to derive macroscopic properties (equations of states, phase diagrams, fluctuations, etc) from (1) as a starting point. A very simplifying aspect of (1) is that it depends neither on the precise nature of the couplings with the heat baths (at least when these couplings are weak) nor on the details of the dynamics.

When the two temperatures T_a and T_b are different (see figure 1), the system reaches in the long-time limit a non-equilibrium steady state [1]–[4], but there does not exist [5, 6] an expression which generalizes (1) for the steady state weights $P(C)$ of the microscopic configurations

$$P_{\text{non-equilibrium}}(C) = ?.$$

In fact, for a non-equilibrium system, the steady state measure $P(C)$ depends in general on the dynamics of the system and on its couplings with the heat baths.

Beyond trying to know the steady state measure $P(C)$, which can be done only for a very few examples [7]–[13], one might wish to determine a number of properties of non-equilibrium steady states like the temperature or energy profiles [14, 15], the average flow of energy through the system [16]–[20], the probability distribution of this energy flow, the fluctuations of the internal energy or of the density.

- (2) *A system in contact with two reservoirs of particles at densities ρ_a and ρ_b .*

Another non-equilibrium steady state situation one can consider is that of a system exchanging particles with two reservoirs [21] at densities ρ_a and ρ_b (see figure 2). When $\rho_a \neq \rho_b$ (and in the absence of an external field) there is a flow of particles through the system. One can then ask the same questions as for the previous case: for example, what is the average current of particles between the two reservoirs, what is the density profile through the system, what are the fluctuations or the large deviations of this current or of the density.

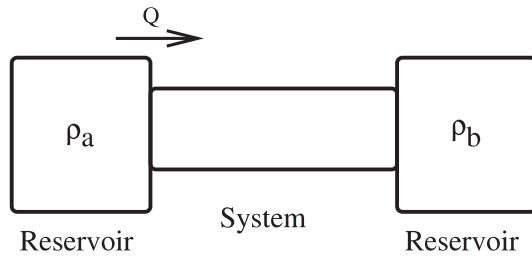


Figure 2. A system in contact with two reservoirs at densities ρ_a and ρ_b .

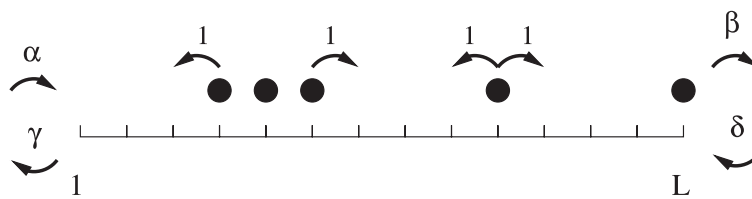


Figure 3. The symmetric simple exclusion process.

(3) *The symmetric simple exclusion process (SSEP)*

The SSEP [22]–[25] is one of the simplest models of a system maintained out of equilibrium by contact with two reservoirs at densities ρ_a and ρ_b . The model is defined as a one-dimensional lattice of L sites with open boundaries, each site being either occupied by a single particle or empty (see figure 3). During every infinitesimal time interval dt , each particle has a probability dt of jumping to its left neighbouring site if this site is empty, and a probability dt of jumping to its right neighbouring site if this right neighbouring site is empty. At the two boundaries the dynamics is modified to mimic the coupling with reservoirs of particles: at the left boundary, during each time interval dt , a particle is injected on site 1 with probability αdt (if this site is empty) and a particle is removed from site 1 with probability γdt (if this site is occupied). Similarly on site L , particles are injected at rate δ and removed at rate β .

We will see ((43) below and [26]–[28]) that these choices of the rates $\alpha, \gamma, \beta, \delta$ correspond to the left boundary being connected to a reservoir at density ρ_a and the right boundary to a reservoir at density ρ_b with ρ_a and ρ_b given by

$$\rho_a = \frac{\alpha}{\alpha + \gamma}; \quad \rho_b = \frac{\delta}{\beta + \delta}. \tag{2}$$

One can also think of the SSEP as a simple model of heat transport, if one interprets the particles as quanta of energy. Then if each particle carries an energy ϵ , the SSEP becomes the model of a system in contact with two heat baths at temperatures T_a and T_b given by (see section 2)

$$\exp\left[\frac{\epsilon}{kT_a}\right] = \frac{\alpha}{\gamma}; \quad \exp\left[\frac{\epsilon}{kT_b}\right] = \frac{\delta}{\beta}. \tag{3}$$

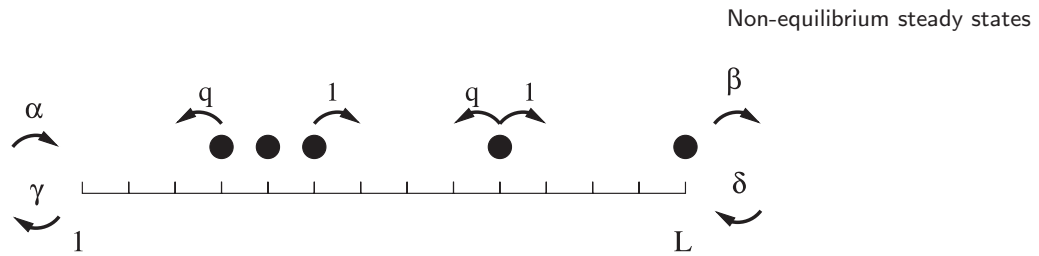


Figure 4. The asymmetric simple exclusion process.

(4) *Driven diffusive systems*

One can add to the systems described above an electric or a gravity field which tends to push the particles in a preferred direction.

For example (see figure 4), adding a field to the SSEP means that the hopping rates to the left become q (the hopping rates to the right still being 1). The model becomes then the ASEP (the asymmetric simple exclusion process) [9], [29]–[32] which appears in many contexts [33, 34], such as hopping conductivity [35], models of traffic [36], growth [37] or polymer dynamics [38]. In the presence of this external field, the system reaches a non-equilibrium steady state even for a ring geometry, without need of a reservoir.

The large scale of the ASEP differs noticeably from the SSEP. For example, in the ASEP on the infinite line, one can observe shock waves whereas the SSEP is purely diffusive. In fact, on large scales the ASEP is described [37] by the Kardar–Parisi–Zhang equation [39] while the SSEP is in the universality class of the Edwards–Wilkinson equation [40, 41].

The outline of these lectures is as follows:

In section 2 it is recalled how detailed balance should be modified to describe systems in contact with several heat baths at unequal temperatures or several reservoirs at different densities.

In section 3 the large deviation functional of the density is introduced and there is a comparison between its properties in equilibrium and in non-equilibrium steady states.

In section 4, the connection between the non-locality of the large deviation functional of the density and the presence of long range correlations is discussed.

In section 5 it is shown how to write the evolution equations of the profile and of the correlation functions for the symmetric simple exclusion process.

Section 6 describes the matrix ansatz [10] which gives an exact expression of the weights in the non-equilibrium steady state of the symmetric exclusion process.

Using an additivity relation established in section 7 as a consequence of the matrix ansatz, the large deviation functional [26, 27] of the density for the SSEP is calculated in section 8.

The macroscopic fluctuation theory of Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim [42]–[45] is recalled in section 9, which shows how the calculation of a large deviation functional of the density can be formulated as an optimization problem.

The definition of the large deviation function of the current and the fluctuation theorem [46]–[50] are recalled in section 10 from which the fluctuation–dissipation theorem for energy or particle currents can be recovered (section 11).

A perturbative approach [51] to calculate the large deviation function of the current for the SSEP is sketched in section 12.

The additivity principle, which predicts the cumulants and the large deviation function of the current, is presented in section 13.

The last four sections are devoted to the ASEP: the matrix ansatz for the ASEP is recalled in section 14. It is shown in section 15 how to obtain the phase diagram of the TASEP from the matrix ansatz. An additivity relation from which one can compute the large deviation functional of the density [53, 54] is established in section 16. Lastly in section 17 it is shown that the fluctuations of density are non-Gaussian [55] in the maximal current phase of the TASEP.

2. How to generalize detailed balance to non-equilibrium systems

As in non-equilibrium systems, the steady state measure $P(C)$ depends on the couplings to the heat baths and on the dynamics of the system, each model of a non-equilibrium has to incorporate a description of these couplings and of the dynamics (various ways of modelling the effect of heat baths or of reservoirs are described in, for example, [1, 56]). It is often theoretically simpler to represent the effect of the heat baths (or of the reservoirs of particles) by some stochastic terms such as Langevin forces corresponding to the temperatures of the heat baths. In practice the dynamics becomes a Markov process.

For a system with stochastic dynamics given by a Markov process (such as the SSEP or mechanical systems with heat baths represented by Langevin forces) the evolution is specified by a transition matrix $W(C', C)$ which represents the rate at which the system jumps from a configuration C to a configuration C' (i.e. the probability that the system jumps from C to C' during an infinitesimal time interval dt is given by $W(C', C) dt$). For simplicity, we will limit the discussion to the case where the total number of accessible configurations is finite. The probability $P_t(C)$ of finding the system in configuration C at time t evolves therefore according to the Master equation

$$\frac{dP_t(C)}{dt} = \sum_{C'} W(C, C')P_t(C') - W(C', C)P_t(C). \quad (4)$$

One can then wonder what should be assumed on the transition matrix $W(C', C)$ to describe a system in contact with one or several heat baths (as, for example, in figure 1).

At equilibrium, (i.e. when the system is in contact with a single heat bath at temperature T) one usually requires that the transition matrix satisfies *detailed balance*

$$W(C', C)e^{-E(C)/kT} = W(C, C')e^{-E(C')/kT}. \quad (5)$$

This ensures the time reversal symmetry of the microscopic dynamics: at equilibrium (i.e. if the initial condition is chosen according to (1)), the probability of observing any given history of the system $\{C_s, 0 < s < t\}$ is equal to the probability of observing the reversed history

$$\text{Pro}(\{C_s, 0 < s < t\}) = \text{Pro}(\{C_{t-s}, 0 < s < t\}). \quad (6)$$

Therefore, if ϵ is the energy transferred from the heat bath at temperature T to the system, and $W_\epsilon(C', C) dt$ is the probability that the system jumps during dt from C to

C' by receiving an energy ϵ from the heat bath, one can rewrite the detailed balance condition (5) as

$$W_{\epsilon}(C', C) = e^{-\epsilon/kT} W_{-\epsilon}(C, C'). \quad (7)$$

If detailed balance gives a good description of the coupling with a single heat bath at temperature T , the straightforward generalization of (7) for a system coupled to two heat baths at unequal temperatures like in figure 1 is [57]

$$W_{\epsilon_a, \epsilon_b}(C', C) = \exp\left[-\frac{\epsilon_a}{kT_a} - \frac{\epsilon_b}{kT_b}\right] W_{-\epsilon_a, -\epsilon_b}(C, C') \quad (8)$$

where ϵ_a, ϵ_b are the energies transferred from the heat baths at temperatures T_a, T_b to the system when the system jumps from configuration C to configuration C' . By comparing with (7), this simply means that the exchanges of energy with the heat bath at temperature T_a tend to equilibrate the system at temperature T_a and the exchanges with the heat bath at temperature T_b tend to equilibrate the system at temperature T_b .

For a system in contact with two reservoirs of particles at fugacities z_a and z_b , as in figure 2, the generalized detailed balance (8) becomes

$$W_{q_a, q_b}(C', C) = z_a^{q_a} z_b^{q_b} W_{-q_a, -q_b}(C, C') \quad (9)$$

where q_a and q_b are the numbers of particles transferred from the two reservoirs to the system when the system jumps from configuration C to configuration C' .

From the definition of the dynamics of the SSEP, it is easy to check that it satisfies (9) with

$$z_a = \frac{\alpha}{\gamma}; \quad z_b = \frac{\delta}{\beta}. \quad (10)$$

One can also check from (3) that if one interprets the particles as quanta of energy, (8) is satisfied.

One way of justifying (8) is to consider the composite system made up of the system we want to study and of the two reservoirs. This composite system is isolated and therefore its total energy \mathcal{E}

$$\mathcal{E} = E(C) + E_a + E_b \quad (11)$$

is conserved by the dynamics. In (11) $E(C)$ is the energy of the system we want to study and E_a, E_b are the energies of the two reservoirs (for simplicity we assume that the energy of the coupling between the reservoirs and the system is small). Whenever there is an evolution step in the dynamics, the system jumps from the microscopic configuration C to the configuration C' and the energies of the reservoirs jump from E_a, E_b to E'_a, E'_b . For the composite system to be able to reach the microcanonical distribution and for microcanonical detailed balance to hold one needs that the transition rates satisfy

$$\begin{aligned} & \exp\left[\frac{S_a(E_a) + S_b(E_b)}{k}\right] \text{Pro}(\{C, E_a, E_b\} \rightarrow \{C', E'_a, E'_b\}) \\ &= \exp\left[\frac{S_a(E'_a) + S_b(E'_b)}{k}\right] \text{Pro}(\{C', E'_a, E'_b\} \rightarrow \{C, E_a, E_b\}) \end{aligned} \quad (12)$$

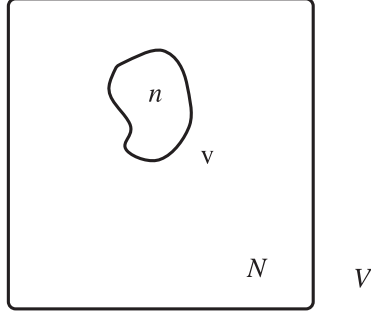


Figure 5. For a system of N particles in total volume V , the probability $P_v(n)$ of having n particles in a large subvolume v is given by (14).

where $S_a(E_a)$ and $S_b(E_b)$ are the entropies of the two reservoirs at energies E_a and E_b . Then if the heat baths are large enough, one has (using the microcanonical definition of the temperature $1/T = dS/dE$ for each reservoir)

$$S(E_a) - S(E'_a) = \frac{E_a - E'_a}{T_a}; \quad S(E_b) - S(E'_b) = \frac{E_b - E'_b}{T_b} \quad (13)$$

where T_a and T_b are the (microcanonical) temperatures of the two heat baths and (12) reduces to (8).

Remark. The quantity $-(\epsilon_a/T_a) - (\epsilon_b/T_b)$ in (8) is the entropy produced in the reservoirs. In fact, in the theory of non-equilibrium phenomena, one can associate to an arbitrary Markov process, defined by transition rates $W(C', C)$, an entropy production [46]–[48], [50, 58, 59] (in the surrounding heat baths) given by

$$\Delta S(C \rightarrow C') = k \log \frac{W(C', C)}{W(C, C')}$$

and (8) appears as one particular case of this general definition.

3. Free energy and the large deviation function

At equilibrium the free energy is defined by

$$F = -kT \log Z = -kT \log \left[\sum_C \exp \left(-\frac{E(C)}{T} \right) \right].$$

In this section we are going to see that the knowledge of the free energy gives also the distribution of the fluctuations and the large deviation function of the density. This will enable us to extend the notion of free energy to non-equilibrium systems by considering the large deviation functional [22, 60, 61] of the density.

If one considers a box of volume V containing N particles, as in figure 5, the probability $P_v(n)$ of finding n particles in a subvolume v located near a position \vec{r} has the following large v dependence:

$$P_v(n) \sim \exp \left[-va_{\vec{r}} \left(\frac{n}{v} \right) \right] \quad (14)$$

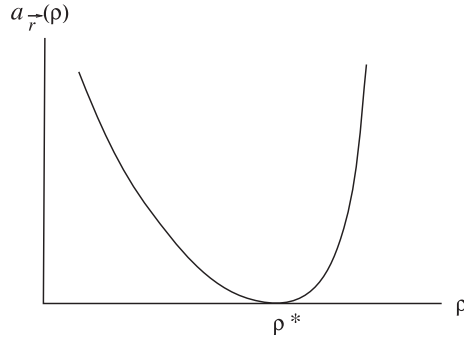


Figure 6. A typical shape of the large deviation function $a_{\vec{r}}(\rho)$. The most likely density ρ^* is the value where $a_{\vec{r}}(\rho)$ vanishes.

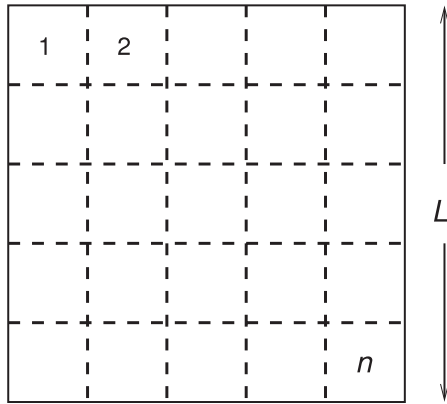


Figure 7. In (15) one specifies the densities ρ_i in each box i .

where $a_{\vec{r}}(\rho)$ is a large deviation function. Figure 6 shows a typical shape of $a_{\vec{r}}(\rho)$ for a homogeneous system (i.e. not at a coexistence between different phases) with a single minimum at $\rho = \rho^*$ where $a_{\vec{r}}(\rho)$ vanishes.

One can also define the large deviation functional \mathcal{F} for an arbitrary density profile. If one divides (as in figure 7) a system of linear size L into n boxes of linear size l (in dimension d , one has of course $n = L^d/l^d$ such boxes), one can try to determine the probability of finding a certain density profile $\{\rho_1, \rho_2, \dots, \rho_n\}$, i.e. the probability of seeing $l^d \rho_1$ particles in the first box, $l^d \rho_2$ particles in the second box, \dots $l^d \rho_n$ in the n th box. For large L one expects the following L dependence of this probability:

$$\text{Pro}(\rho_1, \dots, \rho_n) \sim \exp[-L^d \mathcal{F}(\rho_1, \rho_2, \dots, \rho_n)] \tag{15}$$

where \mathcal{F} is a large deviation function which generalizes $a_{\vec{r}}(\rho)$ defined in (14). If one introduces a reduced coordinate \vec{x}

$$\vec{r} = L\vec{x} \tag{16}$$

and if one takes the limit $L \rightarrow \infty, l \rightarrow \infty$ with $l \ll L$ so that the number n of boxes becomes large, this becomes a functional $\mathcal{F}(\rho(\vec{x}))$ for an arbitrary density profile $\rho(\vec{x})$

$$\text{Pro}(\rho(\vec{x})) \sim \exp[-L^d \mathcal{F}(\rho(\vec{x}))]. \tag{17}$$

Clearly the large deviation function $a_{\vec{r}}(\rho)$ or the large deviation functional $\mathcal{F}(\rho(\vec{x}))$ can be defined for equilibrium systems as well as for non-equilibrium systems.

For equilibrium systems, one can show that $a_{\vec{r}}(\rho)$ is closely related to the free energy: if the volume v is sufficiently large, for short-ranged interactions and in the absence of external potential, the large deviation function $a_{\vec{r}}(\rho)$ is independent of \vec{r} and its expression is given by

$$a_{\vec{r}}(\rho) = a(\rho) = \frac{f(\rho) - f(\rho^*) - (\rho - \rho^*)f'(\rho^*)}{kT} \quad (18)$$

where $f(\rho)$ is the free energy per unit volume at density ρ and $\rho^* = N/V$. This can be seen by noticing that, if $v^{1/d}$ is much larger than the range of the interactions and if $v \ll V$, one has

$$P_v(n) = \frac{Z_v(n)Z_{V-v}(N-n)}{Z_V(N)} \exp[\mathcal{O}(v^{(d-1)/d})] \quad (19)$$

where $Z_V(N)$ is the partition function of N particles in a volume V and the term $\exp[\mathcal{O}(v^{(d-1)/d})]$ represents the interactions between all pairs of particles, one of which is the volume v and the other one is $V - v$. Then taking the log of (19) and using the fact that the free energy $f(\rho)$ per unit volume is defined by

$$\lim_{V \rightarrow \infty} \frac{\log Z_V(V\rho)}{V} = -\frac{f(\rho)}{kT} \quad (20)$$

one gets (18). The functional \mathcal{F} can also be expressed in terms of $f(\rho)$: if one considers $V\rho^*$ particles in a volume $V = L^d$, one can generalize (19) for systems with short-range interactions and no external potential

$$\text{Pro}(\rho_1, \dots, \rho_n) = \frac{Z_v(v\rho_1) \cdots Z_v(v\rho_n)}{Z_V(V\rho^*)} \exp\left[\mathcal{O}\left(\frac{L^d}{l}\right)\right] \quad (21)$$

where $v = l^d$. Comparing with (15), in the limit $L \rightarrow \infty, l \rightarrow \infty$, keeping n fixed gives

$$\mathcal{F}(\rho_1, \rho_2, \dots, \rho_n) = \frac{1}{kT} \frac{1}{n} \sum_{i=1}^n [f(\rho_i) - f(\rho^*)]. \quad (22)$$

In the limit of an infinite number of boxes, this becomes

$$\mathcal{F}(\rho(\vec{x})) = \frac{1}{kT} \int d\vec{x} [f(\rho(\vec{x})) - f(\rho^*)]. \quad (23)$$

Thus for a system with short-range interactions, at equilibrium, the large deviation functional \mathcal{F} is fully determined by the knowledge of the free energy $f(\rho)$ per unit volume. In (23), we see that

- The functional \mathcal{F} is a *local* functional of $\rho(\vec{x})$.
- It is also a *convex* functional of the profile $\rho(\vec{x})$, i.e. for two arbitrary density profiles $\rho_1(\vec{x})$ and $\rho_2(\vec{x})$ one has for $0 < \alpha < 1$

$$\mathcal{F}(\alpha\rho_1(\vec{x}) + (1 - \alpha)\rho_2(\vec{x})) \leq \alpha\mathcal{F}(\rho_1(\vec{x})) + (1 - \alpha)\mathcal{F}(\rho_2(\vec{x})) \quad (24)$$

as the free energy $f(\rho)$ is itself a convex function of the density ρ , (i.e. $f(\alpha\rho_1 + (1 - \alpha)\rho_2) \leq \alpha f(\rho_1) + (1 - \alpha)f(\rho_2)$ for $0 < \alpha < 1$).

- When $f(\rho)$ can be expanded around ρ^* (i.e. at densities where the free energy $f(\rho)$ is not singular) one obtains also from (23) that the fluctuations of the density profile are Gaussian. In fact, if one expands (18) near ρ^* and one replaces it into (14) one gets that the distribution of the number n of particles in the subvolume v is Gaussian (if v is large enough)

$$P_v(n) \sim \exp \left[-v \frac{f''(\rho^*)}{2kT} (\rho - \rho^*)^2 \right] = \exp \left[-\frac{f''(\rho^*)}{2vkT} (n - v\rho^*)^2 \right] \quad (25)$$

and its variance, as predicted by Smoluchowki and Einstein, is given by

$$\langle n^2 \rangle - \langle n \rangle^2 = v \frac{kT}{f''(\rho^*)} = vkT\kappa(\rho^*) \quad (26)$$

where the compressibility $\kappa(\rho)$ is defined by

$$\kappa(\rho) = \frac{1}{\rho} \frac{d\rho}{dp} \quad (27)$$

(and the pressure p is given as usual by $p = -(d/dV)[Vf(N/V)] = \rho^* f'(\rho^*) - f(\rho^*)$). Note that, at a phase transition, $f(\rho)$ is singular and the fluctuations of density are in general non-Gaussian.

- One also knows (by the Landau argument) that, with short-range interactions, there is no phase transition if the dimension of space is one dimensional.

In contrast to equilibrium systems, one can observe in non-equilibrium steady states of systems such as the ones described in figures 1 and 2.

- The large deviation functional \mathcal{F} may be non-local. For example, in the case of the SSEP, we will see in section 8 that the functional is given for $\rho_a - \rho_b$ small by (see (74) below):

$$\begin{aligned} \mathcal{F}(\{\rho(x)\}) &= \int_0^1 dx \left[\rho(x) \log \frac{\rho(x)}{\rho^*(x)} + (1 - \rho(x)) \log \frac{1 - \rho(x)}{1 - \rho^*(x)} \right] \\ &\quad + \frac{(\rho_a - \rho_b)^2}{[\rho_a(1 - \rho_a)]^2} \int_0^1 dx \int_x^1 dy x(1 - y)(\rho(x) - \rho^*(x))(\rho(y) - \rho^*(y)) \\ &\quad + O(\rho_a - \rho_b)^3 \end{aligned} \quad (28)$$

where $\rho^*(x)$ is the most likely profile

$$\rho^*(x) = (1 - x)\rho_a + x\rho_b. \quad (29)$$

- For the ASEP, there is a range of parameters where the functional \mathcal{F} is non-convex (see [53, 54] and section 16 below).
- There are also cases where, in the maximal current phase, the density fluctuations are non-Gaussian (see [55] and section 17 below).
- In non-equilibrium systems nothing prevents the existence of phase transitions in one dimension [9]–[11], [32], [62]–[72].

4. Non-locality of the large deviation functional of the density and long-range correlations

A feature characteristic of non-equilibrium systems is the presence of weak long-range correlations [73]–[78]. For example, for the SSEP, we will see [73] in the next section (45) and (46) that for large L the correlation function of the density is given for $0 < x < y < 1$

$$\langle \rho(x)\rho(y) \rangle_c = -\frac{(\rho_a - \rho_b)^2}{L}x(1 - y). \quad (30)$$

We are going to see in this section that the presence of these long-range correlations is directly related to the non-locality of the large deviation functional \mathcal{F} . Let us introduce the generating function $\mathcal{G}(\{\alpha(x)\})$ of the density defined by

$$\exp[L\mathcal{G}(\{\alpha(x)\})] = \left\langle \exp \left[L \int_0^1 \alpha(x)\rho(x) dx \right] \right\rangle \quad (31)$$

where $\alpha(x)$ is an arbitrary function and $\langle \cdot \rangle$ denotes an average over the profile $\rho(x)$ in the steady state. As the probability of this profile is given by (17) the average in (31) is dominated, for large L , by an optimal profile, which depends on $\alpha(x)$, and \mathcal{G} is the Legendre transform of \mathcal{F}

$$\mathcal{G}(\{\alpha(x)\}) = \max_{\{\rho(x)\}} \left[\int_0^1 \alpha(x)\rho(x) dx - \mathcal{F}(\{\rho(x)\}) \right]. \quad (32)$$

It is clear from (32) that, if the large deviation \mathcal{F} is local (as in (23)), then the generating function \mathcal{G} is also local.

By taking derivatives of (31) with respect to $\alpha(x)$ one gets that the average profile and the correlation functions are given by

$$\rho^*(x) \equiv \langle \rho(x) \rangle = \left. \frac{\delta \mathcal{G}}{\delta \alpha(x)} \right|_{\alpha(x)=0} \quad (33)$$

$$\langle \rho(x)\rho(y) \rangle_c \equiv \langle \rho(x)\rho(y) \rangle - \langle \rho(x) \rangle \langle \rho(y) \rangle = \left. \frac{1}{L} \frac{\delta^2 \mathcal{G}}{\delta \alpha(x)\delta \alpha(y)} \right|_{\alpha(x)=0}. \quad (34)$$

This shows that the non-locality of \mathcal{G} is directly related to the existence of long-range correlations.

Derivation of (34). To understand the L dependence in (34) let us assume that the non-local functional \mathcal{G} can be expanded as

$$\mathcal{G}(\alpha(x)) = \int_0^1 dx A(x)\alpha(x) + \int_0^1 dx B(x)\alpha(x)^2 + \int_0^1 dx \int_x^1 dy C(x,y)\alpha(x)\alpha(y) + \dots \quad (35)$$

If one comes back to a lattice gas of L sites with a number n_i of particles on site i and one considers the generating function of these occupation numbers, one has for large L

$$\log \left[\left\langle \exp \sum_i \alpha_i n_i \right\rangle \right] \simeq L\mathcal{G}(\alpha(x)) \quad (36)$$

when α_i is a slowly varying function of i of the form $\alpha_i = \alpha(i/L)$. By expanding the lhs of (36) in powers of the α_i one has

$$\log \left[\left\langle \exp \sum_i \alpha_i n_i \right\rangle \right] = \sum_{i=1}^L A_i \alpha_i + \sum_{i=1}^L B_i \alpha_i^2 + \sum_{i<j} C_{i,j} \alpha_i \alpha_j + \dots \quad (37)$$

and therefore

$$\langle n_i \rangle = A_i; \quad \langle n_i^2 \rangle_c = 2B_i; \quad \langle n_i n_j \rangle_c = C_{i,j}. \quad (38)$$

Comparing (35) and (37) in (36) one sees that

$$C_{i,j} = \frac{1}{L} C \left(\frac{i}{L}, \frac{j}{L} \right) \quad (39)$$

which leads to (34). \square

A similar reasoning would show that

$$\langle \rho(x_1) \rho(x_2) \dots \rho(x_k) \rangle_c = \frac{1}{L^{k-1}} \frac{\delta^k \mathcal{G}}{\delta \alpha(x_1) \dots \delta \alpha(x_k)} \Big|_{\alpha(x)=0}. \quad (40)$$

This $1/L^{k-1}$ dependence of the k point function can indeed be proved in the SSEP [78]. We see that all the correlation functions can in principle be obtained by expanding, when this expansion is meaningful (see [53, 54] for counter-examples), the large deviation function \mathcal{G} in powers of $\alpha(x)$.

5. The symmetric simple exclusion model

For the SSEP, the calculation of the average profile or of the correlation functions can be done directly from the definition of the model. If $\tau_i = 0$ or 1 is a binary variable indicating whether site i is occupied or empty, one can write the time evolution of the average occupation $\langle \tau_i \rangle$

$$\begin{aligned} \frac{d\langle \tau_1 \rangle}{dt} &= \alpha - (\alpha + \gamma + 1)\langle \tau_1 \rangle + \langle \tau_2 \rangle \\ \frac{d\langle \tau_i \rangle}{dt} &= \langle \tau_{i-1} \rangle - 2\langle \tau_i \rangle + \langle \tau_{i+1} \rangle \quad \text{for } 2 \leq i \leq L-1 \\ \frac{d\langle \tau_L \rangle}{dt} &= \langle \tau_{L-1} \rangle - (1 + \beta + \delta)\langle \tau_L \rangle + \delta. \end{aligned} \quad (41)$$

The steady state density profile (obtained by writing that $d\langle \tau_i \rangle/dt = 0$) is [27, 79]

$$\langle \tau_i \rangle = \frac{\rho_a(L + 1/(\beta + \delta) - i) + \rho_b(i - 1 + 1/(\alpha + \gamma))}{L + 1/(\alpha + \gamma) + 1/(\beta + \delta) - 1} \quad (42)$$

with ρ_a and ρ_b defined as in (2). One can notice that for large L , if one introduces a macroscopic coordinate $i = Lx$, this becomes

$$\langle \tau_i \rangle = \rho^*(x) = (1 - x)\rho_a + x\rho_b \quad (43)$$

and one recovers (29). For large L one can also remark that $\langle \tau_1 \rangle \rightarrow \rho_a$ and $\langle \tau_L \rangle \rightarrow \rho_b$, indicating that ρ_a and ρ_b defined by (2) represent the densities of the left and right

reservoirs. One can, in fact, show [26]–[28] that the rates $\alpha, \gamma, \beta, \delta$ do correspond to the left and right boundaries being connected respectively to reservoirs at densities ρ_a and ρ_b .

The average current in the steady state is given by

$$\langle J \rangle = \langle \tau_i(1 - \tau_{i+1}) - \tau_{i+1}(1 - \tau_i) \rangle = \langle \tau_i - \tau_{i+1} \rangle = \frac{\rho_a - \rho_b}{L + \frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta} - 1}. \quad (44)$$

This shows that for large L , the current $\langle J \rangle \simeq (\rho_a - \rho_b)/L$ is proportional to the gradient of the density (with a coefficient of proportionality which is here simply 1) and therefore follows Fick's law.

One can write down the equations which generalize (41) and govern the time evolution of the two-point function or higher correlations. For example, one finds [73, 78] in the steady state for $1 \leq i < j \leq L$

$$\langle \tau_i \tau_j \rangle_c \equiv \langle \tau_i \tau_j \rangle - \langle \tau_i \rangle \langle \tau_j \rangle = -\frac{(\frac{1}{\alpha+\gamma} + i - 1)(\frac{1}{\beta+\delta} + L - j)}{(\frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta} + L - 1)^2 (\frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta} + L - 2)} (\rho_a - \rho_b)^2. \quad (45)$$

For large L , if one introduces macroscopic coordinates $i = Lx$ and $j = Ly$, this becomes for $x < y$

$$\langle \tau_{Lx} \tau_{Ly} \rangle_c = -\frac{x(1-y)}{L} (\rho_a - \rho_b)^2 \quad (46)$$

which is the expression (30).

One could believe that these weak, but long-range, correlations play no role in the large- L limit. However, if one considers macroscopic quantities such as the total number N of particles in the system, one can see that these two-point correlations give a leading contribution to the variance of N

$$\begin{aligned} \langle N^2 \rangle - \langle N \rangle^2 &= \sum_i [\langle \tau_i \rangle - \langle \tau_i \rangle^2] + 2 \sum_{i < j} \langle \tau_i \tau_j \rangle_c \simeq L \left[\int dx \rho^*(x)(1 - \rho^*(x)) \right. \\ &\quad \left. - 2(\rho_a - \rho_b)^2 \int_0^1 dx \int_x^1 dy x(1-y) \right]. \end{aligned} \quad (47)$$

For the SSEP (see section 1 for the definition), one can write down the steady state equations satisfied by higher correlation functions to get, for example, for $x < y < z$

$$\langle \tau_{Lx} \tau_{Ly} \tau_{Lz} \rangle_c = -2 \frac{x(1-2y)(1-z)}{L^2} (\rho_a - \rho_b)^3 \quad (48)$$

but solving these equations become quickly too complicated. We will see in the next section that the matrix ansatz gives an algebraic procedure to calculate all these correlation functions [78].

6. The matrix ansatz for the symmetric exclusion process

The matrix ansatz is an approach inspired by the construction of exact eigenstates in quantum spin chains [80]–[82]. It gives an algebraic way of calculating exactly the weights of all the configurations in the steady state. In [10] it was shown that the probability

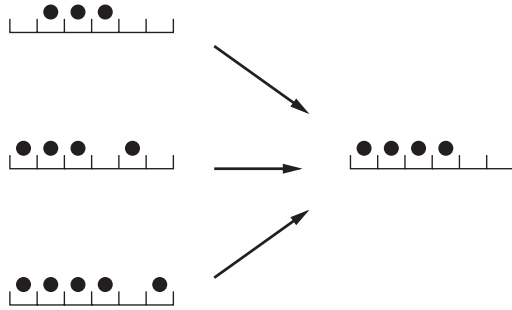


Figure 8. The three configurations which appear on the left-hand side of (53) and from which one can jump to the configuration which appears on the right-hand side of (53).

of a microscopic configuration $\{\tau_1, \tau_2, \dots, \tau_L\}$ can be written as the matrix element of a product of L matrices

$$\text{Pro}(\{\tau_1, \tau_2, \dots, \tau_L\}) = \frac{\langle W | X_1 X_2 \dots X_L | V \rangle}{\langle W | (D + E)^L | V \rangle} \quad (49)$$

where the matrix X_i depends on the occupation τ_i of site i

$$X_i = \tau_i D + (1 - \tau_i) E \quad (50)$$

and the matrices D and E satisfy the following algebraic rules

$$\begin{aligned} DE - ED &= D + E \\ \langle W | (\alpha E - \gamma D) &= \langle W | \\ (\beta D - \delta E) | V \rangle &= | V \rangle. \end{aligned} \quad (51)$$

Let us check on the simple example of figure 8 that expression (49) does give the steady state weights: if one chooses the configuration where the first p sites on the left are occupied and the remaining $L - p$ sites on the right are empty, the weight of this configuration is given by

$$\frac{\langle W | D^p E^{L-p} | V \rangle}{\langle W | (D + E)^L | V \rangle}. \quad (52)$$

For (49) to be the weights of all configurations in the steady state, one needs that the rate at which the system enters each configuration and the rate at which the system leaves it should be equal. In the case of the configuration whose weight is (52), this means that the following steady state identity should be satisfied (see figure 8):

$$\begin{aligned} \alpha \frac{\langle W | E D^{p-1} E^{L-p} | V \rangle}{\langle W | (D + E)^L | V \rangle} + \frac{\langle W | D^{p-1} E D E^{L-p-1} | V \rangle}{\langle W | (D + E)^L | V \rangle} + \beta \frac{\langle W | D^p E^{L-p-1} D | V \rangle}{\langle W | (D + E)^L | V \rangle} \\ = (\gamma + 1 + \delta) \frac{\langle W | D^p E^{L-p} | V \rangle}{\langle W | (D + E)^L | V \rangle}. \end{aligned} \quad (53)$$

This equality is easy to check by rewriting (53) as

$$\begin{aligned} & \frac{\langle W | (\alpha E - \gamma D) D^{p-1} E^{L-p} | V \rangle}{\langle W | (D + E)^L | V \rangle} - \frac{\langle W | D^{p-1} (DE - ED) E^{L-p-1} | V \rangle}{\langle W | (D + E)^L | V \rangle} \\ & + \frac{\langle W | D^p E^{L-p-1} (\beta D - \delta E) | V \rangle}{\langle W | (D + E)^L | V \rangle} = 0 \end{aligned} \quad (54)$$

and by using (51). A similar reasoning [10] allows one to prove that the corresponding steady state identity holds for any other configuration.

A priori one should construct the matrices D and E (which might be infinite-dimensional [10]) and the vectors $\langle W |$ and $|V\rangle$ satisfying (51) to calculate the weights (49) of the microscopic configurations. However, these weights do not depend on the particular representation chosen and can be calculated directly from (51). This can be easily seen by using the two matrices A and B defined by

$$\begin{aligned} A &= \beta D - \delta E \\ B &= \alpha E - \gamma D \end{aligned} \quad (55)$$

which satisfy

$$AB - BA = (\alpha\beta - \gamma\delta)(D + E) = (\alpha + \delta)A + (\beta + \gamma)B. \quad (56)$$

Each product of D 's and E 's can be written as a sum of products of A 's and B 's which can be ordered using (56) by pushing all the A 's to the right and all the B 's to the left. One then gets a sum of terms of the form $B^p A^q$, the matrix elements of which can be evaluated easily ($\langle W | B^p A^q | V \rangle = \langle W | V \rangle$) from (51) and (55).

One can calculate with the weights (49) the average density profile

$$\langle \tau_i \rangle = \frac{\langle W | (D + E)^{i-1} D (D + E)^{L-i} | V \rangle}{\langle W | (D + E)^L | V \rangle}$$

as well as all the correlation functions

$$\langle \tau_i \tau_j \rangle = \frac{\langle W | (D + E)^{i-1} D (D + E)^{j-i-1} D (D + E)^{L-j} | V \rangle}{\langle W | (D + E)^L | V \rangle}$$

and one can recover that way (42) and (45).

Using the fact that the average current between sites i and $i + 1$ is given by

$$\langle J \rangle = \frac{\langle W | (D + E)^{i-1} (DE - ED) (D + E)^{L-i-1} | V \rangle}{\langle W | (D + E)^L | V \rangle} = \frac{\langle W | (D + E)^{L-1} | V \rangle}{\langle W | (D + E)^L | V \rangle}$$

(of course in the steady state the current does not depend on i) and from the expression (44) one can calculate the normalization

$$\frac{\langle W | (D + E)^L | V \rangle}{\langle W | V \rangle} = \frac{1}{(\rho_a - \rho_b)^L} \frac{\Gamma(L + \frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta})}{\Gamma(\frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta})} \quad (57)$$

where $\Gamma(z)$ is the usual Gamma function which satisfies $\Gamma(z + 1) = z\Gamma(z)$. (see equation (3.11) of [27] for an alternative derivation of this expression.)

Remark. When $\rho_a = \rho_b = r$, the two reservoirs are at the same density and the steady state becomes the equilibrium (Gibbs) state of the lattice gas at this density r . In this case, the weights of the configurations are those of a Bernoulli measure at density r , that is

$$\text{Pro}(\{\tau_1, \tau_2, \dots, \tau_L\}) = \prod_{i=1}^L [r\tau_i + (1-r)(1-\tau_i)]. \quad (58)$$

This case corresponds to a limit where the matrices D and E commute (it can be recovered by making all the calculations with the matrices (49) and (51) for $\rho_a \neq \rho_b$ and by taking the limit $\rho_a \rightarrow \rho_b$ in the final expressions, as all the expectations, for a lattice of finite size L , are rational functions of ρ_a and ρ_b).

7. Additivity as a consequence of the matrix ansatz

In this section we are going to show how, from the matrix ansatz, to establish an identity (65) which will be used in section 8 to relate the large deviation function \mathcal{F} of a system to those of its subsystems.

As in (49) the weight of each configuration is written as the matrix element of a product of L matrices, one can try to insert at a position L_1 a complete basis in order to relate the properties of a lattice of L sites to those of two subsystems of sizes L_1 and $L - L_1$. To do so let us define the following left and right eigenvectors of the operators $\rho_a E - (1 - \rho_a)D$ and $(1 - \rho_b)D - \rho_b E$

$$\begin{aligned} \langle \rho_a, a | [\rho_a E - (1 - \rho_a)D] &= a \langle \rho_a, a | \\ [(1 - \rho_b)D - \rho_b E] | \rho_b, b \rangle &= b | \rho_b, b \rangle. \end{aligned} \quad (59)$$

It is easy to see, using the definition (2), that the vectors $\langle W |$ and $|V\rangle$ are given by

$$\begin{aligned} \langle W | &= \langle \rho_a, (\alpha + \gamma)^{-1} | \\ |V\rangle &= | \rho_b, (\beta + \delta)^{-1} \rangle. \end{aligned} \quad (60)$$

It is then possible to show, using simply the fact (51) that $DE - ED = D + E$ and the definition of the eigenvectors (59), that (for $\rho_b < \rho_a$)

$$\frac{\langle \rho_a, a | Y_1 Y_2 | \rho_b, b \rangle}{\langle \rho_a, a | \rho_b, b \rangle} = \oint_{\rho_b < |\rho| < \rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)^{a+b}}{(\rho_a - \rho)^{a+b}(\rho - \rho_b)} \frac{\langle \rho_a, a | Y_1 | \rho, b \rangle}{\langle \rho_a, a | \rho, b \rangle} \frac{\langle \rho, 1 - b | Y_2 | \rho_b, b \rangle}{\langle \rho, 1 - b | \rho_b, b \rangle} \quad (61)$$

where Y_1 and Y_2 are arbitrary polynomials of the matrices D and E .

Proof of (61). To prove (61) it is sufficient to choose Y_1 of the form $[\rho_a E - (1 - \rho_a)D]^n [D + E]^{n'}$ (clearly any polynomial of the matrices D and E can be rewritten as a polynomial of $A \equiv D + E$ and $B \equiv \rho_a E - (1 - \rho_a)D$. Then as $AB - BA = A$, which is a consequence of $DE - ED = D + E$, one can push all the A 's to the right and all the B 's to the left. Therefore any polynomial can be written as a sum of terms of the form $[\rho_a E - (1 - \rho_a)D]^n [D + E]^{n'}$). Similarly one can choose Y_2 of the form

$[D + E]^{n''}[(1 - \rho_b)D - \rho_b E]^{n''}$. Therefore proving (61) for such choices of Y_1 and Y_2 reduces to proving

$$\frac{\langle \rho_a, a | (D + E)^{n'+n''} | \rho_b, b \rangle}{\langle \rho_a, a | \rho_b, b \rangle} = \oint_{\rho_b < |\rho| < \rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)^{a+b}}{(\rho_a - \rho)^{a+b}(\rho - \rho_b)} \frac{\langle \rho_a, a | (D + E)^{n'} | \rho, b \rangle}{\langle \rho_a, a | \rho, b \rangle} \times \frac{\langle \rho, 1 - b | (D + E)^{n''} | \rho_b, b \rangle}{\langle \rho, 1 - b | \rho_b, b \rangle}. \tag{62}$$

As from (57) one has

$$\frac{\langle \rho_a, a | (D + E)^L | \rho, b \rangle}{\langle \rho_a, a | \rho, b \rangle} = \frac{\Gamma(L + a + b)}{(\rho_a - \rho_b)^L \Gamma(a + b)}. \tag{63}$$

Then (61) and (62) follow as one can easily check that

$$\frac{\Gamma(n' + n'' + a + b)}{(\rho_a - \rho_b)^{n'+n''}} = \oint_{\rho_b < |\rho| < \rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)^{a+b}}{(\rho_a - \rho)^{a+b+n'}(\rho - \rho_b)^{n''+1}} \frac{\Gamma(n' + a + b)\Gamma(n'' + 1)}{\Gamma(a + b)}. \tag{64}$$

□

An additivity relation more general than (61) can be proved for the ASEP [54]. The special case of the TASEP will be discussed in section 16 below.

If one normalizes (61) by (57) one gets

$$\frac{\langle \rho_a, a | Y_1 Y_2 | \rho_b, b \rangle}{\langle \rho_a, a | (D + E)^{L+L'} | \rho_b, b \rangle} = \frac{\Gamma(L + L' + a + b)}{\Gamma(L + a + b)\Gamma(L' + 1)} \oint_{\rho_b < |\rho| < \rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)^{a+b+L+L'}}{(\rho_a - \rho)^{a+b+L}(\rho - \rho_b)^{1+L'}} \times \frac{\langle \rho_a, a | Y_1 | \rho, b \rangle}{\langle \rho_a, a | (D + E)^L | \rho, b \rangle} \frac{\langle \rho, 1 - b | Y_2 | \rho_b, b \rangle}{\langle \rho, 1 - b | (D + E)^{L'} | \rho_b, b \rangle}. \tag{65}$$

8. Large deviation function of density profiles

We are going to see now how the large deviation functional $\mathcal{F}(\rho(x))$ of the density can be calculated for the SSEP from the additivity relation (65).

If one divides a chain of L sites into n boxes of linear size l (there are of course $n = L/l$ such boxes), one can try to determine the probability of finding a certain density profile $\{\rho_1, \rho_2, \dots, \rho_n\}$, i.e. the probability of seeing $l\rho_1$ particles in the first box, $l\rho_2$ particles in the second box, $\dots, l\rho_n$ in the n th box. For large L one expects (see (15)) the following L dependence of this probability

$$\text{Pro}_L(\rho_1, \dots, \rho_n | \rho_a, \rho_b) \sim \exp[-L\mathcal{F}_n(\rho_1, \rho_2, \dots, \rho_n | \rho_a, \rho_b)]. \tag{66}$$

If one defines a reduced coordinate x by

$$i = Lx \tag{67}$$

and if one takes the limit $l \rightarrow \infty$ with $l \ll L$ so that the number of boxes becomes infinite, one gets as in (17) the large deviation functional $\mathcal{F}(\rho(x))$

$$\text{Pro}_L(\{\rho(x)\}) \sim \exp[-L\mathcal{F}(\{\rho(x)\} | \rho_a, \rho_b)]. \tag{68}$$

For the SSEP (in one dimension), the functional $\mathcal{F}(\rho(x) | \rho_a, \rho_b)$ is given by the following exact expressions:

At equilibrium, i.e. for $\rho_a = \rho_b = r$

$$\mathcal{F}(\{\rho(x)\}|r, r) = \int_0^1 B(\rho(x), r) dx \tag{69}$$

where

$$B(\rho, r) = (1 - \rho) \log \frac{1 - \rho}{1 - r} + \rho \log \frac{\rho}{r}. \tag{70}$$

This can be derived easily. When $\rho_a = \rho_b = r$, the steady state is a Bernoulli measure (58) where all the sites are occupied independently with probability r . Therefore, if one divides a chain of length L into L/l intervals of length l , one has

$$\text{PROL}(\rho_1, \dots, \rho_n|r, r) = \prod_i^{L/l} \frac{l!}{[l\rho_i]![l(1-\rho_i)]!} r^{l\rho_i} (1-r)^{l(1-\rho_i)} \tag{71}$$

and using Stirling's formula one gets (69) and (70).

For the non-equilibrium case, i.e. for $\rho_a \neq \rho_b$, it was shown in [26, 27, 43] that

$$\mathcal{F}(\{\rho(x)\}|\rho_a, \rho_b) = \int_0^1 dx \left[B(\rho(x), F(x)) + \log \frac{F'(x)}{\rho_b - \rho_a} \right] \tag{72}$$

where the function $F(x)$ is the monotone solution of the differential equation

$$\rho(x) = F + \frac{F(1-F)F''}{F'^2} \tag{73}$$

satisfying the boundary conditions $F(0) = \rho_a$ and $F(1) = \rho_b$. This expression shows that \mathcal{F} is a *non-local* functional of the density profile $\rho(x)$ as $F(x)$ depends on the profile $\rho(y)$ at all points y . For example, if the difference $\rho_a - \rho_b$ is small, one can expand \mathcal{F} and obtain the expression (28) where the non-local character of the functional is clearly visible: at second order in $\rho_a - \rho_b$, one can check that

$$\begin{aligned} F &= \rho_a - (\rho_a - \rho_b)x - \frac{(\rho_a - \rho_b)^2}{\rho_a(1 - \rho_a)} \left[(1-x) \int_0^x y(\rho(y) - \rho_a) dy \right. \\ &\quad \left. + x \int_x^1 (1-y)(\rho(y) - \rho_a) dy \right] + O((\rho_a - \rho_b)^3) \\ &= \rho^*(x) - \frac{(\rho_a - \rho_b)^2}{\rho_a(1 - \rho_a)} \left[(1-x) \int_0^x y(\rho(y) - \rho^*(x)) dy \right. \\ &\quad \left. + x \int_x^1 (1-y)(\rho(y) - \rho^*(x)) dy \right] + O((\rho_a - \rho_b)^3) \end{aligned} \tag{74}$$

is a solution of (73) and this leads to (28) by replacing into (72).

Derivation of (72), (73). In the original derivation of (72) and (73) from the matrix ansatz [26, 27] the idea was to decompose the chain into L/l boxes of l sites and to sum the weights given by the matrix ansatz (49) and (51) over all the microscopic configurations for which the number of particles is $l\rho_1$ in the first box, $l\rho_2$ in the second box \dots , $l\rho_n$ in the n th box.

An easier way of deriving (72) and (73) (for simplicity we do it here in the particular case where $a + b = 1$, i.e. $1/(\alpha + \gamma) + 1/(\beta + \delta) = 1$, and $\rho_b < \rho_a$ but the extension to

other cases is easy) is to use (65) when Y_1 and Y_2 represent sums over all configurations with kl sites with a density ρ_1 in the first l sites, \dots ρ_k in the k th l sites and Y_2 a similar sum for the $(n - k)l$ remaining sites:

$$P_{nl}(\rho_1, \rho_2 \dots \rho_n | \rho_a, \rho_b) = \frac{(kl)!((n - k)l)!}{(nl)!} \oint_{\rho_b < |\rho| < \rho_a} \frac{d\rho}{2i\pi} \times \frac{(\rho_a - \rho_b)^{nl+1}}{(\rho_a - \rho)^{kl+1}(\rho - \rho_b)^{(n-k)l+1}} P_{kl}(\rho_1 \dots \rho_k | \rho_a, \rho) P_{(n-k)l}(\rho_{k+1} \dots \rho_n | \rho, \rho_b). \tag{75}$$

Note that in (75) the density ρ has become a complex variable. This is not a difficulty as all the weights (and therefore the probabilities which appear in (75)) are rational functions of ρ_a and ρ_b .

For large nl , if one writes $k = nx$, one gets by evaluating (75) at the saddle point

$$\mathcal{F}_n(\rho_1, \rho_2, \dots, \rho_n | \rho_a, \rho_b) = \max_{\rho_b < F < \rho_a} x \mathcal{F}_k(\rho_1, \dots, \rho_k | \rho_a, F) + (1 - x) \mathcal{F}_{n-k}(\rho_{k+1}, \dots, \rho_n | F, \rho_b) + x \log\left(\frac{\rho_a - F}{x}\right) + (1 - x) \log\left(\frac{F - \rho_b}{1 - x}\right) - \log(\rho_a - \rho_b). \tag{76}$$

(To estimate (75) by a saddle point method, one should find the value F of ρ which maximizes the integrand over the contour. As the contour is perpendicular to the real axis at their crossing point, this becomes a minimum when ρ varies along the real axis.) If one repeats the same procedure n times, one gets

$$\mathcal{F}_n(\rho_1, \rho_2, \dots, \rho_n | \rho_a, \rho_b) = \max_{\rho_b = F_0 < F_1 < \dots < F_i < \dots < F_n = \rho_a} \frac{1}{n} \sum_{i=1}^n \mathcal{F}_1(\rho_i | F_{i-1}, F_i) + \log\left(\frac{(F_{i-1} - F_i)n}{\rho_a - \rho_b}\right). \tag{77}$$

For large n , as F_i is monotone, the difference $F_{i-1} - F_i$ is small for almost all i and one can replace $\mathcal{F}_1(\rho_i | F_{i-1}, F_i)$ by its equilibrium value $\mathcal{F}_1(\rho_i | F_i, F_i) = B(\rho_i, F_i)$. If one writes F_i as a function of i/n

$$F_i = F\left(\frac{i}{n}\right) \tag{78}$$

(77) becomes

$$\mathcal{F}(\{\rho(x)\} | \rho_a, \rho_b) = \max_{F(x)} \int_0^1 dx \left[B(\rho(x), F(x)) + \log \frac{F'(x)}{\rho_b - \rho_a} \right] \tag{79}$$

where the maximum is over all the monotone functions $F(x)$ which satisfy $F(0) = \rho_a$ and $F(1) = \rho_b$ and one gets (72), (73). \square

Remark. One can easily get from (72) and (73) the generating function $\mathcal{G}(\{\alpha(x)\})$ of the density (31) for the SSEP:

$$\mathcal{G}(\{\alpha(x)\}) = \int_0^1 dx \left[\log(1 - F + F e^{\alpha(x)}) - \log \frac{F'}{\rho_b - \rho_a} \right] \tag{80}$$

where F is the monotone solution of

$$F'' + \frac{F'^2(1 - e^{\alpha(x)})}{1 - F + Fe^{\alpha(x)}} = 0 \quad (81)$$

with $F(0) = \rho_a$ and $F(1) = \rho_b$. For small $\alpha(x)$ the solution of (81) is, to second order in the difference $\rho_a - \rho_b$

$$F(x) = \rho^*(x) - (\rho_a - \rho_b)^2 \left[(1-x) \int_0^x y \alpha(y) dy + x \int_x^1 (1-y) \alpha(y) dy \right]. \quad (82)$$

This leads to $\mathcal{G}(\alpha(x))$ at order $(\rho_a - \rho_b)^2$

$$\begin{aligned} \mathcal{G}(\{\alpha(x)\}) = & \int_0^1 dx \left[\rho^*(x) \alpha(x) + \frac{\rho^*(x)(1 - \rho^*(x))}{2} \alpha(x)^2 \right] \\ & - (\rho_a - \rho_b)^2 \int_0^1 dx \int_x^1 dy x(1-y) \alpha(x) \alpha(y) \end{aligned} \quad (83)$$

and one recovers through (34) the expression of the two-point correlation function (30).

9. The macroscopic fluctuation theory

For a general diffusive one-dimensional system (figure 2) of linear size L the average current and the fluctuations of this current near equilibrium can be characterized by two quantities $D(\rho)$ and $\sigma(\rho)$ defined by

$$\lim_{t \rightarrow \infty} \frac{\langle Q_t \rangle}{t} = \frac{D(\rho)}{L} (\rho_a - \rho_b) \quad \text{for } (\rho_a - \rho_b) \text{ small} \quad (84)$$

$$\lim_{t \rightarrow \infty} \frac{\langle Q_t^2 \rangle}{t} = \frac{\sigma(\rho)}{L} \quad \text{for } \rho_a = \rho_b \quad (85)$$

where Q_t is the total number of particles transferred from the left reservoir to the system during time t .

Starting from the hydrodynamic large deviation theory [22, 25, 73] Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim [42]–[44] have developed a general approach, *the macroscopic fluctuation theory*, to calculate the large deviation functional \mathcal{F} of the density (17) in the non-equilibrium steady state of a system in contact with two (or more) reservoirs as in figure 2. Let us briefly sketch their approach. For diffusive systems (such as the SSEP), the density $\rho_i(t)$ near position i at time t and the total flux $Q_i(t)$ flowing through position i between time 0 and time t are, for a large system of size L and for times of order L^2 , scaling functions of the form

$$\rho_i(t) = \hat{\rho} \left(\frac{i}{L}, \frac{t}{L^2} \right), \quad \text{and} \quad Q_i(t) = L \hat{Q} \left(\frac{i}{L}, \frac{t}{L^2} \right). \quad (86)$$

(Note that, due to the conservation of the number of particles, the scaling form of $\rho_i(t)$ implies the scaling form of $Q_i(t)$.) If one introduces the instantaneous (rescaled) current defined by

$$\hat{j}(x, \tau) = \frac{\partial \hat{Q}(x, \tau)}{\partial \tau} \quad (87)$$

the conservation of the number of particles implies that

$$\frac{\partial \widehat{\rho}(x, \tau)}{\partial \tau} = -\frac{\partial^2 \widehat{Q}(x, \tau)}{\partial \tau \partial x} = -\frac{\partial \widehat{j}(x, \tau)}{\partial x}. \tag{88}$$

Note that the total flux of particles through position $i = [Lx]$ during the macroscopic time interval $d\tau$, i.e. during the microscopic time interval $L^2 d\tau$, is $L\widehat{j}(x, \tau) d\tau$. Thus the microscopic current is of order $1/L$ while the rescaled current \widehat{j} remains of order 1.

The *macroscopic fluctuation theory* [42]–[44] starts from the probability of observing a certain density profile $\widehat{\rho}(x, \tau)$ and current profile $\widehat{j}(x, \tau)$ over the rescaled time interval $\tau_1 < \tau < \tau_2$

$$Q_{\tau_1, \tau_2}(\{\widehat{\rho}(x, \tau), \widehat{j}(x, \tau)\}) \sim \exp \left[-L \int_{\tau_1}^{\tau_2} d\tau' \int_0^1 dx \frac{[\widehat{j}(x, \tau') + D(\widehat{\rho}(x, \tau')) \frac{\partial \widehat{\rho}(x, \tau')}{\partial x}]^2}{2\sigma(\widehat{\rho}(x, \tau'))} \right] \tag{89}$$

where the current $\widehat{j}(x, s)$ is related to the density profile $\widehat{\rho}(x, s)$ by the conservation law (88) and the functions $D(\rho)$ and $\sigma(\rho)$ are defined by (84) and (85). Similar expressions were obtained in [83, 84] by considering stochastic models in the context of shot noise in mesoscopic quantum conductors.

Then Bertini *et al* [42] show that to calculate the probability of observing a density profile $\rho(x)$ in the steady state, at time τ , one has to find out how this deviation is produced. For large L , one has to find the optimal path $\{\widehat{\rho}(x, s), \widehat{j}(x, s)\}$ for $-\infty < s < \tau$ in the space of density and current profiles and

$$\text{Pro}(\rho(x)) \sim \max_{\{\widehat{\rho}(x, s), \widehat{j}(x, s)\}} Q_{-\infty, \tau}(\{\widehat{\rho}(x, s), \widehat{j}(x, s)\}) \tag{90}$$

which goes from the typical profile $\rho^*(x)$ to the desired profile

$$\widehat{\rho}(x, -\infty) = \rho^*(x); \quad \widehat{\rho}(x, \tau) = \rho(x). \tag{91}$$

This means that the large deviation functional \mathcal{F} of the density (68) is given by

$$\mathcal{F}(\rho(x)) = \min_{\{\widehat{\rho}(x, s), \widehat{j}(x, s)\}} \int_{-\infty}^{\tau} d\tau' \int_0^1 dx \frac{[\widehat{j}(x, \tau') + D(\widehat{\rho}(x, \tau')) \frac{\partial \widehat{\rho}(x, \tau')}{\partial x}]^2}{2\sigma(\widehat{\rho}(x, \tau'))} \tag{92}$$

where the density and the current profiles satisfy the conservation law (88) and the boundary conditions (91). Obviously (90) or (92) do not depend on τ as the probability of producing a certain deviation $\rho(x)$ in the steady state does not depend on the time τ at which this deviation occurs.

Finding this optimal path $\widehat{\rho}(x, s), \widehat{j}(x, s)$ with the boundary conditions (91) is usually a hard problem. Bertini *et al* [42] were, however, able to write an equation satisfied by \mathcal{F} : as (92) does not depend on τ , one can isolate in the integral (92) the contribution of the last time interval $(\tau - \delta\tau, \tau)$ and (92) becomes

$$\mathcal{F}(\rho(x)) = \min_{\delta\rho(x), j(x)} \left[\mathcal{F}(\rho(x) - \delta\rho(x)) + \delta\tau \int_0^1 dx \frac{[j(x) + D(\rho(x))\rho'(x)]^2}{2\sigma(\rho(x))} \right] \tag{93}$$

where $\rho(x) - \delta\rho(x) = \widehat{\rho}(x, \tau - d\tau)$ and $j(x) = \widehat{j}(x, \tau)$. Then if one defines $U(x)$ by

$$U(x) = \frac{\delta\mathcal{F}(\{\rho(x)\})}{\delta\rho(x)} \quad (94)$$

and one uses the conservation law $\delta\rho(x) = -(dj(x)/dx) d\tau$ one should have, according to (93), that the optimal current $j(x)$ is given by

$$j(x) = -D(\rho(x))\rho'(x) + \sigma(\rho(x))U'(x). \quad (95)$$

Therefore starting with $\widehat{\rho}(x, \tau) = \rho(x)$ and using the time evolution

$$\frac{d\widehat{\rho}(x, s)}{ds} = -\frac{d\widehat{j}(x, s)}{dx} \quad (96)$$

with \widehat{j} related to $\widehat{\rho}$ by (95) one should get the whole time-dependent optimal profile $\widehat{\rho}(x, s)$ which converges to $\rho^*(x)$ in the limit $s \rightarrow -\infty$. The problem, of course, is that $\mathcal{F}(\rho(x))$ is in general not known and so is $U(x)$ defined in (94).

One can write from (93) (after an integration by parts and using the fact that $U(0) = U(1) = 0$ if $\rho(0) = \rho_a$ and $\rho(1) = \rho_b$) the equation satisfied by $U'(x)$

$$\int_0^1 dx \left[\left(\frac{D\rho'}{\sigma} - U' \right)^2 - \left(\frac{D\rho'}{\sigma} \right)^2 \right] \frac{\sigma}{2} = 0 \quad (97)$$

which is the Hamilton–Jacobi [42] equation of Bertini *et al.* For general $D(\rho)$ and $\sigma(\rho)$ one does not know how to find the solution $U'(x)$ of (97) for an arbitrary $\rho(x)$ and thus one does not know how to get a more explicit expression of the large deviation function $\mathcal{F}(\{\rho(x)\})$.

One can, however, check rather easily whether a given expression of $\mathcal{F}(\{\rho(x)\})$ satisfies (97) since $U'(x)$ can be calculated from (94). For the SSEP one gets from (79), (94)

$$U(x) = \log \left[\frac{\rho(x)(1 - F(x))}{(1 - \rho(x))F(x)} \right] \quad (98)$$

with $F(x)$ related to $\rho(x)$ by (73). One can then check that (97) is indeed satisfied using the expressions of $D = 1$ and $\sigma = 2\rho(1 - \rho)$ for the SSEP (see (117) below).

In fact, when \mathcal{F} is known, one can obtain the whole optimal path $\widehat{\rho}(x, s)$ from the evolution (96) with \widehat{j} related to $\widehat{\rho}$ by (95) which becomes for the SSEP

$$\widehat{j}(x, s) = -\frac{d\widehat{\rho}(x, s)}{dx} + \sigma(\widehat{\rho}(x, s)) \log \left[\frac{\widehat{\rho}(x, s)(1 - \widehat{F}(x, s))}{(1 - \widehat{\rho}(x, s))\widehat{F}(x, s)} \right] \quad (99)$$

where \widehat{F} is related to $\widehat{\rho}$ by (73). For (72) and (73) to coincide with (92), the optimal profile $\widehat{\rho}$ evolving according to (96) should converge to $\rho^*(x)$ as $s \rightarrow -\infty$. One can check that this evolution of $\widehat{\rho}(x, s)$ is equivalent to the following evolution [43] of \widehat{F}

$$\frac{d\widehat{F}(x, s)}{ds} = -\frac{d^2\widehat{F}(x, s)}{dx^2} \quad (100)$$

where \widehat{F} is related to $\widehat{\rho}$ by (73). Clearly (100) is a diffusion equation and, because of the minus sign, $\widehat{F}(x, s) \rightarrow \rho^*(x)$ and therefore $\widehat{\rho}(x, s) \rightarrow \rho^*(x)$ as $s \rightarrow -\infty$. Thus (96)

and (99) do give the optimal path in (92) with the right boundary conditions (91) and (92) coincides for the SSEP with the prediction (72) and (73) of the matrix approach.

Apart for the SSEP, the large deviation functional \mathcal{F} of the density is so far known only in a very few cases: the Kipnis–Marchioro–Presutti model [85, 86], the weakly asymmetric exclusion process [28, 87] and the ABC model [64, 71] on a ring for equal densities of the three species.

10. Large deviation of the current and the fluctuation theorem

For a system in contact with two reservoirs at densities ρ_a and ρ_b , as in figure 2, one can try to study the probability distribution of the total number Q_t of particles which flows through the system during time t . For finite t , this distribution depends on the initial condition of the system as well as on the place where the flux Q_t is measured (along an arbitrary section of the system, at the boundary with the left reservoir or at the boundary with the right reservoir). In the long-time limit, however, if the system has a finite relaxation time and if the number of particles in the system is bounded (i.e. infinitely many particles cannot accumulate in the system) the probability distribution of Q_t takes the form

$$\text{Pro} \left(\frac{Q_t}{t} = j \right) \sim e^{-tF(j)} \tag{101}$$

where the large deviation function $F(j)$ of the current j depends neither on the initial condition nor on where the flux Q_t is measured. This large deviation function $F(j)$ has usually a shape similar to $a_{\bar{r}}(\rho)$ in figure 6, with a minimum at the typical value $j^* = \langle J \rangle$ (the average current) where $F(j^*) = 0$.

It is often as convenient to work with the generating function $\langle e^{\lambda Q_t} \rangle$. In the long-time limit

$$\langle e^{\lambda Q_t} \rangle \sim e^{\mu(\lambda)t} \tag{102}$$

where $\mu(\lambda)$ is clearly the Legendre transform of the large deviation function $F(j)$

$$\mu(\lambda) = \max_j [\lambda j - F(j)]. \tag{103}$$

As in section 4, the knowledge of $\mu(\lambda)$ determines the cumulants of Q_t

$$\lim_{t \rightarrow \infty} \frac{\langle Q_t^k \rangle_c}{t} = \left. \frac{d^k \mu(\lambda)}{d\lambda^k} \right|_{\lambda=0} \tag{104}$$

when the expansion in powers of λ is justified.

According to the *fluctuation theorem* [46]–[50], [58, 59], [88]–[92], the large deviation function $F(j)$ of the current satisfies the following symmetry property

$$F(j) - F(-j) = -j[\log z_a - \log z_b] \quad \text{and} \quad \mu(\lambda) = \mu(-\lambda + \log z_b - \log z_a). \tag{105}$$

Proof. Following previous derivations [49, 50, 90] for stochastic dynamics the fluctuation theorem (105) can be easily recovered [57] from the *generalized detailed balance relation* (9). This can be seen by comparing the probabilities of a trajectory in phase space and of its time reversal for a system in contact with two reservoirs. A trajectory ‘Traj’ is

specified by a sequence of successive configurations C_1, \dots, C_k visited by the system, the times t_1, \dots, t_k spent in each of these configurations and the number of particles $q_{a,i}, q_{b,i}$ transferred from the reservoirs to the system when the system jumps from C_i to C_{i+1}

$$\text{Pro}(\text{Traj}) = dt^{k-1} \left[\prod_{i=1}^{k-1} W_{q_{a,i}, q_{b,i}}(C_{i+1}, C_i) \right] \exp \left[- \sum_{i=1}^k t_i r(C_i) \right]$$

where $r(C) = \sum_{C'} \sum_{q_a, q_b} W_{q_a, q_b}(C', C)$ and dt is the infinitesimal time interval over which jumps occur.

For the trajectory ‘-Traj’ obtained from ‘Traj’ by time reversal, i.e. for which the system visits successively the configurations C_k, \dots, C_1 , exchanging $-q_{a,i}, -q_{b,i}$ particles with the reservoirs each time the system jumps from C_{i+1} to C_i , one has

$$\text{Pro}(-\text{Traj}) = dt^{k-1} \left[\prod_{i=1}^{k-1} W_{-q_{a,i}, -q_{b,i}}(C_i, C_{i+1}) \right] \exp \left[- \sum_{i=1}^k t_i r(C_i) \right].$$

One can see from the generalized detailed balance relation (9) that

$$\frac{\text{Pro}(\text{Traj})}{\text{Pro}(-\text{Traj})} = \exp \left[\sum_{i=1}^{k-1} q_{a,i} \log z_a - q_{b,i} \log z_b \right] = \exp [Q_t^{(a)} \log z_a - Q_t^{(b)} \log z_b] \quad (106)$$

where $Q_t^{(a)} = \sum_i q_{a,i}$ and $Q_t^{(b)} = \sum_i q_{b,i}$ are the total number of particles transferred from the reservoirs a and b to the system during time t .

In general $Q_t^{(a)}$ and $Q_t^{(b)}$ grow with time but their sum remains bounded (if one assumes that particles cannot accumulate in the system—see [93] for a counter-example). Therefore for large time $Q_t \equiv Q_t^{(a)} = -Q_t^{(b)} + o(t)$ and

$$\frac{\text{Pro}(\text{Traj})}{\text{Pro}(-\text{Traj})} \sim \exp [Q_t (\log z_a - \log z_b)]. \quad (107)$$

Summing over all trajectories [57], taking the log and then the long-time limit (101) leads to the fluctuation theorem (105). \square

Remark. The fluctuation theorem predicts a symmetry relation similar to (105) for the heat current for a system in contact with two heat baths at unequal temperatures as in figure 1. Under similar conditions as for the current of particles (the energy of the system is bounded and the relaxation time is finite—see [94]–[96] for counter-examples where the energy is not bounded in which case the fluctuation theorem has to be modified) one gets that the distribution of the energy Q_t flowing through the system during a long time t is given by (101) and that the large deviation function $F(j)$ or its Legendre transform satisfy

$$F(j) - F(-j) = -j \left(\frac{1}{kT_b} - \frac{1}{kT_a} \right); \quad \mu(\lambda) = \mu \left(-\lambda + \frac{1}{kT_a} - \frac{1}{kT_b} \right) \quad (108)$$

which states that the difference $F(j) - F(-j)$ is linear in j with a universal slope related to the difference of the inverse temperatures. Note that $j(1/T_b - 1/T_a)$ is the rate of entropy production which is the quantity generally used to state the fluctuation theorem [46, 47, 50, 59].

11. The fluctuation–dissipation theorem

In this section we are going to see how the fluctuation–dissipation theorem can be recovered from the fluctuation theorem of section 10 when the system is close to equilibrium.

In the limit of small $T_a - T_b$ (i.e. close to equilibrium), the *fluctuation–dissipation theorem* relates the response to a small temperature gradient

$$\frac{\langle Q_t \rangle}{t} \rightarrow (T_a - T_b) \tilde{D} \quad \text{for } T_a - T_b \text{ small} \tag{109}$$

and the variance of the energy flux at equilibrium

$$\frac{\langle Q_t^2 \rangle}{t} \rightarrow \tilde{\sigma} \quad \text{for } T_a = T_b. \tag{110}$$

In fact from these definitions of \tilde{D} and $\tilde{\sigma}$, one has for $\mu(\lambda)$ defined in (102)

$$\mu(\lambda) = (T_a - T_b) \tilde{D} \lambda + \frac{\tilde{\sigma}}{2} \lambda^2 + O(\lambda^3, \lambda^2(T_a - T_b), \lambda(T_a - T_b)^2) \tag{111}$$

and using the fluctuation theorem (108), one gets that the coefficients $\tilde{\sigma}$ and \tilde{D} have to satisfy

$$\tilde{\sigma} = 2kT_a^2 \tilde{D} \tag{112}$$

which is the usual fluctuation–dissipation relation. In general both \tilde{D} and $\tilde{\sigma}$ depend on the temperature T_a .

The same close-to-equilibrium expansion of (105) for a current of particles leads to

$$\tilde{\sigma} = 2 \frac{d\rho}{d \log z} \tilde{D} = 2kT \rho^2 \kappa(\rho) \tilde{D} \tag{113}$$

where the coefficients $\tilde{\sigma}$ and \tilde{D} are defined as in (109), (110) by

$$\frac{\langle Q_t \rangle}{t} \rightarrow (\rho_a - \rho_b) \tilde{D} \quad \text{for } \rho_a - \rho_b \text{ small} \quad \text{and} \quad \frac{\langle Q_t^2 \rangle}{t} \rightarrow \tilde{\sigma} \quad \text{for } \rho_a = \rho_b \tag{114}$$

and where $\kappa(\rho)$ is the compressibility (27) at equilibrium.

To see why the compressibility appears in (113), one can write $\log Z = -F/kT = -Vf(N/V)/kT$ where F is the total free energy and f the free energy per unit volume. One then uses the facts that the fugacity z is given by $kT \log z = dF/dN = f'(\rho)$, that $p = -dF/dV = \rho f'(\rho) - f(\rho)$ and thus $d\rho/d \log z = kT/f''(\rho) = kT \rho d\rho/dp = kT \rho^2 \kappa(\rho)$.

In the case of the SSEP, one has from (44) and (84) that $D_{\text{SSEP}} = 1$. As the free energy $f(\rho)$ of the SSEP (at equilibrium at density ρ) is

$$f(\rho) = kT[\rho \log \rho + (1 - \rho) \log(1 - \rho)] \tag{115}$$

one has

$$\log z = \log \frac{\rho}{1 - \rho}. \tag{116}$$

Thus $d\rho/d \log z = kT/f''(\rho) = \rho(1 - \rho)$ and, thanks to (113) and (44) and (84), one gets

$$D_{\text{SSEP}} = 1; \quad \sigma_{\text{SSEP}} = 2\rho(1 - \rho). \tag{117}$$

Note that in (84) and (85) there is, compared with ((110), (109) and (114)), an extra $1/L$ factor in the definition of σ and D to get a finite large L limit of σ and D . Of course, with this extra $1/L$ factor, both (112) and (113) remain valid.

12. Current fluctuations in the SSEP

For the SSEP, if Q_t is the total number of particles transferred from the left reservoir to the system during a long time t , one has (102)

$$\langle e^{\lambda Q_t} \rangle \sim e^{\mu(\lambda)t}. \quad (118)$$

The fluctuation theorem (105) implies (116) a symmetry relation satisfied by $\mu(\lambda)$

$$\mu(\lambda) = \mu \left(-\lambda - \log \frac{\rho_a}{1 - \rho_a} + \log \frac{\rho_b}{1 - \rho_b} \right) \quad (119)$$

but of course this symmetry does not determine $\mu(\lambda)$. In this section we are going to see that, because the evolution is Markovian, $\mu(\lambda)$ can be determined as the largest eigenvalue of a certain matrix [51], [97]–[99] and we will sketch an approach allowing us to determine $\mu(\lambda)$ perturbatively in λ .

The probability $P_t(C)$ of finding the system in a configuration C at time t evolves according to (4)

$$\frac{dP_t(C)}{dt} = \sum_{C'} W(C, C') P_t(C') - W(C', C) P_t(C). \quad (120)$$

Among all the matrix elements $W(C, C')$, some correspond to exchanges of particles with the left reservoir and others represent internal moves in the bulk or exchanges with the right reservoir. Thus one can decompose the matrix $W(C, C')$ into three matrices

$$W(C, C') = W_1(C, C') + W_0(C, C') + W_{-1}(C, C') \quad (121)$$

where here the index is the number of particles transferred from the left reservoir to the system during time dt , when the system jumps from the configuration C' to the configuration C . One can then show [51, 97, 98] that $\mu(\lambda)$ is simply the largest eigenvalue (more precisely the eigenvalue with the largest real part) of the matrix M_λ defined by

$$M_\lambda(C, C') = e^\lambda W_1(C, C') + W_0(C, C') + e^{-\lambda} W_{-1}(C, C') - \delta(C, C') \sum_{C''} W(C'', C). \quad (122)$$

In fact the joint probability $P_t(C, Q_t)$ of C and Q_t evolves according to

$$\frac{dP_t(C, Q_t)}{dt} = \sum_{C'} \sum_{q=-1,0,1} W_q(C, C') P_t(C', Q_t - q) - \sum_{C'} W(C', C) P_t(C, Q_t). \quad (123)$$

Then if $\tilde{P}_t(C) = \sum_{Q_t} e^{\lambda Q_t} P_t(C, Q_t)$ one has

$$\frac{d\tilde{P}_t(C, Q_t)}{dt} = \sum_{C'} M_\lambda(C, C') \tilde{P}_t(C') \quad (124)$$

and this shows that $\mu(\lambda)$ is the eigenvalue with largest real part of the matrix M_λ .

The size of the matrix M_λ grows like 2^L (which is the total number of possible configurations of a chain of L sites). In [51] a perturbative approach was developed to calculate $\mu(\lambda)$ in powers of λ . Let us sketch briefly this approach: one can write

down exact expressions for the time evolution $\langle e^{\lambda Q_t} \rangle$ or of $\langle e^{\lambda Q_t} H(C) \rangle$ where $H(C)$ is an arbitrary function of the configuration C at time t . For example

$$Q_{t+dt} = \begin{cases} Q_t & \text{with probability } 1 - \alpha(1 - \tau_1) dt - \gamma\tau_1 dt \\ Q_t + 1 & \text{with probability } \alpha(1 - \tau_1) dt \\ Q_t - 1 & \text{with probability } \gamma\tau_1 dt \end{cases} \quad (125)$$

and therefore

$$\frac{d\langle e^{\lambda Q_t} \rangle}{dt} = \alpha(e^\lambda - 1)\langle (1 - \tau_1)e^{\lambda Q_t} \rangle + \gamma(e^{-\lambda} - 1)\langle \tau_1 e^{\lambda Q_t} \rangle. \quad (126)$$

Similarly one can show that for $1 < i < L$

$$\frac{d\langle \tau_i e^{\lambda Q_t} \rangle}{dt} = \alpha(e^\lambda - 1)\langle (1 - \tau_1)\tau_i e^{\lambda Q_t} \rangle + \gamma(e^{-\lambda} - 1)\langle \tau_1 \tau_i e^{\lambda Q_t} \rangle + \langle (\tau_{i+1} - 2\tau_i + \tau_{i-1})e^{\lambda Q_t} \rangle \quad (127)$$

the cases $i = 1$ and $i = L$ being slightly different

$$\frac{d\langle \tau_1 e^{\lambda Q_t} \rangle}{dt} = \alpha e^\lambda \langle (1 - \tau_1)e^{\lambda Q_t} \rangle - \gamma \langle \tau_1 e^{\lambda Q_t} \rangle + \langle (\tau_2 - \tau_1)e^{\lambda Q_t} \rangle \quad (128)$$

$$\begin{aligned} \frac{d\langle \tau_L e^{\lambda Q_t} \rangle}{dt} &= \alpha(e^\lambda - 1)\langle (1 - \tau_1)\tau_L e^{\lambda Q_t} \rangle - \gamma(e^{-\lambda} - 1)\langle \tau_1 \tau_L e^{\lambda Q_t} \rangle + \langle (\tau_{L-1} - \tau_L)e^{\lambda Q_t} \rangle \\ &\quad + \delta \langle (1 - \tau_L)e^{\lambda Q_t} \rangle - \beta \langle \tau_L e^{\lambda Q_t} \rangle. \end{aligned} \quad (129)$$

In the long-time limit $\langle e^{\lambda Q_t} \rangle \sim e^{\mu(\lambda)t}$ and one can define a measure $\langle \cdot \rangle_\lambda$ on the configurations C

$$\langle H(C) \rangle_\lambda = \lim_{t \rightarrow \infty} \frac{\langle H(C) e^{\lambda Q_t} \rangle}{\langle e^{\lambda Q_t} \rangle}. \quad (130)$$

From (126)–(129) one gets

$$\mu(\lambda) = \alpha(e^\lambda - 1)\langle (1 - \tau_1) \rangle_\lambda + \gamma(e^{-\lambda} - 1)\langle \tau_1 \rangle_\lambda \quad (131)$$

$$\mu(\lambda)\langle \tau_i \rangle_\lambda = \alpha(e^\lambda - 1)\langle (1 - \tau_1)\tau_i \rangle_\lambda + \gamma(e^{-\lambda} - 1)\langle \tau_1 \tau_i \rangle_\lambda + \langle (\tau_{i+1} - 2\tau_i + \tau_{i-1}) \rangle_\lambda \quad (132)$$

$$\mu(\lambda)\langle \tau_1 \rangle_\lambda = \alpha e^\lambda \langle (1 - \tau_1) \rangle_\lambda - \gamma \langle \tau_1 \rangle_\lambda + \langle (\tau_2 - \tau_1) \rangle_\lambda \quad (133)$$

$$\begin{aligned} \mu(\lambda)\langle \tau_L \rangle_\lambda &= \alpha(e^\lambda - 1)\langle (1 - \tau_1)\tau_L \rangle_\lambda - \gamma(e^{-\lambda} - 1)\langle \tau_1 \tau_L \rangle_\lambda \\ &\quad + \langle (\tau_{L-1} - \tau_L) \rangle_\lambda + \delta \langle (1 - \tau_L) \rangle_\lambda - \beta \langle \tau_L \rangle_\lambda. \end{aligned} \quad (134)$$

We see that to get $\mu(\lambda)$ at order λ^k , one needs to know (131) the one-point function $\langle \tau_i \rangle_\lambda$ at order λ^{k-1} , the two-point functions $\langle \tau_i \tau_j \rangle_\lambda$ at order λ^{k-2} (see (132)–(134)) and so on up to the k -point functions at order λ^0 . As the steady state weights $P(C)$ for the SSEP are known exactly (sections 5 and 6) [10, 26, 27], all the correlation functions are known at order λ^0 and one can truncate the hierarchy at the level of the k -point functions.

In [51] this perturbation theory based on the hierarchy (131)–(134) was developed to calculate $\mu(\lambda)$ in powers of λ . The main outcome of this perturbation theory [51] is that

$\mu(\lambda)$, which in principle depends on L , λ and on the four parameters $\alpha, \beta, \gamma, \delta$, takes for large L a simple form

$$\mu(\lambda) = \frac{1}{L}R(\omega) + \mathcal{O}\left(\frac{1}{L^2}\right) \quad (135)$$

where ω is defined by

$$\omega = (e^\lambda - 1)\rho_a + (e^{-\lambda} - 1)\rho_b - (e^\lambda - 1)(1 - e^{-\lambda})\rho_a\rho_b \quad (136)$$

where ρ_a and ρ_b are given in (2). The perturbation theory gives up to fourth order in ω

$$R(\omega) = \omega - \frac{\omega^2}{3} + \frac{8\omega^3}{45} - \frac{4\omega^4}{35} + \mathcal{O}(\omega^5). \quad (137)$$

The fact that $\mu(\lambda)$ depends only on ρ_a, ρ_b and λ through the single parameter ω is the outcome of the calculation, but so far there is no physical explanation why it is so. However ω remains unchanged under a number of symmetries [51] (left–right, particle–hole, the Gallavotti–Cohen symmetry (119)), implying that $\mu(\lambda)$ remains unchanged as it should under these symmetries.

From the knowledge of $R(\omega)$ up to fourth order in ω , one can determine [51] the first four cumulants (104) of the integrated current Q_t for arbitrary ρ_a and ρ_b :

- For $\rho_a = 1$ and $\rho_b = 0$, one finds

$$\frac{\langle Q_t \rangle}{t} = \frac{1}{L} + \mathcal{O}\left(\frac{1}{L^2}\right) \quad (138)$$

$$\frac{\langle Q_t^2 \rangle_c}{t} = \frac{1}{3L} + \mathcal{O}\left(\frac{1}{L^2}\right) \quad (139)$$

$$\frac{\langle Q_t^3 \rangle_c}{t} = \frac{1}{15L} + \mathcal{O}\left(\frac{1}{L^2}\right) \quad (140)$$

$$\frac{\langle Q_t^4 \rangle_c}{t} = \frac{-1}{105L} + \mathcal{O}\left(\frac{1}{L^2}\right). \quad (141)$$

These cumulants are the same as the ones known for a different problem of current flow: the case of non-interacting fermions through a mesoscopic disordered conductor [100, 101]. This can be understood as a theory [84] similar to the macroscopic fluctuation theory of Bertini *et al* [42]–[45] can be written for these mesoscopic conductors with the same $D(\rho)$ and $\sigma(\rho)$ as for the SSEP (117).

- For $\rho_a = \rho_b = \frac{1}{2}$ which corresponds to an equilibrium case with the same density 1/2 in the two reservoirs, one finds that all odd cumulants vanish as they should and that

$$\frac{\langle Q_t^2 \rangle_c}{t} = \frac{1}{2L} + \mathcal{O}\left(\frac{1}{L^2}\right) \quad (142)$$

$$\frac{\langle Q_t^4 \rangle_c}{t} = \mathcal{O}\left(\frac{1}{L^2}\right). \quad (143)$$

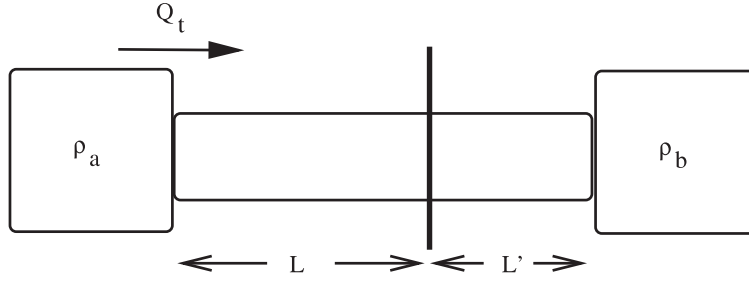


Figure 9. In the additivity principle one tries to relate the large deviation function of the current $F_{L+L'}(j)$ of a system of size $L + L'$ to the large deviation functions $F_L(j)$ and $F_{L'}(j)$ of its two subsystems (147).

Because $\mu(\lambda)$ depends on the parameters ρ_a, ρ_b and λ through the single parameter ω , if one knows $\mu(\lambda)$ for one single choice of ρ_a and ρ_b , then (136) and (137) determine $\mu(\lambda)$ for all other choices of ρ_a, ρ_b . In [51], it was conjectured that, for the particular case $\rho_a = \rho_b = \frac{1}{2}$, not only the fourth cumulant vanishes as in (143), but also all the higher cumulants vanish, so that the distribution of Q_t is Gaussian (to leading order in $1/L$). This fully determines the function $R(\omega)$ to be

$$R(\omega) = [\log(\sqrt{1 + \omega} + \sqrt{\omega})]^2. \tag{144}$$

One can then check that, with this expression of $R(\omega)$, not only (138) and (141) but all the higher cumulants of Q_t in the case $\rho_a = 1$ and $\rho_b = 0$ coincide with those of fermions through mesoscopic conductors [51, 100].

13. The additivity principle

In [52], another conjecture, *the additivity principle* based on a simpler physical interpretation, was formulated which leads for the SSEP to the same expression (136) and (144) as predicted in section 12 and can be generalized to obtain $F(j)$ or $\mu(\lambda)$ defined in (101) and (102) for more general diffusive systems.

For a system of length $L + L'$ in contact with two reservoirs of particles at densities ρ_a and ρ_b , the probability of observing, during a long time t , an integrated current $Q_t = jt$ has the following form (101)

$$\text{Pro}_{L+L'}(j, \rho_a, \rho_b) \sim e^{-tF_{L+L'}(j, \rho_a, \rho_b)}. \tag{145}$$

The idea of the additivity principle (see figure 9) is to try to relate the large deviation function $F_{L+L'}(j, \rho_a, \rho_b)$ of the current to the large deviation functions of subsystems by writing that for large t

$$\text{Pro}_{L+L'}(j, \rho_a, \rho_b) \sim \max_{\rho} [\text{Pro}_L(j, \rho_a, \rho) \times \text{Pro}_{L'}(j, \rho, \rho_b)]. \tag{146}$$

This means that the probability of transporting a current j over a distance $L + L'$ between two reservoirs at densities ρ_a and ρ_b is the same (up to boundary effects which give for large L subleading contributions) as the probability of transporting the same current j over a distance L between two reservoirs at densities ρ_a and ρ times the probability of

transporting the current j over a distance L' between two reservoirs at densities ρ and ρ_b . One can then argue that choosing the optimal density ρ makes this probability maximum. From (146) one gets the following additivity property of the large deviation function

$$F_{L+L'}(j, \rho_a, \rho_b) = \min_{\rho} [F_L(j, \rho_a, \rho) + F_{L'}(j, \rho, \rho_b)]. \quad (147)$$

Thus the large deviation function of the current for a system of length $L + L'$ between two reservoirs at densities ρ_a and ρ_b is the same as the sum of the large deviations of two subsystems of lengths L and L' with a fictitious reservoir at density ρ between them.

Suppose that we consider a diffusive system for which we know the two functions $D(\rho)$ and $\sigma(\rho)$ defined in (84) and (85). If one accepts the additivity property (147) of the large deviation function, one can cut the system into more and more pieces so that

$$F_L(j, \rho_a, \rho_b) = \min_{\rho_1, \dots, \rho_{n-1}} \left\{ \sum_{i=0}^{n-1} F_{L/n}(j, \rho_i, \rho_{i+1}) \right\} \quad (148)$$

where $\rho_0 = \rho_a$ and $\rho_n = \rho_b$.

For large n , the optimal choice of the ρ_i 's is such that the differences $\rho_i - \rho_{i+1}$ are small. For a current j of order $1/L$, and for $\rho_i - \rho_{i+1}$ small, one can replace (84) and (85) F_l for $l = L/k$ by

$$F_l(j, \rho_i, \rho_{i+1}) \simeq \frac{[j - (D(\rho_i)(\rho_i - \rho_{i+1})/l)]^2}{2(\sigma(\rho_i)/l)}. \quad (149)$$

In the limit $n \rightarrow \infty$ (keeping $l = L/n$ large for (84) and (85) to be still valid) (148) becomes [52]

$$F_L(j, \rho_a, \rho_b) = \frac{1}{L} \min_{\rho(x)} \left[\int_0^1 \frac{[jL + D(\rho)\rho']^2}{2\sigma(\rho)} dx \right] \quad (150)$$

where the optimal profile $\rho(x)$ (for large n , the optimal ρ_i in (148) is given by $\rho_i = \rho(i/n)$) should satisfy $\rho(0) = \rho_a$ and $\rho(1) = \rho_b$.

One can show [52, 57] that the optimal profile in (150) (when $\rho_a \neq \rho_b$ and the deviation of current j is small enough for this optimal profile to be still monotone) is given by

$$\rho'(x)^2 = \frac{(Lj)^2(1 + 2K\sigma(\rho(x)))}{D^2(\rho(x))} \quad (151)$$

where the constant K is adjusted to ensure that $\rho(0) = \rho_a$ and $\rho(1) = \rho_b$. Replacing $\rho(x)$ by (151) in (150) leads to

$$F_L(j, \rho_a, \rho_b) = j \int_{\rho_b}^{\rho_a} \left[\frac{1 + K\sigma(\rho)}{[1 + 2K\sigma(\rho)]^{1/2}} - 1 \right] \frac{D(\rho)}{\sigma(\rho)} d\rho \quad (152)$$

where the constant K is fixed from (151) by the boundary conditions ($\rho(0) = \rho_a$ and $\rho(1) = \rho_b$)

$$Lj = \int_{\rho_b}^{\rho_a} \frac{D(\rho)}{[1 + 2K\sigma(\rho)]^{1/2}} d\rho. \quad (153)$$

Expressions (152) and (153) give therefore $F_L(j)$ in a parametric form.

The optimal profile (150) remains unchanged when $j \rightarrow -j$ (simply the sign of $[1 + 2K\sigma(\rho)]^{1/2}$ is changed) in (152) and (153) and one gets that (113)

$$F_L(j) - F_L(-j) = -2j \int_{\rho_b}^{\rho_a} \frac{D(\rho)}{\sigma(\rho)} d\rho = -j(\log z_a - \log z_b). \quad (154)$$

Thus the expressions (152) and (153) do satisfy the fluctuation theorem (105).

From (152) and (153) one can calculate $\mu(\lambda)$ by (103) and one gets [52, 57] a parametric form

$$\mu(\lambda, \rho_a, \rho_b) = -\frac{K}{L} \left[\int_{\rho_b}^{\rho_a} \frac{D(\rho) d\rho}{\sqrt{1 + 2K\sigma(\rho)}} \right]^2, \quad (155)$$

with $K = K(\lambda, \rho_a, \rho_b)$ is the solution of

$$\lambda = \int_{\rho_b}^{\rho_a} d\rho \frac{D(\rho)}{\sigma(\rho)} \left[\frac{1}{\sqrt{1 + 2K\sigma(\rho)}} - 1 \right]. \quad (156)$$

One can then get [52], by eliminating K (perturbatively in λ) the expansion of $\mu(\lambda)$ in powers of λ and therefore the cumulants (104) in the long-time limit for arbitrary ρ_a and ρ_b

$$\begin{aligned} \frac{\langle Q_t \rangle}{t} &= \frac{1}{L} I_1, & \frac{\langle Q_t^2 \rangle - \langle Q_t \rangle^2}{t} &= \frac{1}{L} \frac{I_2}{I_1}, & \frac{\langle Q_t^3 \rangle_c}{t} &= \frac{1}{L} \frac{3(I_3 I_1 - I_2^2)}{I_1^3}, \\ \frac{\langle Q_t^4 \rangle_c}{t} &= \frac{1}{L} \frac{3(5I_4 I_1^2 - 14I_1 I_2 I_3 + 9I_2^3)}{I_1^5} \end{aligned} \quad (157)$$

where

$$I_n = \int_{\rho_b}^{\rho_a} D(\rho) \sigma(\rho)^{n-1} d\rho. \quad (158)$$

Using the fact (117) that for the SSEP $D(\rho) = 1$ and $\sigma(\rho) = 2\rho(1-\rho)$, one can recover [52] from (155)–(157) the above expressions (138)–(141) and (144). The validity of (152) and (153) has also been checked for weakly interacting lattice gases [102].

It was understood by Bertini *et al* [103, 104] that the additivity principle (146) and (148) and its consequences (150)–(157) are not always valid. As explained in section 9 the macroscopic fluctuation theory gives the probability (89) of arbitrary (rescaled) density and current profiles $\hat{\rho}, \hat{j}$. Therefore, according to the macroscopic fluctuation theory, to observe (101) an average current j over a long time t one should have

$$F(j) = \lim_{t \rightarrow \infty} \frac{1}{t} L \min_{\hat{\rho}(x,\tau), \hat{j}(x,\tau)} \int_0^{t/L^2} d\tau \int_0^1 dx \frac{\left[\hat{j}(x, \tau) + D(\hat{\rho}(x, \tau)) \frac{\partial \hat{\rho}(x, \tau)}{\partial x} \right]^2}{2\sigma(\hat{\rho}(x, \tau))} \quad (159)$$

with the constraint that

$$jL = \frac{L^2}{t} \int_0^{t/L^2} \hat{j}(x, \tau) d\tau. \quad (160)$$

Comparing (150) and (159) we see that the two expressions coincide when the optimal $\hat{\rho}, \hat{j}$ in (159) are independent of the time τ . Therefore the additivity principle gives the

large deviation function $F(j)$ of the current only when the optimal profile $\widehat{\rho}(x, \tau)$ in (159) is time-independent.

Bertini *et al* [103, 104] pointed out that it can happen, for some $\sigma(\rho)$ and $D(\rho)$, that the expression (150), (152) and (153) is non-convex and therefore cannot be the right expression of the large deviation function $F(j)$ (which is always convex). In such cases, the expression (150) is no longer valid (it becomes [103, 104] simply an upper bound of $F(j)$). This is because the optimal profile in (159) is no longer constant in time. When this optimal profile is time-dependent, one has to solve a much harder optimization problem [57, 105] than (150).

Restrictions on $\sigma(\rho)$ and $D(\rho)$ for (150) to be valid have been given in [104] and there are cases, such as the weakly asymmetric exclusion process (for which the hopping rate q of figure 4 is close to 1: $q - 1 = O(L^{-1})$) on a ring [57, 105], for which by varying λ or the asymmetry one can observe a phase transition between a phase where the optimal profile in (159) is constant in time and a phase where it becomes time-dependent.

14. The matrix approach for the asymmetric exclusion process

The matrix ansatz of section 6 (which gives the weights of the microscopic configurations in the steady state) has been generalized to describe the steady state of several other systems [12, 63], [106]–[126], with of course modified algebraic rules for the matrices the vectors $\langle W|$ and $|V\rangle$.

For example, for the asymmetric exclusion process (ASEP), for which the definition is the same as the SSEP except that particles jump at rate 1 to their right and at rate $q \neq 1$ to their left if the target site is empty (see figure 4), one can show [10, 107, 118, 120] that the weights are still given by (49) with the algebra (51) replaced by

$$DE - qED = D + E \tag{161}$$

$$\langle W|(\alpha E - \gamma D) = \langle W| \tag{162}$$

$$(\beta D - \delta E)|V\rangle = |V\rangle. \tag{163}$$

One should notice that for the ASEP, the direct approach of calculating, as in section 5, the steady state properties by writing the time evolution leads nowhere. Indeed (41) becomes

$$\begin{aligned} \frac{d\langle\tau_1\rangle}{dt} &= \alpha - (\alpha + \gamma + 1)\langle\tau_1\rangle + q\langle\tau_2\rangle + (1 - q)\langle\tau_1\tau_2\rangle \\ \frac{d\langle\tau_i\rangle}{dt} &= \langle\tau_{i-1}\rangle - (1 + q)\langle\tau_i\rangle + q\langle\tau_{i+1}\rangle - (1 - q)(\langle\tau_{i-1}\tau_i\rangle - \langle\tau_i\tau_{i+1}\rangle) \\ \frac{d\langle\tau_L\rangle}{dt} &= \langle\tau_{L-1}\rangle - (q + \beta + \delta)\langle\tau_L\rangle + \delta - (1 - q)\langle\tau_{L-1}\tau_L\rangle \end{aligned} \tag{164}$$

and the equations which determine the one-point functions are no longer closed. Therefore all the correlation functions have to be determined at the same time and this is what the matrix ansatz (49) does. Alternative combinatorial methods to calculate the steady state weights of exclusion processes with open boundary conditions have been obtained in [127, 128].

The large deviation function \mathcal{F} of the density defined by (68) has been calculated for the ASEP [28, 53, 54] by an extension of the approach of sections 7 and 8 (see section 16).

15. The phase diagram of the totally asymmetric exclusion process

The last three sections 15–17 present, as examples, three results which can be obtained rather easily from the matrix ansatz (161)–(163) for the totally asymmetric case (TASEP), i.e. for $q = 0$ (in the particular case where particles are injected only at the left boundary and removed only at the right boundary, i.e. when the input rates $\gamma = \delta = 0$). In this case the algebra (161) becomes

$$DE = D + E \tag{165}$$

$$\langle W|\alpha E = \langle W| \tag{166}$$

$$\beta D|V\rangle = |V\rangle. \tag{167}$$

As for the SSEP the average current $\langle J \rangle$ is still given in terms of the vectors $\langle W|, |V\rangle$ and of the matrices D and E by

$$\langle J \rangle = \frac{\langle W|(D + E)^{L-1}|V\rangle}{\langle W|(D + E)^L|V\rangle}. \tag{168}$$

However, as the algebraic rules have changed, the expression of the current is different for the SSEP and the ASEP. From the relation $DE = D + E$ it is easy to prove by recurrence that

$$DF(E) = F(1)D + E \frac{F(E) - F(1)}{E - 1}$$

for any polynomial $F(E)$ and

$$(D + E)^N = \sum_{p=1}^N \frac{p(2N - 1 - p)!}{N!(N - p)!} (E^p + E^{p-1}D + \dots + D^p).$$

Using the fact that

$$\frac{\langle W|E^m D^n|V\rangle}{\langle W|V\rangle} = \frac{1}{\alpha^m} \frac{1}{\beta^n},$$

one gets [10]

$$\frac{\langle W|(D + E)^N|V\rangle}{\langle W|V\rangle} = \sum_{p=1}^N \frac{p(2N - 1 - p)!}{N!(N - p)!} \frac{1/\alpha^{p+1} - 1/\beta^{p+1}}{1/\alpha - 1/\beta}. \tag{169}$$

For large N this sum is dominated either by $p \sim 1$, or $p \sim N$ depending on the values of α and β and one obtains

$$\frac{\langle W|(D + E)^N|V\rangle}{\langle W|V\rangle} \sim \begin{cases} 4^N & \text{if } \alpha > \frac{1}{2} & \text{and } \beta > \frac{1}{2} \\ [\beta(1 - \beta)]^{-N} & \text{if } \beta < \alpha & \text{and } \beta < \frac{1}{2} \\ [\alpha(1 - \alpha)]^{-N} & \text{if } \beta > \alpha & \text{and } \alpha < \frac{1}{2}. \end{cases} \tag{170}$$

This leads to three different expressions of the current (168) for large L , corresponding to the three different phases:

- the low density phase ($\beta > \alpha$ and $\alpha < \frac{1}{2}$) where $\langle J \rangle = \alpha(1 - \alpha)$;
- the high density phase ($\alpha > \beta$ and $\beta < \frac{1}{2}$) where $\langle J \rangle = \beta(1 - \beta)$;
- the maximal current phase ($\alpha > \frac{1}{2}$ and $\beta > \frac{1}{2}$) where $\langle J \rangle = \frac{1}{4}$;

which is the exact phase diagram of the TASEP [9]–[11], [32]. The existence of phase transitions [65], [67]–[69] in these driven lattice gases is one of the striking properties of non-equilibrium steady states, as it is well known that one-dimensional systems at equilibrium with short-range interactions cannot exhibit phase transitions.

16. Additivity and large deviation function for the TASEP

Let us now see how the additivity relation (61) can be generalized for the TASEP in order to obtain the large deviation functional of the density. For the algebra (165), if one introduces the following eigenvectors

$$\langle \rho | E = \frac{1}{\rho} \langle \rho |; \quad D | \rho \rangle = \frac{1}{1 - \rho} | \rho \rangle \tag{171}$$

it is clear that

$$\langle W | = \langle \rho_a |; \quad | V \rangle = | \rho_b \rangle \tag{172}$$

with $\rho_a = \alpha$ and $\rho_b = 1 - \beta$. Note that in general $\langle \rho_a | \rho_b \rangle \neq 0$ even when $\rho_a \neq \rho_b$. Now one can prove, as in (61), that for $\rho_b < \rho_a$

$$\frac{\langle \rho_a | Y_1 Y_2 | \rho_b \rangle}{\langle \rho_a | \rho_b \rangle} = \oint_{\rho_b < |\rho| < \rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)}{(\rho_a - \rho)(\rho - \rho_b)} \frac{\langle \rho_a | Y_1 | \rho \rangle}{\langle \rho_a | \rho \rangle} \frac{\langle \rho | Y_2 | \rho_b \rangle}{\langle \rho | \rho_b \rangle} \tag{173}$$

where Y_1 and Y_2 are arbitrary polynomials in D and E .

Proof of (173). Any polynomial Y of the operators D and E can be written, using $DE = D + E$, as

$$Y = \sum_{n,n'} a_{n,n'} E^n D^{n'} \tag{174}$$

by pushing all the D 's to the right and all the E s to the left. Therefore to prove (173) it is sufficient to do it for Y_1 and Y_2 of the form

$$Y_1 = E^{n_1} D^{n'_1}, \quad Y_2 = E^{n_2} D^{n'_2} \tag{175}$$

If $n'_1 = 0$ or $n_2 = 0$, the identity (173) is easy to check. Then one can prove it by recursion on $n'_1 + n_2$: if $Y_1 = Z_1 D$ and $Y_2 = E Z_2$, and one assumes that the identity (173) is valid for $Z_1 D Z_2$ and $Z_1 E Z_2$, the lhs of (173) can be written as (165)

$$\begin{aligned} \frac{\langle \rho_a | Z_1 D E Z_2 | \rho_b \rangle}{\langle \rho_a | \rho_b \rangle} &= \frac{\langle \rho_a | Z_1 (D + E) Z_2 | \rho_b \rangle}{\langle \rho_a | \rho_b \rangle} = \oint_{\rho_b < |\rho| < \rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)}{(\rho_a - \rho)(\rho - \rho_b)} \left[\frac{1}{\rho} + \frac{1}{1 - \rho} \right] \\ &\times \frac{\langle \rho_a | Z_1 | \rho \rangle}{\langle \rho_a | \rho \rangle} \frac{\langle \rho | Z_2 | \rho_b \rangle}{\langle \rho | \rho_b \rangle} \end{aligned}$$

and simply because $1/\rho + 1/(1 - \rho) = 1/(\rho(1 - \rho))$ this becomes

$$\oint_{\rho_b < |\rho| < \rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)}{(\rho_a - \rho)(\rho - \rho_b)} \frac{1}{\rho(1 - \rho)} \frac{\langle \rho_a | Z_1 | \rho \rangle \langle \rho | Z_2 | \rho_b \rangle}{\langle \rho_a | \rho \rangle \langle \rho | \rho_b \rangle}$$

$$= \oint_{\rho_b < |\rho| < \rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)}{(\rho_a - \rho)(\rho - \rho_b)} \frac{\langle \rho_a | Z_1 D | \rho \rangle \langle \rho | E Z_2 | \rho_b \rangle}{\langle \rho_a | \rho \rangle \langle \rho | \rho_b \rangle}$$

which is the rhs of (173). □

We are now going to see, as an example, how the large deviation function \mathcal{F} of the density can be derived for the TASEP from (173) when $\rho_a > \rho_b$. If one defines $K(\rho_a, \rho_b)$ by

$$K(\rho_a, \rho_b) = \lim_{L \rightarrow \infty} \frac{1}{L} \log \frac{\langle \rho_a | (D + E)^L | \rho_b \rangle}{\langle \rho_a | \rho_b \rangle} \tag{176}$$

one can easily check from (170) that for $\rho_b (= 1 - \beta) < \rho_a (= \alpha)$

$$K(\rho_a, \rho_b) = - \max_{\rho_b < \rho < \rho_a} \log(\rho(1 - \rho)). \tag{177}$$

Using a saddle-point method in (173) when Y_1 and Y_2 are sums of long products of D 's and E s, one gets

$$\frac{\langle \rho_a | Y_1 Y_2 | \rho_b \rangle}{\langle \rho_a | \rho_b \rangle} \simeq \min_{\rho_b \leq F \leq \rho_a} \frac{\langle \rho_a | Y_1 | F \rangle \langle F | Y_2 | \rho_b \rangle}{\langle \rho_a | F \rangle \langle F | \rho_b \rangle}. \tag{178}$$

(Note that in applying the saddle-point method, one needs to find the maximum F over the circular integration contour. This maximum is at the same time a *minimum* when F varies along the real axis.) Then as for a system of large size L (176) and (177) one has

$$\frac{\langle \rho_a | Y | \rho_b \rangle}{\langle \rho_a | (D + E)^L | \rho_b \rangle} \sim e^{-K(\rho_a, \rho_b)L} \frac{\langle \rho_a | Y | \rho_b \rangle}{\langle \rho_a | \rho_b \rangle}. \tag{179}$$

One can, of course, repeat (178) several times to relate a large system of size L to its subsystems (as long as these subsystems are large). Therefore one gets

$$\frac{\langle \rho_a | Y_1 Y_2 \cdots Y_k | \rho_b \rangle}{\langle \rho_a | (D + L)^L | \rho_b \rangle} \sim e^{-K(\rho_a, \rho_b)L} \min_{\rho_a \geq F_1 \geq F_2 \geq \cdots \geq F_{n-1} > \rho_b} \prod_{i=1}^n \left[\frac{\langle F_{i-1} | Y_i | F_i \rangle}{\langle F_{i-1} | (D + E)^l | F_i \rangle} e^{K(F_{i-1}, F_i)l} \right] \tag{180}$$

where $F_0 = \rho_a$, $F_n = \rho_b$ and $l = L/n$. If Y_i is the sum of the matrix elements of all configurations of l sites with $l\rho_i$ particles one gets for the large deviation function \mathcal{F}_n defined in (15)

$$\mathcal{F}_n(\rho_1, \rho_2, \dots, \rho_n | \rho_a, \rho_b)$$

$$= K(\rho_a, \rho_b) + \max_{\rho_b = F_0 < F_1 < \cdots < F_i < \cdots < F_n = \rho_a} \frac{1}{n} \sum_{i=1}^n \mathcal{F}_1(\rho_i | F_{i-1}, F_i) - K(F_{i-1}, F_i). \tag{181}$$

For large n , almost all the differences $F_{i-1} - F_i$ are small, so that

$$\mathcal{F}_1(\rho_i | F_{i-1}, F_i) \simeq \mathcal{F}_1(\rho_i | F_i, F_i) = \rho_i \log \frac{\rho_i}{F_i} + (1 - \rho_i) \log \frac{1 - \rho_i}{1 - F_i} \equiv B(\rho_i, F_i)$$

since when the two densities F_{i-1} and F_i are equal, the steady state measure is Bernoulli and this leads to

$$\mathcal{F}(\{\rho(x)\}) = - \max_{\rho_b < r < \rho_a} [\log(r(1-r))] + \sup_F \int_0^1 dx [B(\rho(x), F(x)) + \log(F(x)(1-F(x)))] \tag{182}$$

which is the expression of the large deviation function of the density of the TASEP (and also of the ASEP [53, 54]) for $\rho_a > \rho_b$.

For $\rho_a > \rho_b$, one can also obtain [28, 53, 54] this large deviation function, starting from a relation similar to (173) obtained by deforming the circular contour to ensure that ρ_b remains inside and ρ_a outside. One can note that, when Y_1 and Y_2 are polynomials in D and E , all the matrix elements in (173) are rational functions of ρ_a and ρ_b which can be easily analytically continued from the case $\rho_a > \rho_b$ to the case $\rho_a < \rho_b$. The result is [53, 54]

$$\mathcal{F}(\{\rho(x)\}) = \inf_{0 < y < 1} \left[\int_0^y dx \left(B(\rho(x), \rho_a) + \log \frac{\rho_a(1-\rho_a)}{\langle J \rangle} \right) + \int_y^1 dx \left(B(\rho(x), \rho_b) + \log \frac{\rho_b(1-\rho_b)}{\langle J \rangle} \right) \right] \tag{183}$$

For the TASEP one knows [10, 11] that along the line $\rho_a = 1 - \rho_b < \frac{1}{2}$ there is a first-order phase transition line. Along this line $\langle J \rangle = \rho_a(1 - \rho_a) = \rho_b(1 - \rho_b)$ and the typical configurations $\rho_z(x)$ are shocks [115, 117, 129] located at arbitrary positions z between a region of density ρ_a and a region of density $1 - \rho_a$

$$\rho_z(x) = \begin{cases} \rho_a & \text{for } 0 < x < z \\ 1 - \rho_a & \text{for } z < x < 1. \end{cases} \tag{184}$$

For all these profiles $\rho_z(x)$, the functional (183) vanishes. It is also easy to check that $\mathcal{F}(\rho(x)) > 0$ for a profile of the form

$$\rho(x) = \alpha \rho_z(x) + (1 - \alpha) \rho_{z'}(x) \tag{185}$$

and this shows that \mathcal{F} is non-convex. Therefore, in contrast to equilibrium systems (24), the functional $\mathcal{F}(\rho(x))$ may be non-convex in non-equilibrium steady states.

17. Correlation functions in the TASEP and Brownian excursions

In this last example, we will see that the fluctuations of the density are non-Gaussian in the maximal current phase of the TASEP. In this maximal current phase ($\alpha > \frac{1}{2}$ and $\beta > \frac{1}{2}$) one can show [55], using the matrix ansatz, that the correlation function of the occupations of k sites at positions $i_1 = Lx_1, i_2 = Lx_2, \dots, i_k = Lx_k$ with $x_1 < x_2 < \dots < x_k$ are given by

$$\left\langle \left(\tau_{Lx_1} - \frac{1}{2} \right) \dots \left(\tau_{Lx_k} - \frac{1}{2} \right) \right\rangle = \frac{1}{2^k} \frac{1}{L^{k/2}} \frac{d^k}{dx_1 \dots dx_k} \langle y(x_1) \dots y(x_k) \rangle, \tag{186}$$

where $y(x)$ is a Brownian excursion between 0 and 1 (a Brownian excursion is a Brownian path constrained to $y(x) > 0$ for $0 < x < 1$ with the boundaries $y(0) = y(1) = 0$). The

probability $P(y_1 \dots y_k; x_1 \dots x_k)$ of finding the Brownian excursion at positions $y_1 \dots y_k$ for $0 < x_1 < \dots < x_k < 1$ is

$$P(y_1 \dots y_k; x_1 \dots x_k) = \frac{h_{x_1}(y_1)g_{x_2-x_1}(y_1, y_2) \dots g_{x_k-x_{k-1}}(y_{k-1}, y_k)h_{1-x_k}(y_k)}{\sqrt{\pi}}, \quad (187)$$

where h_x and g_x are defined by

$$\begin{cases} h_x(y) = \frac{2y}{x^{3/2}}e^{-y^2/x} \\ g_x(y, y') = \frac{1}{\sqrt{\pi x}}(e^{-(y-y')^2/x} - e^{-(y+y')^2/x}). \end{cases}$$

One can derive easily (186) in the particular case $\alpha = \beta = 1$ using a representation of (165) which consists of two infinite-dimensional bidiagonal matrices

$$D = \sum_{n \geq 1} |n\rangle\langle n| + |n\rangle\langle n+1| = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 1 & 0 & 0 & 0 & \dots \\ 0 & 0 & 1 & 1 & 0 & 0 & \dots \\ 0 & 0 & 0 & 1 & 1 & 0 & \dots \\ & & & & \ddots & \ddots & \ddots \end{pmatrix}$$

$$E = \sum_{n \geq 1} |n\rangle\langle n+1| + |n\rangle\langle n| = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & \dots \\ 1 & 1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 1 & 0 & 0 & 0 & \dots \\ 0 & 0 & 1 & 1 & 0 & 0 & \dots \\ & & & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

with

$$\begin{aligned} \langle W| = \langle 1| &= (1, 0, 0 \dots) \\ \langle V| = \langle 1| &= (1, 0, 0 \dots). \end{aligned}$$

With this representation one can write $\langle W|(D + E)^L|V\rangle$ as a sum over a set \mathcal{M}_L of one-dimensional random walks w of L steps which remain positive. Each walk w is defined by a sequence $(n_i(w))$ of $L - 1$ heights ($n_i(w) \geq 1$) (with at the boundaries $n_0(w) = n_L(w) = 1$ and the constraint $|n_{i+1} - n_i| \leq 1$):

$$\langle W|(D + E)^L|V\rangle = \sum_{w \in \mathcal{M}_L} \Omega(w),$$

where

$$\Omega(w) = \prod_{i=1}^L v(n_{i-1}, n_i) \quad \text{with } v(n, n') = \begin{cases} 2 & \text{if } |n - n'| = 0 \\ 1 & \text{if } |n - n'| = 1. \end{cases}$$

One has $v(n, n') = \langle n|D + E|n'\rangle$ since $D + E$ has a tridiagonal form

$$D + E = \begin{pmatrix} 2 & 1 & & (0) \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ (0) & & 1 & 2 \end{pmatrix}.$$

Then from the matrix expression one gets $\langle \tau_i \rangle$ and $\langle \tau_i \tau_j \rangle$:

$$\left\langle \left(\tau_{i_1} - \frac{1}{2} \right) \cdots \left(\tau_{i_k} - \frac{1}{2} \right) \right\rangle = \frac{1}{2^k} \sum_w \nu(w) (n_{i_1} - n_{i_1-1}) \cdots (n_{i_k} - n_{i_k-1}), \quad (188)$$

where $\nu(w)$ is the probability of the walk w induced by the weights Ω :

$$\nu(w) = \frac{\Omega(w)}{\sum_w \Omega(w')}.$$

The expression (188) is the discrete version of (186).

The result (186) can be extended [55] to arbitrary values of α and β in the maximal current phase (i.e. for $\alpha > 1/2$ and $\beta > 1/2$). From (186) one can, in particular, recover the leading $1/L$ correction to the flat profile [130]

$$\left\langle \tau_i - \frac{1}{2} \right\rangle \simeq \frac{1}{2\sqrt{\pi L}} \frac{1 - 2x}{\sqrt{x(1-x)}}$$

for $i = Lx$.

From this link between the density fluctuations and Brownian excursions, one can also show that, for a TASEP of L sites, the number N of particles between sites Lx_1 and Lx_2 , has non-Gaussian fluctuations in the maximal current phase: if one defines the reduced density

$$\mu = \frac{N - L(x_2 - x_1)/2}{\sqrt{L}} \quad (189)$$

one can show [55] that for large L

$$P(\mu) = \int_0^\infty dy_1 \int_0^\infty dy_2 \frac{1}{\sqrt{2\pi(x_2 - x_1)}} \exp\left(-\frac{(2\mu + y_1 - y_2)^2}{x_2 - x_1}\right). \quad (190)$$

This contrasts with the Gaussian fluctuations of the density (25) at equilibrium. According to numerical simulations [55] the distribution (189) and (190) (properly rescaled) of the fluctuations of the density remains valid for more general driven systems in their maximal current phase. Of course, proving it in a more general case is an interesting open question.

18. Conclusion

These lectures have presented a number of recent results concerning the fluctuations and the large deviation functions of the density or of the current in non-equilibrium steady states.

For general diffusive systems, the macroscopic fluctuation theory [42]–[45], [103, 104] discussed in section 9 gives a framework to calculate the large deviation of the density $\mathcal{F}(\rho(x))$ leading to equations (97), (96) and (95) which are, in general, difficult to solve. One can, however, check that the expressions (72), (73) and (79) obtained [26, 27] in sections 6–8 by the matrix ansatz do solve these equations. So far the large deviation functional is only known for very few examples [26]–[28], [86]. There remains a lot to be done to understand the general properties of the functional $\mathcal{F}(\rho(x))$. For example, with

Thierry Bodineau we tried, so far without success, to calculate $\mathcal{F}(\rho(x))$ (97), (96) and (95) for general D and σ in powers of $\rho_a - \rho_b$. Also for the SSEP, we did not succeed in obtaining the large deviation functional of the density $\mathcal{F}(\rho(x))$ for the λ -measure defined in (130). Other situations which would be interesting to consider are the cases of several species of particles, several conserved quantities [131, 132] or non-conserved quantities [133].

For driven diffusive systems, the situation is worse: so far $\mathcal{F}(\rho(x))$ is only known for the ASEP [53, 54] and, to my knowledge, there does not exist so far a general theory to calculate this large deviation functional for general driven diffusive systems [134]. In contrast to equilibrium systems, for the ASEP, the large deviation functional may be non-convex (section 16) or fluctuations of the density may be non-Gaussian (section 17).

For current fluctuations in diffusive systems, the additivity principle gives explicit expressions (section 13) of the large deviation function of the current for general diffusive systems. In some cases, however, these expressions are not valid, when the profile to produce a deviation of current becomes time-dependent. In such cases the calculation of the large deviation function $F(j)$ of the current is much harder [57]. So far the predictions (150), (152), (153), (155)–(157) of the additivity principle remain to be checked in specific examples: even for the SSEP, only the first four cumulants are known to agree with (157) but a direct calculation of $F(j)$ for the SSEP is, to my knowledge, still missing. It would be nice to see whether this could be done by a Bethe ansatz calculation for the SSEP with open boundaries [135]. It would also be useful to test the predictions of the additivity principle on other diffusive systems and to try to extend them to more complicated situations, in particular when there is more than a single conserved quantity [131, 132].

Concerning the fluctuations or the large deviations of the current of driven diffusive systems, there has been lots of progress over the last ten years [136]–[141]. On the infinite line exact results for the TASEP and the PNG (polynuclear growth model) lead to a universal distribution of current characteristic of the KPZ universality class. On the ring too, Bethe ansatz calculations [66, 97, 98], [142]–[150], allow us to calculate the large deviation function of the current which exhibits a universal shape in the scaling regime. For driven diffusive systems, however, there is not yet a general approach allowing us to calculate the large deviation function or the fluctuations of the current for all geometries, including finite systems with open boundary conditions [135]. Of course it would be nice to extend the macroscopic fluctuation theory to get a framework allowing us to calculate both the large deviation functions of the current and of the density for general driven diffusive systems.

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