Work, dissipation, and fluctuations in nonequilibrium physics

Cumulants and large deviations of the current through non-equilibrium steady states ☆

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Abstract

Using a generalisation of detailed balance for systems maintained out of equilibrium by contact with 2 reservoirs at unequal temperatures or at unequal densities, one can recover the fluctuation theorem for the large deviation function of the current. For large diffusive systems, we show how the large deviation function of the current can be computed using a simple additivity principle. The validity of this additivity principle and the occurrence of phase transitions are discussed in the framework of the macroscopic fluctuation theory. ***To cite this article: T. Bodineau, B. Derrida, C. R. Physique 8 (2007).***
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Résumé

Cumulants et grandes déviations du courant dans des états stationnaires hors équilibre. En généralisant la relation de bilan détaillé à des systèmes maintenus hors équilibre par contact avec deux réservoirs à des températures ou à des densités différentes, nous retrouvons le théorème de fluctuations pour la fonction de grandes déviations du courant. Pour de grands systèmes diffusifs, nous montrons comment la fonction de grandes déviations du courant peut être calculée simplement à l'aide d'un principe d'additivité. La validité de ce principe d'additivité et l'existence de transitions de phase sont discutées dans le cadre d'une théorie des fluctuations à l'échelle macroscopique. ***Pour citer cet article : T. Bodineau, B. Derrida, C. R. Physique 8 (2007).***
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1. Introduction

A physical system in contact with two heat baths at unequal temperatures T_a and T_b is one of the simplest situations for which one can observe a non-equilibrium steady state (Fig. 1). At equilibrium, i.e. when the two heat baths are at
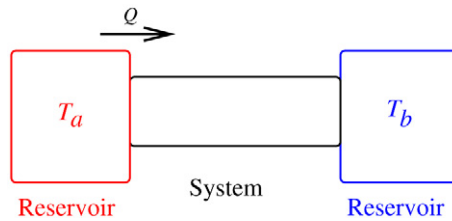
Fig. 1. A system maintained in contact with two heat baths at unequal temperatures reaches in the long time limit a non-equilibrium steady state.
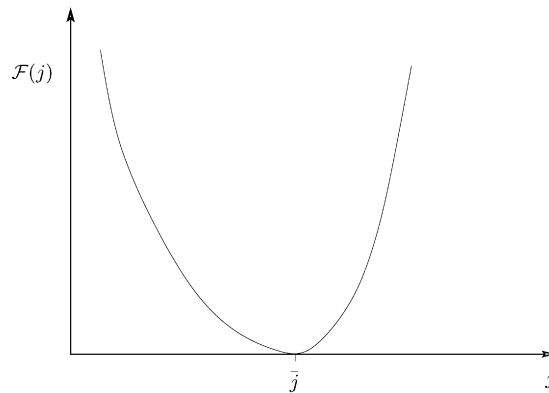

Fig. 2. A typical shape of the large deviation function $\mathcal{F}(j)$ which vanishes at the typical current $\bar{j}$.

the same temperature ($T_a = T_b = T$), the probability $P(C)$ of finding the system in a given microscopic configuration C is given by the usual Boltzmann–Gibbs weight

$$P(C) = Z^{-1} \exp\left[-\frac{E(C)}{kT}\right] \tag{1}$$

where $E(C)$ is the internal energy of the system in configuration C. Over the whole 20th century, studies in equilibrium statistical mechanics have been based on this expression or its microcanonical counterpart, and the great success of the theory was to show that (1) was the right starting point to explain the equilibrium properties of a large variety of physical systems (fluids, magnets, alloys, plasmas, ...) and to understand all kinds of effects, in particular phase transitions and critical phenomena. A very simplifying aspect of (1) is that it depends neither on the precise nature of the coupling with the heat bath (at least when this coupling is weak) nor on the detailed dynamics of the system.

As soon as the two temperatures T_a and T_b are different [1], there is not such a simple expression [2,3] which generalizes (1) for the steady state weights $P(C)$ of the microscopic configurations. In fact, for a non-equilibrium system, the steady state measure $P(C)$ depends in general on the precise description of the dynamics of the system, of the heat baths and on their couplings. So far the exact expression of these weights is known only for a few non-equilibrium models [4–7].

In addition to the steady state weights, one might be interested in the flow of energy through the system. For an interval of time t, one may consider Q_t, the energy transfered from the heat bath at temperature T_a to the system. In the steady state, this energy fluctuates and one might try to predict its various *cumulants* $\langle Q_t^n \rangle_c$ or *its large deviation function* $\mathcal{F}(j)$ defined as

$$\mathrm{Pro}\left(\frac{Q_t}{t} = j\right) \sim \exp\left[-t\mathcal{F}(j)\right] \quad \text{for large } t \tag{2}$$

A typical shape of this large deviation function is shown in Fig. 2.

We refer to [8,9] for a full account on the large deviation theory. Note also that other definitions of the current distribution have been considered in [10,11].

The whole distribution of Q_t and a fortiori its cumulants depend in principle on the initial configuration $C_{initial}$, on the final configuration C_{final} and on the place where the flux of energy is measured. However if the internal energy of the system is bounded ($\max_C |E(C)| < \infty$), the cumulants of Q_t (in the long time limit) and the large deviation function $\mathcal{F}(j)$ do not depend on where the flow of energy is measured. In particular, if one measures the flux of energy between the system and the other heat bath, the large deviation function $\mathcal{F}(j)$ is unchanged. Also if the system relaxes faster than the time t over which Q_t is measured, the cumulants $\langle Q_t^n \rangle_c$ divided by t and the large deviation function $\mathcal{F}(j)$ do not depend on the initial and final configurations $C_{initial}, C_{final}$. In fact in this case it is elementary to verify that $\mathcal{F}(j)$ is *convex*, that is if $0 \leqslant \alpha \leqslant 1$

$$\mathcal{F}\big(\alpha j_1 + (1 - \alpha) j_2\big) \leqslant \alpha \mathcal{F}(j_1) + (1 - \alpha)\mathcal{F}(j_2) \tag{3}$$

as the probability distribution $\mathrm{Pro}(Q_t | C_{initial}, C_{final})$ of Q_t, given the initial and final configurations $C_{initial}$ and C_{final}, satisfies

$$\mathrm{Pro}(Q | C_{initial}, C_{final}) = \sum_{C_\tau} \sum_q \mathrm{Pro}(q | C_{initial}, C_\tau)\,\mathrm{Pro}(Q - q | C_\tau, C_t)$$
$$\geqslant \mathrm{Pro}(q | C_{initial}, C_\tau)\,\mathrm{Pro}(Q - q | C_\tau, C_{final})$$

which leads to (3) in the long time limit when $\tau = \alpha t$, $q = j_1 \alpha t$, $Q - q = j_2(1 - \alpha)t$. The importance of convexity was understood in [12] (see Section 5 below).

It is sometimes easier to work with the generating function of Q_t. For large t one has

$$\big\langle e^{\lambda Q_t} \big\rangle \sim e^{t\mu(\lambda)} \tag{4}$$

where $\langle \cdot \rangle$ denotes the expectation over the dynamics and $\mu(\lambda)$ is the Legendre transform of the large deviation function $\mathcal{F}$

$$\mu(\lambda) = \max_j \big[j\lambda - \mathcal{F}(j) \big] \tag{5}$$

From the knowledge of $\mu(\lambda)$, one can often determine the cumulants of Q_t in the long time limit by

$$\lim_{t \to \infty} \frac{\langle Q_t^n \rangle_c}{t} = \frac{d^n \mu(\lambda)}{d\lambda^n}\bigg|_{\lambda=0} \tag{6}$$

This relation is based on the assumption that the order of the limits $t \to \infty$ and $\lambda \to 0$ can be exchanged. One can show that these limits can be exchanged only for very few examples, although one believes that the assumption remains valid for general diffusive systems. There are however cases where these limits do not commute and for which the moments of the fluctuations cannot be deduced from the knowledge of the large deviation function [13].

2. Generalized detailed balance and the fluctuation theorem

In principle, determining the evolution of Q_t requires the integration of the evolution equations of the system in presence of the heat baths. This is a difficult task, in particular because the heat baths are often described by an infinite number of degrees of freedom. Nevertheless, it can be shown in some cases that integrating the variables of the heat baths leads to effective reservoirs with stochastic noise. We refer to [14,15] and references therein for various ways of describing thermostats.

Instead of considering mechanical systems, it is simpler to model the interactions with the heat baths by a stochastic term in the equations of motion of the system (like in a Langevin equation). The microscopic dynamics becomes then stochastic. This means that the evolution is given by a Markov chain with 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 $W(C', C)\,dt$).

At equilibrium, one usually requires that the transition matrix satisfies *detailed balance*

$$W(C', C)e^{-\frac{E(C)}{T}} = W(C, C')e^{-\frac{E(C')}{T}} \tag{7}$$

which ensures the time reversal symmetry of the microscopic dynamics. If one introduces q the energy transfered from the heat bath at temperature T to the system, and $W_q(C', C)\, \mathrm{d}t$, the probability that the system jumps during $\mathrm{d}t$ from C to C' by receiving an energy q from the heat bath, one can rewrite (7)

$$\mathrm{e}^{\frac{q}{T}} W_q(C', C) = W_{-q}(C, C') \tag{8}$$

If one accepts that detailed balance gives a good description of the coupling with a single heat bath at temperature T, one can wonder what would be the right way of describing the dynamics of a system coupled to several heat baths at unequal temperatures like in Fig. 1. When the system jumps from one configuration C to another configuration C', energies $q_a, q_b, q_c, \ldots$ are transferred from the heat baths at temperatures $T_a, T_b, T_c, \ldots$ to the system. The straightforward generalization of (8) is

$$\mathrm{e}^{\frac{q_a}{T_a} + \frac{q_b}{T_b} + \frac{q_c}{T_c} + \cdots} W_{q_a, q_b, q_c, \ldots}(C', C) = W_{-q_a, -q_b, -q_c, \ldots}(C, C') \tag{9}$$

For a system in contact with several reservoirs at temperature $T_a, T_b, T_c, \ldots$, this simply means, by comparing with (8), that the exchanges of energy with the heat bath at temperature T_a tend to equilibrate the system at temperature T_a, the exchanges with the heat bath at temperature T_b tend to equilibrate the system at temperature T_b and so on.

The fluctuation theorem [16,17] can be easily recovered from the *generalized detailed balance relation* (9). To see this, one can compare the probability of a trajectory in phase space and its time reversal for a system in contact with two reservoirs. Similar approaches have been implemented for stochastic dynamics in [18–21]. A trajectory '*Traj*' is specified by a sequence of successive configurations $C_1, \ldots, C_k$ visited by the system, the times $t_1, \ldots, t_k$ spent in each of these configurations, and the energies $q_{a,i}, q_{b,i}$ transfered from the heat baths to the system when the system jumps from C_i to C_{i+1}.

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

where $r(C) = \sum_{C'} \sum_{q_a, q_b} W_{q_a, q_b}(C', C)$ and $\mathrm{d}t$ 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 $C_k, \ldots, C_1$, exchanging the energies $-q_{a,i}, -q_{b,i}$ each time the system jumps from C_{i+1} to C_i, one has

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

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

$$\frac{\mathrm{Pro}(Traj)}{\mathrm{Pro}(-Traj)} = \exp\left[-\sum_{i=1}^{k-1} \frac{q_{a,i}}{T_a} + \frac{q_{b,i}}{T_b} \right] = \exp\left[-\frac{Q_t^{(a)}}{T_a} - \frac{Q_t^{(b)}}{T_b} \right] \tag{10}$$

where $Q_t^{(a)} = \sum_i q_{a,i}$ and $Q_t^{(b)} = \sum_i q_{b,i}$ are the total energies transfered from the heat baths a and b to the system during time t. If the internal energy of the system is bounded, energy conservation implies that $|Q_t^{(a)} + Q_t^{(b)}| < E$, and one gets

$$\exp\left[Q_t^{(a)} \left(\frac{1}{T_b} - \frac{1}{T_a} \right) - \frac{E}{T_b} \right] < \frac{\mathrm{Pro}(Traj)}{\mathrm{Pro}(-Traj)} < \exp\left[Q_t^{(a)} \left(\frac{1}{T_b} - \frac{1}{T_a} \right) + \frac{E}{T_b} \right] \tag{11}$$

If $P(C)$ is the steady state probability of configuration C, the probability that $Q_t \equiv Q_t^{(a)}$ is the total energy transfered from the heat bath a to the system is given by

$$\mathrm{Pro}(Q_t) = \sum_{C_{\mathrm{initial}}} \sum_{C_{\mathrm{final}}} \sum_{Traj(C_{\mathrm{initial}}, C_{\mathrm{final}}, Q_t)} P(C_{\mathrm{initial}}) \, \mathrm{Pro}\big(Traj(C_{\mathrm{initial}}, C_{\mathrm{final}}, Q_t)\big)$$

where the sums are over all initial configurations C_{initial}, final configurations C_{final} and all trajectories $Traj(C_{\mathrm{initial}}, C_{\mathrm{final}}, Q_t)$ starting in configuration C_{initial}, ending in configuration C_{final} with a total transfer of energy Q_t. Now as

$$\mathrm{Pro}(-Q_t) = \sum_{C_{\mathrm{initial}}} \sum_{C_{\mathrm{final}}} \sum_{Traj(C_{\mathrm{final}}, C_{\mathrm{initial}}, -Q_t)} P(C_{\mathrm{final}}) \, \mathrm{Pro}\big(Traj(C_{\mathrm{final}}, C_{\mathrm{initial}}, -Q_t)\big)$$

one can see that, if for any pair of configurations the ratio of their steady state weights remains bounded

$$\forall C, C' \quad 0 < A < \frac{P(C)}{P(C')} < B < \infty$$

one has because of (11) that

$$\frac{A}{B} \exp\left[-\frac{E}{T_b} + Q_t\left(\frac{1}{T_b} - \frac{1}{T_a}\right)\right] < \frac{\mathrm{Pro}(Q_t)}{\mathrm{Pro}(-Q_t)} < \frac{B}{A} \exp\left[\frac{E}{T_b} + Q_t\left(\frac{1}{T_b} - \frac{1}{T_a}\right)\right]$$

Taking the log and then the long time limit (2) leads to the *fluctuation theorem*

$$\mathcal{F}(j) - \mathcal{F}(-j) = -j\left(\frac{1}{T_b} - \frac{1}{T_a}\right) \tag{12}$$

which states that the difference $\mathcal{F}(j) - \mathcal{F}(-j)$ is linear in j with a universal slope related to the difference of the inverse temperatures.

We see that in the framework of stochastic dynamics, the fluctuation theorem is an elementary consequence of the generalized detailed balance relation (9) satisfied by the dynamics and of the assumptions that the energy is bounded (see [22–24] for examples where the energy is not bounded in which case the fluctuation theorem has to be modified) and the fact that the time t is much longer than the relaxation times in the system. In terms of the Legendre transform (4), (5) the fluctuation theorem becomes

$$\mu(\lambda) = \mu\left(-\lambda + \frac{1}{T_a} - \frac{1}{T_b}\right) \tag{13}$$

Remarks:

(i) In the limit of small $T_a - T_b$ (i.e. close to equilibrium), one can recover from (13) the fluctuation–dissipation relation between the variance of the current at equilibrium

$$\frac{\langle Q_t^2 \rangle}{t} \to \tilde{\sigma} \quad \text{for } T_a = T_b \tag{14}$$

and the response to a small temperature gradient

$$\frac{\langle Q_t \rangle}{t} \to (T_a - T_b)\tilde{D} \quad \text{for } T_a - T_b \text{ small} \tag{15}$$

In fact from these definitions of $\tilde{\sigma}$ and $\tilde{D}$, one has

$$\mu(\lambda) = (T_a - T_b)\tilde{D}\lambda + \frac{\tilde{\sigma}}{2}\lambda^2 + \mathrm{O}\left(\lambda^3, \lambda^2(T_a - T_b), \lambda(T_a - T_b)^2\right) \tag{16}$$

and for this expression to satisfy the fluctuation theorem (13), the coefficients $\tilde{\sigma}$ and $\tilde{D}$ have to satisfy

$$\tilde{\sigma} = 2T_a^2 \tilde{D} \tag{17}$$

which is the usual Einstein fluctuation–dissipation relation between the response coefficient $\tilde{D}$ and the fluctuation coefficient $\tilde{\sigma}$. Note that in general both $\tilde{D}$ and $\tilde{\sigma}$ depend on the temperature T_a.

(ii) One can easily extend the generalized detailed balance (9) and the fluctuation theorem (12), (13) to other types of currents. For example, in the case of a current of particles, (9) becomes

$$z_a^{-q_a} z_b^{-q_b} W_{q_a, q_b}(C', C) = W_{-q_a, -q_b}(C, C') \tag{18}$$

where z_a and z_b are the fugacities associated to the reservoirs of particles and q_a and q_b are the numbers of particles transfered from the reservoirs while the system jumps from configuration C to configuration C'. The fluctuation theorem (12), (13) becomes then

$$\mathcal{F}(j) - \mathcal{F}(-j) = j[\log z_b - \log z_a] \quad \text{and} \quad \mu(\lambda) = \mu(-\lambda + \log z_b - \log z_a) \tag{19}$$

Close to equilibrium, if one defines as in (14), (15), the fluctuation and the response coefficients for a system in contact with two reservoirs

$$\frac{\langle Q_t^2 \rangle}{t} \to \tilde{\sigma} \quad \text{for } \rho_a = \rho_b \quad \text{and} \quad \frac{\langle Q_t \rangle}{t} \to (\rho_a - \rho_b)\tilde{D} \quad \text{for } \rho_a - \rho_b \text{ small} \tag{20}$$

where $\tilde{D}$ and $\tilde{\sigma}$ are now functions of the density ρ_a. One can show, by expanding in powers of λ and of $z_a - z_b$ as in (16) that

$$\tilde{\sigma} = 2\tilde{D}\frac{d\rho}{d\log z} = 2\tilde{D}T\rho^2\kappa \tag{21}$$

where $\kappa = \rho^{-1}\,d\rho/dp$ is the compressibility. (To see why the compressibility appears, one can write $\log Z = -\mathbb{F}/T = -Vf(N/V)/T$ where $\mathbb{F}$ is the free energy and f the free energy per unit volume; one uses the facts that $T\log z = d\mathbb{F}/dN = f'(\rho)$ and that $p = -d\mathbb{F}/dV = \rho f'(\rho) - f(\rho)$; then one can see that $d\rho/d\log z = T/f''(\rho) = T\rho\,d\rho/dp$.)

(iii) Another easy extension is to consider systems with several types of currents (for example a current of particles and a current of energy, or several types of particles, or systems in contact with more than two reservoirs). The extension of the fluctuation theorem to these cases allows one to recover Onsager's reciprocity relations in the close-to-equilibrium limit [25,20].

(iv) The fluctuation theorem is usually formulated in terms of entropy production [26,27,21] as, in the steady state, the entropy of the system remains stationary whereas a current j of energy from the heat bath at temperature T_a into a heat bath at temperature T_b gives a rate $j(1/T_b - 1/T_a)$ of increase of entropy.

2.1. An example: the symmetric simple exclusion process (SSEP) [28–31]

There are only few examples of non-equilibrium steady states for which the cumulants $\langle Q_t^n \rangle_c$ or the large deviation function $\mathcal{F}(j)$ of the current can be calculated [32–34]. One of the simplest cases is the symmetric simple exclusion process shown in Fig. 3.

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. During every infinitesimal time interval dt, each particle has a probability dt of jumping to the left if the neighboring site on its left is empty, dt of jumping to the right if the neighboring site on its right 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 $\alpha\,dt$ (if this site is empty) and a particle is removed from site 1 with probability $\gamma\,dt$ (if this site is occupied). Similarly on site L, particles are injected at rate δ and removed at rate β. (Note that one could consider that in the SSEP the particles represent quanta of energy and all the properties could be interpreted in terms of heat transport.)

From the definition of the model, one can see that the dynamics satisfies the generalized detailed balance relation (18) with

$$z_a = \frac{\alpha}{\gamma}; \qquad z_b = \frac{\delta}{\beta}$$

If τ_i is a binary variable which indicates whether site i is occupied ($\tau_i = 1$) or empty ($\tau_i = 0$), it is easy to calculate the steady state profile [32]

$$\langle \tau_i \rangle = \rho_b + \frac{L - i + b}{L + 1 + a + b}(\rho_a - \rho_b) \tag{22}$$

where

$$\rho_a = \frac{\alpha}{\alpha + \gamma}, \quad \rho_b = \frac{\delta}{\beta + \delta} \quad \text{and} \quad a = \frac{1}{\alpha + \gamma}, \quad b = \frac{1}{\beta + \delta}$$

Clearly, in the expression (22) of the profile, ρ_a and ρ_b represent the densities in the reservoirs at the two ends of the chain. The calculation of the first cumulants can be done either directly or by a perturbation theory in λ by using the generating function [32].
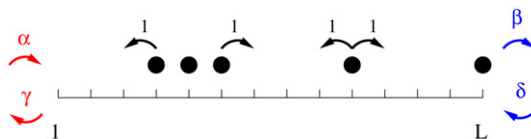

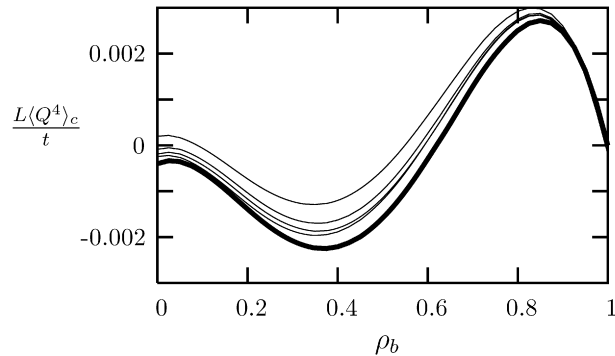Fig. 3. The symmetric simple exclusion process.

Fig. 4. The fourth cumulant versus ρ_b for $\rho_a = 1$. The thin lines represent the fourth cumulant obtained from exact calculations of $\mu_L(\lambda)$ for system sizes $L = 5, 9, 13, 17$, whereas the thick line represents expression (23) valid in the limit $L \to \infty$.

$$\lim_{t \to \infty} \frac{\langle Q_t \rangle}{t} = \frac{\rho_a - \rho_b}{L + a + b - 1}$$

$$\lim_{t \to \infty} \frac{\langle Q_t^2 \rangle_c}{t} = \frac{1}{L_1}(\rho_a + \rho_b - 2\rho_a\rho_b)$$

$$+ \frac{a(a-1)(2a-1) + b(b-1)(2b-1) - L_1(L_1-1)(2L_1-1)}{3L_1^3(L_1-1)}(\rho_a - \rho_b)^2$$

where $L_1 = L + a + b - 1$. For large L, the first four cumulants (see Fig. 4, for a graphical representation of the fourth) are given by:

$$\lim_{t \to \infty} \frac{\langle Q_t \rangle}{t} \simeq \frac{\rho_a - \rho_b}{L}$$

$$\lim_{t \to \infty} \frac{\langle Q_t^2 \rangle_c}{t} \simeq \frac{1}{L}\left[\rho_a + \rho_b - \frac{2\rho_a^2 + 2\rho_a\rho_b + 2\rho_b^2}{3} \right]$$

$$\lim_{t \to \infty} \frac{\langle Q_t^3 \rangle_c}{t} \simeq \frac{1}{L}\left[\rho_a - \rho_b - 2(\rho_a^2 - \rho_b^2) + \frac{16\rho_a^3 + 12\rho_a^2\rho_b - 12\rho_a\rho_b^2 - 16\rho_b^3}{15} \right]$$

$$\lim_{t \to \infty} \frac{\langle Q_t^4 \rangle_c}{t} \simeq \frac{1}{L}\left[\rho_a + \rho_b - \frac{14\rho_a^2 + 2\rho_a\rho_b + 14\rho_b^2}{3} + \frac{32\rho_a^3 + 8\rho_a^2\rho_b + 8\rho_a\rho_b^2 + 32\rho_b^3}{5} \right.$$

$$\left. - \frac{96\rho_a^4 + 64\rho_a^3\rho_b - 40\rho_a^2\rho_b^2 + 64\rho_a\rho_b^3 + 96\rho_b^4}{35} \right] \tag{23}$$

3. The additivity principle

One can formulate a conjecture, *the additivity principle* [35], based on a simple physical picture, which allows one to determine all the cumulants and the large deviation function $\mathcal{F}(j)$ for more general one dimensional diffusive systems. Applied to the SSEP, this leads to the same expression of the cumulants (23) and provide a way of calculating all the higher cumulants. Here we will limit the discussion to non-equilibrium steady states of systems in contact with two reservoirs of particles. As shown below everything can be easily generalized to systems in contact with two heat baths. 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 (2)

$$\text{Pro}_{L+L'}(j, \rho_a, \rho_b) \sim e^{-t F_{L+L'}(j, \rho_a, \rho_b)} \tag{24}$$

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

$$\text{Pro}_{L+L'}(j, \rho_a, \rho_b) \sim \max_r \left[\text{Pro}_L(j, \rho_a, r) \times \text{Pro}_{L'}(j, r, \rho_b) \right] \tag{25}$$

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 r times the probability of transporting the current j over a distance L' between two reservoirs at densities r and ρ_b. One can then argue that one should choose for r the density which makes this probability maximum. From (25) one gets the following additivity property of the large deviation function:

$$F_{L+L'}(j, \rho_a, \rho_b) = \min_r \left[F_L(j, \rho_a, r) + F_{L'}(j, r, \rho_b) \right] \tag{26}$$

By repeating this procedure, one gets that

$$F_L(j, \rho_a, \rho_b) = \min_{r_1, \ldots, r_{k-1}} \left\{ \sum_{i=0}^{k-1} F_l(j, r_i, r_{i+1}) \right\} \tag{27}$$

where $k = L/l$, $r_0 = \rho_a$ and $r_k = \rho_b$.

For large L and k (with L/k still very large), if one considers current fluctuations of order $1/L$, it is advantageous, to minimize (27), to make the differences $r_i - r_{i+1}$ small. As the current j is also small one can consider that each piece of length l is close to equilibrium and has Gaussian fluctuations at the leading order

$$F_l(j, r_i, r_{i+1}) \simeq \frac{[j - \frac{D(r_i)(r_i - r_{i+1})}{l}]^2}{2 \frac{\sigma(r_i)}{l}} \tag{28}$$

where the parameters D and σ are defined for a system of length l in contact with two reservoirs at densities ρ_a and ρ_b by

$$\frac{\langle Q_t^2 \rangle}{t} \to \frac{\sigma(\rho_a)}{l} \quad \text{for } \rho_a = \rho_b \tag{29}$$

$$\frac{\langle Q_t \rangle}{t} \to (\rho_a - \rho_b) \frac{D(\rho_a)}{l} \quad \text{for } \rho_a - \rho_b \text{ small} \tag{30}$$

These are the same parameters as in (14), (15), (20) up to a factor l. (In the definitions (29), (30), one should take first the $t \to \infty$ limit, i.e. $\sigma(\rho_a) = \lim_{l \to \infty} \lim_{t \to \infty} \frac{l \langle Q_t^2 \rangle}{t}$.)

If for large k, the optimal density r_i in (27) varies slowly with i

$$r_i = \rho \left(i \frac{l}{L} \right)$$

for some smooth density $\rho(x)$ (see Fig. 5) then combining (27) and (28), we get

$$F_L(j, \rho_a, \rho_b) = \min_{\{r_i\}} \sum_{i=0}^{k-1} \frac{[j - \frac{D(r_i)(r_i - r_{i+1})}{l}]^2}{2 \frac{\sigma(r_i)}{l}} = \min_{\rho(x)} \frac{1}{L} \int_0^1 \frac{[Lj + \rho'(x) D(\rho(x))]^2}{2 \sigma(\rho(x))} \, dx \tag{31}$$

with $\rho(0) = \rho_a$ and $\rho(1) = \rho_b$. Note that (28) is a local equilibrium assumption, i.e. that both the current j and the difference $r_i - r_{i+1}$ are small. Therefore one cannot expect (31) to be valid when the current deviation j is not of order $1/L$.
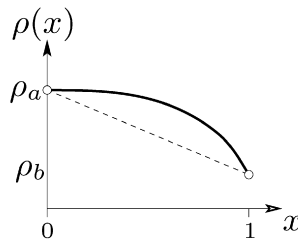

Fig. 5. The dashed line represents the steady state profile. The optimal density in (31) changes in the bulk to facilitate the deviation of the current.

The steady state profile $\bar{\rho}(x)$ is the one which makes vanish the large deviation function F_L. It therefore satisfies

$$L\bar{j} + D\big(\bar{\rho}(x)\big)\bar{\rho}(x)' = 0$$

where the most likely current $\bar{j}$ is fixed by the boundary conditions

$$\bar{j} = \frac{1}{L} \int\limits_{\rho_b}^{\rho_a} D(\rho)\,\mathrm{d}\rho$$

4. The large deviation function obtained from the additivity principle

4.1. The optimal profile

The profile $\rho_0(x)$ which optimizes (31) satisfies

$$\frac{\mathrm{d}}{\mathrm{d}\rho} \frac{L^2 j^2}{2\sigma(\rho_0(x))} - \rho_0'(x)^2 \frac{\mathrm{d}}{\mathrm{d}\rho} \frac{D^2(\rho_0(x))}{2\sigma(\rho_0(x))} - 2\rho_0''(x) \frac{D^2(\rho_0(x))}{2\sigma(\rho_0(x))} = 0$$

If one multiplies this expression by $\rho_0'(x)$, one can integrate once. Finally one gets that the optimal profile satisfies

$$\rho_0'(x)^2 = \frac{(Lj)^2(1 + 2K\sigma(\rho_0(x)))}{D^2(\rho_0(x))} \tag{32}$$

where the integration constant K is fixed by the boundary conditions $\rho_0(0) = \rho_a$ and $\rho_0(1) = \rho_b$.

Suppose that $\rho_a > \rho_b$ and that the deviations are not too large so that the optimal profile remains monotone, i.e.

$$\rho_0'(x) = -Lj \frac{\sqrt{1 + 2K\sigma(\rho_0(x))}}{D(\rho_0(x))} \tag{33}$$

one can rewrite (31) as

$$F_L(j, \rho_a, \rho_b) = j \int\limits_{\rho_b}^{\rho_a} \left[\frac{1 + K\sigma(\rho)}{[1 + 2K\sigma(\rho)]^{1/2}} - 1 \right] \frac{D(\rho)}{\sigma(\rho)}\,\mathrm{d}\rho \tag{34}$$

where the constant K is fixed from (33) by the boundary condition ($\rho(0) = \rho_a$ and $\rho(1) = \rho_b$), i.e.

$$Lj = \int\limits_{\rho_b}^{\rho_a} \frac{D(\rho)}{[1 + 2K\sigma(\rho)]^{1/2}}\,\mathrm{d}\rho \tag{35}$$

The optimal profile (33) remains unchanged when $j \to -j$ (simply the sign of $[1 + 2K\sigma(\rho)]^{1/2}$ is changed) in (34), (35) and one gets that

$$F_L(j) - F_L(-j) = -2j \int\limits_{\rho_b}^{\rho_a} \frac{D(\rho)}{\sigma(\rho)}\,\mathrm{d}\rho \tag{36}$$

which is the fluctuation theorem (19). In fact already in (31) it was clear by expanding the square that the optimal $\rho_0(x)$ does not depend on the sign of j and that (36) had to be satisfied.

The physical meaning of the optimal profile ρ_0 (32) is that adopting this profile is the easiest way to flow through the system an atypical current j. The large deviation functional (31) shows that the optimal density profile ρ_0 and the current deviation j are coupled in a non-trivial way. One can think of the system as a pipe with diameter $\sigma(\rho)$ depending on the local density. The easiest way to increase the particle current is to adjust the size of the pipe $\sigma(\rho)$ and therefore the local density, in order to facilitate the flow of particles. In the example of the SSEP with reservoirs at equal densities $\rho = \rho_a = \rho_b$, the variance of the current $\sigma(\rho) = 2\rho(1-\rho)$ is maximum at density $\rho = 1/2$. When $\rho_a = \rho_b < 1/2$, it is favorable to have in the bulk a density $\rho_0(x) > \rho_a$ in order to facilitate the flow of particles and the optimal way of doing it is by choosing the profile $\rho_0(x)$ which satisfies (32). If $\rho_a = \rho_b = 1/2$, then the optimal

density profile remains flat for any current deviation and the large deviation functional (31) is quadratic [32,35]. In general the complicated expression of the cumulants (23) expresses the non-trivial coupling between the flux j and the optimal density profile $\rho_0(x)$.

4.2. The cumulants

The parametric expression (34), (35) for the large deviation function $F_L(j)$ can be transformed into another parametric form for $\mu_L(\lambda)$ defined in (4), (5)

$$\mu_L(\lambda, \rho_a, \rho_b) = -\frac{K}{L}\left[\int_{\rho_b}^{\rho_a} \frac{D(\rho)\,\mathrm{d}\rho}{\sqrt{1+2K\sigma(\rho)}}\right]^2 \tag{37}$$

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

$$\lambda = \int_{\rho_b}^{\rho_a} \mathrm{d}\rho\, \frac{D(\rho)}{\sigma(\rho)}\left[\frac{1}{\sqrt{1+2K\sigma(\rho)}} - 1\right] \tag{38}$$

By eliminating K, one can obtain the expansion of μ_L in powers of λ and by taking successive derivatives (5), (6) with respect to λ one gets for the cumulants of the current:

$$\frac{\langle Q_t \rangle}{t} = \frac{1}{L}I_1, \qquad \frac{\langle Q_t^2 \rangle - \langle Q_t \rangle^2}{t} = \frac{1}{L}\frac{I_2}{I_1}$$

$$\frac{\langle Q_t^3 \rangle_c}{t} = \frac{1}{L}\frac{3(I_3 I_1 - I_2^2)}{I_1^3}, \qquad \frac{\langle Q_t^4 \rangle_c}{t} = \frac{1}{L}\frac{3(5I_4 I_1^2 - 14 I_1 I_2 I_3 + 9 I_2^3)}{I_1^5} \tag{39}$$

where the integrals I_n are given by

$$I_n = \int_{\rho_b}^{\rho_a} D(\rho)\sigma(\rho)^{n-1}\,\mathrm{d}\rho$$

In the case of the SSEP, one has $D(\rho) = 1$ and $\sigma(\rho) = 2\rho(1-\rho)$. One can simplify (37), (38) and get

$$\mu_L(\lambda) = \frac{1}{L}\left[\log\left(\sqrt{1+\omega} + \sqrt{\omega}\right)\right]^2 \quad \text{with } \omega = \left(e^\lambda - 1\right)\rho_a + \left(e^{-\lambda} - 1\right)\rho_b - \left(e^\lambda - 1\right)\left(e^{-\lambda} - 1\right)\rho_a \rho_b \tag{40}$$

From this one can recover the cumulants (23) and determine all the higher cumulants. Expressions equivalent to (40) were derived in the theory of shot noise of mesoscopic conductors [36,37].

Remark. The density ρ is the physical relevant parameter. However it can be useful [38] to consider instead the conjugate field $\beta = \log z$ (see (21)). Formula (31) then simplifies as it depends only on one macroscopic input $\sigma(\beta)$

$$F_L(j, \beta_a, \beta_b) = \min_{\beta(x)} \frac{1}{L}\int_0^1 \frac{[Lj + \frac{\sigma(\beta(x))}{2}\beta'(x)]^2}{2\sigma(\beta(x))}\,\mathrm{d}x \tag{41}$$

where the minimum is taken over the chemical potential profiles such that $\beta(0) = \log z_a$ and $\beta(1) = \log z_b$.

4.3. Heat flux

All the above discussion can be generalized to the case of a heat flux in diffusive systems: one has to replace everywhere the density profile $\rho(x)$ by the temperature profile $T(x)$. There is even one simplification as in the thermal case D and σ are related as in (17) so that for $D(T)$ defined as in (30) (i.e. $\langle Q_t \rangle / t = (T_a - T_b)D(T)/L$ for small $T_a - T_b$), one gets

$$Lj = \int_{T_b}^{T_a} \frac{\mathrm{d}T\, D(T)}{[1 + 4KT^2 D(T)]^{1/2}}, \qquad F_L(j) = j\int_{T_b}^{T_a} \frac{\mathrm{d}T}{2T^2}\left[\frac{1+2KT^2 D(T)}{[1+4KT^2 D(T)]^{1/2}} - 1\right] \tag{42}$$

5. The macroscopic fluctuation theory

Building on the hydrodynamic large deviation theory [39,29,30], Bertini et al. developed [40–42] a general framework to determine the steady state large deviation function of non-equilibrium systems. This framework has been extended [12,43] to the current large deviations. Let us sketch briefly their approach. For diffusive systems (such as SSEP), the total flux $Q_i(t)$ flowing through position i between time 0 and time t and the density $\rho_i(t)$ near position i are, for a large system of size L and for times of order L^2, scaling functions of the form

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

It is convenient to introduce the instantaneous current defined in terms of the rescaled time τ

$$\hat{q}(x, \tau) = \frac{\partial \hat{Q}(x, \tau)}{\partial \tau} \tag{43}$$

In fact $L\hat{q}(x, \tau)\,\mathrm{d}\tau$ is simply the total flux of particles through position $[xL]$ during the microscopic time interval $[L^2\tau, L^2(\tau + \mathrm{d}\tau)]$, with $1/L \ll \mathrm{d}\tau \ll 1$ so that there is a large number of particles which contribute to the integrated current but the density does not vary over this small time interval. Remark that the current $\hat{q}$ is defined after a diffusive rescaling, i.e. the space is scaled by $1/L$ and the time by $1/L^2$. Thus unlike the microscopic current, $\hat{q}$ remains of order 1. The conservation of the number of particles implies that

$$\frac{\partial \hat{\rho}(x, \tau)}{\partial \tau} = -\frac{\partial^2 \hat{Q}(x, \tau)}{\partial \tau \, \partial x} = -\frac{\partial \hat{q}(x, \tau)}{\partial x} \tag{44}$$

The *macroscopic fluctuation theory* [12,43] gives for the probability of observing a certain density profile $\hat{\rho}(x, \tau)$ and a current $\hat{q}(x, \tau)$ over the rescaled time interval $0 < \tau' < \tau$

$$\text{Pro}\left(\{\hat{\rho}(x, \tau'), \hat{q}(x, \tau')\}\right) \sim \exp\left[-L \int_0^\tau \mathrm{d}\tau' \int_0^1 \mathrm{d}x \, \frac{[\hat{q}(x, \tau') + D(\hat{\rho}(x, \tau'))\frac{\partial \hat{\rho}(x,\tau')}{\partial x}]^2}{2\sigma(\hat{\rho}(x, \tau'))}\right] \tag{45}$$

Of course $\hat{\rho}$ and $\hat{q}$ have to satisfy the relation (44). (Note that if t is the microscopic time, then $\tau = t/L^2$ plays the role of a macroscopic time.) Similar expression were obtained in [46–48] by considering stochastic models in the context of shot noise in mesoscopic quantum conductors. The functional (45) was used to calculate the large deviation functional of the density for several systems [41,44] and in the case of SSEP the results agree with an exact microscopic derivation [45].

The large deviation function $\mathcal{F}(j)$ (2) for observing the total current j, i.e. the following event

$$Lj = \frac{1}{\tau} \int_0^\tau \mathrm{d}\tau' \int_0^1 \mathrm{d}x \, \hat{q}(x, \tau') \tag{46}$$

as predicted in [12,43] by the macroscopic fluctuation theory (45) becomes

$$\mathcal{F}(j) = \frac{1}{L} \lim_{\tau \to \infty} \frac{1}{\tau} \min_{\substack{\hat{\rho}(x,\tau') \\ \hat{q}(x,\tau')}} \int_0^\tau \mathrm{d}\tau' \int_0^1 \mathrm{d}x \, \frac{[\hat{q}(x, \tau') + D(\hat{\rho}(x, \tau'))\frac{\partial \hat{\rho}(x,\tau')}{\partial x}]^2}{2\sigma(\hat{\rho}(x, \tau'))} \tag{47}$$

where the minimum is over all the density profiles $\{\hat{\rho}(x, \tau'), \ 0 < \tau' < \tau\}$ and the currents $\{\hat{q}(x, \tau'), \ 0 < \tau' < \tau\}$ which satisfy the conservation law (44) and the global constraint (46).

If the optimal density and current profiles are time independent (up to boundary effects for τ' close to 0 or τ which do not contribute in the $\tau \to \infty$ limit), one recovers the predictions of the additivity principle (31) and $\mathcal{F}(j) = F_L(j)$. When the optimal profile is time dependent the additivity principle predictions (31) give only an upper bound: $\mathcal{F}(j) \leqslant F_L(j)$. In [12,43], Bertini et al. provided an example for which the functions F_L and $\mathcal{F}$ are different. In their example, F_L was not a convex function of j and $\mathcal{F}$ was its convex envelope (see (3)). They also proved (see [43] Section 6.1) that $\mathcal{F}$ reduces to F_L under the following global condition on D and σ

$$\text{For all } \rho, \quad D(\rho)\sigma''(\rho) \leqslant D'(\rho)\sigma'(\rho) \tag{48}$$

This holds for the SSEP and the Zero Range process [30]. Condition (48) is however only sufficient.

In general a dynamical phase transition [43,49] may occur where the system switches from a time independent to a time dependent optimal profile. To calculate the large deviation function $\mathcal{F}$ one needs to determine the optimal time dependent profile $\hat{\rho}(x, \tau)$, which is not an easy task as the optimization problem is non-linear. A complete characterization of the regime for which the additivity principle holds ($\mathcal{F}(j) = F_L(j)$) remains a challenging problem.

6. Phase transitions

In this section, we try to determine the phase boundary where the optimal profile becomes time dependent. To do so we consider a more general situation with a small driving force (like an electric field) in the bulk. Adding such a driving force of amplitude ν/L to an open system of length L with reservoirs ρ_a, ρ_b modifies the mean current (30) as follows [29,49]

$$\frac{\langle Q_t \rangle}{t} \rightarrow (\rho_a - \rho_b) \frac{D(\rho_a)}{L} + \frac{\nu}{L} \sigma(\rho_a) \quad \text{for } \rho_a - \rho_b \text{ small} \tag{49}$$

In (49), the conductivity σ which was defined as the variance of the current in (29) can also be understood as the linear response to the small field ν/L. The effect of the field can be easily taken into account in the framework of the macroscopic fluctuation theory [43,49] by arguing that locally the current has Gaussian fluctuations with mean value given by (49). The functional (47) becomes

$$\mathcal{F}(j) = \frac{1}{L} \lim_{\tau \to \infty} \frac{1}{\tau} \min_{\substack{\hat{\rho}(x,\tau') \\ \hat{q}(x,\tau')}} \int_0^\tau \mathrm{d}\tau' \int_0^1 \mathrm{d}x \, \frac{[\hat{q}(x,\tau') + D(\hat{\rho}(x,\tau')) \frac{\partial \hat{\rho}(x,\tau')}{\partial x} - \nu \sigma(\hat{\rho}(x,\tau'))]^2}{2\sigma(\hat{\rho}(x,\tau'))}. \tag{50}$$

with the constraint (46) on the total current.

6.1. Stability of the functional

The time independent optimal profile $\rho_0(x)$ is now a solution of (see (32))

$$\left(D(\rho_0(x))\rho_0'(x)\right)^2 = \left(jL - \nu \sigma(\rho_0(x))\right)^2 + 2K\sigma(\rho_0(x)) \tag{51}$$

where the constant K has to be adjusted so that ρ_0 satisfies the boundary conditions ($\rho_0(0) = \rho_a$ and $\rho_0(1) = \rho_b$). A situation for which $\rho_0(x)$ is certainly not optimal in (50) is when a small time dependent perturbation is sufficient to lower (50). To investigate the stability of $\rho_0(x)$ against such perturbations, one can write

$$\hat{\rho}(x, \tau') = \rho_0(x) + \delta\rho(x, \tau')$$
$$\hat{q}(x, \tau') = j + \delta j(x, \tau')$$

where $\delta\rho$ and δj have zero time averages and are related by (44). Inserting these expressions into (50), one gets at the second order

$$\int_0^\tau \mathrm{d}\tau' \int_0^1 \mathrm{d}x \left\{ \frac{(\delta j)^2}{2\sigma(\rho_0)} - j \frac{\sigma'(\rho_0)}{\sigma^2(\rho_0)} \delta\rho\delta j + A(\rho_0)(\delta\rho')^2 + 2[A'(\rho_0)\rho_0']\delta\rho\delta\rho' + \frac{1}{2}[B''(\rho_0) + A''(\rho_0)(\rho_0')^2](\delta\rho)^2 \right\}$$

where we introduced the functions

$$A(u) = \frac{D^2(u)}{2\sigma(u)}, \quad \text{and} \quad B(u) = \frac{j^2}{2\sigma(u)} + \frac{\nu^2}{2}\sigma(u).$$

The coefficients of the quadratic form are x dependent but time independent. Thus to analyze the stability, one can consider perturbations of the form

$$\delta\rho(x, \tau') = \frac{\mathrm{i}}{\omega} \exp(\mathrm{i}\omega\tau')\varphi_1'(x) - \frac{\mathrm{i}}{\omega} \exp(-\mathrm{i}\omega\tau')\varphi_2'(x)$$
$$\delta j(x, \tau') = \exp(\mathrm{i}\omega\tau')\varphi_1(x) + \exp(-\mathrm{i}\omega\tau')\varphi_2(x) \tag{52}$$

where $\varphi_2(x) = \varphi_1^*(x)$. The quadratic form can be rewritten as

$$\tau \int_0^1 dx \left\{ \frac{\varphi_1\varphi_2}{\sigma(\rho_0)} - j\frac{\sigma'(\rho_0)}{\sigma^2(\rho_0)}\frac{i}{\omega}[\varphi_1'\varphi_2 - \varphi_1\varphi_2'] + \frac{2}{\omega^2}A(\rho_0)\varphi_1''\varphi_2'' \right.$$
$$\left. + \frac{2}{\omega^2}[A'(\rho_0)\rho_0'][\varphi_1'\varphi_2'' + \varphi_1''\varphi_2'] + \frac{1}{\omega^2}[B''(\rho_0) + A''(\rho_0)(\rho_0')^2]\varphi_1'\varphi_2' \right\} \tag{53}$$

For the time independent profile $\rho_0(x)$ to be stable against small time dependent perturbations, the quadratic form (53) has to be positive for all ω. In general, all the coefficients in (53) are spatially dependent through $\rho_0(x)$ and it is difficult to provide from (53) a more explicit characterization of this local stability.

6.2. Periodic systems

For a system of N particles on a ring of length L with density $\bar{\rho} = N/L$, the flat profile $\rho_0(x) = \bar{\rho}$ remains a solution of the Euler–Lagrange equation associated to (50). In this case, the coefficients of the quadratic form have no x dependence and the different spatial modes decouple. One can choose $\varphi_1 = \exp(ikx)$ and $\varphi_2 = \exp(-ikx)$ and the positivity of the quadratic form implies that for any k (multiple of 2π) and ω, one has

$$\frac{1}{\sigma(\bar{\rho})}\left(1 + Lj\frac{k\sigma'(\bar{\rho})}{\omega\sigma(\bar{\rho})}\right)^2 + \frac{k^2}{\omega^2}\left(\frac{k^2 D(\bar{\rho})^2}{\sigma(\bar{\rho})} - (Lj)^2\frac{\sigma''(\bar{\rho})}{2\sigma(\bar{\rho})^2} + v^2\frac{\sigma''(\bar{\rho})}{2}\right) > 0. \tag{54}$$

The first mode to become unstable is the fundamental mode $k = 2\pi$, thus the flat profile is stable when [49]

$$\frac{8\pi^2 D^2(\bar{\rho})}{\sigma(\bar{\rho})} > \sigma''(\bar{\rho})\left[\frac{(Lj)^2}{\sigma^2(\bar{\rho})} - v^2\right] \tag{55}$$

Let j_c be the critical current for which (55) becomes an equality. If $\sigma''(\bar{\rho}) > 0$ (resp. $\sigma''(\bar{\rho}) < 0$), the flat profile becomes unstable for currents $|j| > |j_c|$ (resp. $|j| < |j_c|$). Remark that the instability regime is always symmetric with respect to 0 as predicted by the fluctuation theorem (19) which becomes in presence of a driving force

$$\mathcal{F}(j) - \mathcal{F}(-j) = -2vj - 2j\int_{\rho_b}^{\rho_a} \frac{D(\rho)}{\sigma(\rho)}d\rho$$

Beyond the threshold (55) a bifurcation occurs and a traveling wave of the form $\rho(x - vt)$ is more favorable than the flat profile $\bar{\rho}$. From (54), we get that close to the phase transition, the optimal velocity is given by

$$\omega = -2\pi Lj_c\frac{\sigma'(\bar{\rho})}{\sigma(\bar{\rho})} \quad \Rightarrow \quad v = Lj_c\frac{\sigma'(\bar{\rho})}{\sigma(\bar{\rho})} \tag{56}$$

If we make the *assumption* that no first order transition occurs before the second order transition predicted at j_c, we can compute the expansion of $\mathcal{F}$ close to j_c. We consider small current perturbations

$$Lj = Lj_c + \varepsilon, \quad \text{with } Lj_c = \sqrt{v^2\sigma(\bar{\rho})^2 + \frac{8\pi^2 D(\bar{\rho})^2\sigma(\bar{\rho})}{\sigma''(\bar{\rho})}} \tag{57}$$

Let us limit the discussion to the case $\sigma''(\bar{\rho}) < 0$. Then for $\varepsilon > 0$ the flat profile remains optimal and one expects that the large deviation function is quadratic

$$\forall \varepsilon > 0, \quad \mathcal{F}(j) = \frac{(Lj_c + \varepsilon - v\sigma(\bar{\rho}))^2}{2\sigma(\bar{\rho})} \tag{58}$$

On the other hand for $\sigma''(\bar{\rho}) < 0$, the flat profile is unstable for $\varepsilon < 0$ and the expansion of $\mathcal{F}(j)$ at the second order in ε can be obtained by approximating the travelling wave as follows

$$\rho_0(x, t) \approx \bar{\rho} + \sqrt{-\varepsilon}a_1\sin(2\pi(x - vt)) + \varepsilon a_2\cos(4\pi(x - vt)) \tag{59}$$

where the velocity $v = Lj_c \frac{\sigma'(\bar{\rho})}{\sigma(\bar{\rho})}$ is given by (56). In fact the expansion should also include corrections in ε to the velocity as well as other Fourier modes, but a computation shows that they do not contribute to the second order expansion of $\mathcal{F}$. Inserting the test function (59) in (50) implies that the second order of $\mathcal{F}(j)$ in ε is given by the quartic form

$$
\begin{aligned}
\left(\frac{Lj_c \sigma''(\bar{\rho})}{4\sigma(\bar{\rho})^2} + \left(-\frac{3\pi^2 D'(\bar{\rho})D(\bar{\rho})}{\sigma(\bar{\rho})} + \frac{3\pi^2 D(\bar{\rho})^2 \sigma'(\bar{\rho})}{2\sigma(\bar{\rho})^2} + \frac{\pi^2 D(\bar{\rho})^2 \sigma^{(3)}(\bar{\rho})}{2\sigma(\bar{\rho})\sigma''(\bar{\rho})} \right) a_2 \right) a_1^2 \\
+ \left(-\frac{\pi^2 D(\bar{\rho})^2 \sigma^{(4)}(\bar{\rho})}{16\sigma(\bar{\rho})\sigma''(\bar{\rho})} + \frac{\pi^2 D(\bar{\rho})^2 \sigma'(\bar{\rho})^2}{4\sigma(\bar{\rho})^3} + \frac{\pi^2 D(\bar{\rho})^2 \sigma''(\bar{\rho})}{4\sigma(\bar{\rho})^2} - \frac{\pi^2 D(\bar{\rho})D'(\bar{\rho})\sigma'(\bar{\rho})}{2\sigma(\bar{\rho})^2} \right. \\
\left. + \frac{\pi^2 D(\bar{\rho})D''(\bar{\rho})}{4\sigma(\bar{\rho})} + \frac{\pi^2 D'(\bar{\rho})^2}{4\sigma(\bar{\rho})} + \frac{3v^2 \sigma''(\bar{\rho})^2}{64\sigma(\bar{\rho})} \right) a_1^4 + \frac{3\pi^2 D(\bar{\rho})^2}{\sigma(\bar{\rho})} a_2^2 + \frac{1}{2\sigma(\bar{\rho})}
\end{aligned}
\tag{60}
$$

where $\sigma^{(3)}, \sigma^{(4)}$ denote the third and fourth derivatives. The optimal amplitudes a_1, a_2 of the traveling wave (59) are the minimizers of the quartic form. Note that (60) is not always stable and for some specific choices of the functions D and σ, the minimum of (60) can be $-\infty$. For example the sign of the coefficient a_1^4 depends on $\sigma^{(4)}(\bar{\rho})$ which can a priori take any arbitrary value. The condition for the quartic form (60) to be stable can be written as

$$
\mathbb{A}(\bar{\rho}) > 0,
\tag{61}
$$

where

$$
\begin{aligned}
\mathbb{A}(\bar{\rho}) = {} & 9v^2 \sigma(\bar{\rho})^2 \sigma''(\bar{\rho})^4 - 96\pi^2 D'(\bar{\rho})^2 \sigma(\bar{\rho})^2 \sigma''(\bar{\rho})^2 + 48\pi^2 D(\bar{\rho})D''(\bar{\rho})\sigma(\bar{\rho})^2 \sigma''(\bar{\rho})^2 \\
& + 12\pi^2 D(\bar{\rho})^2 \sigma'(\bar{\rho})^2 \sigma''(\bar{\rho})^2 - 24\pi^2 D(\bar{\rho})^2 \sigma(\bar{\rho})\sigma'(\bar{\rho})\sigma''(\bar{\rho})\sigma^{(3)}(\bar{\rho}) \\
& + 48\pi^2 D(\bar{\rho})^2 \sigma(\bar{\rho})\sigma''(\bar{\rho})^3 + 48\pi^2 D(\bar{\rho})D'(\bar{\rho})\sigma(\bar{\rho})\sigma'(\bar{\rho})\sigma''(\bar{\rho})^2 \\
& + 48\pi^2 D(\bar{\rho})D'(\bar{\rho})\sigma(\bar{\rho})^2 \sigma''(\bar{\rho})\sigma^{(3)}(\bar{\rho}) - 4\pi^2 D(\bar{\rho})^2 \sigma(\bar{\rho})^2 \sigma^{(3)}(\bar{\rho})^2 \\
& - 12\pi^2 D(\bar{\rho})^2 \sigma(\bar{\rho})^2 \sigma''(\bar{\rho})\sigma^{(4)}(\bar{\rho})
\end{aligned}
\tag{62}
$$

If (61) is not satisfied then one expects that a first order transition occurred before j_c.

We suppose as before that $\sigma''(\bar{\rho}) < 0$ and that (61) is satisfied. Then the minimum of (60) is achieved for

$$
a_1 = 2\sqrt{-\frac{6Lj_c \sigma(\bar{\rho})\sigma''(\bar{\rho})^3}{\mathbb{A}(\bar{\rho})}} \quad \text{and} \quad a_2 = \left(\frac{D'(\bar{\rho})}{2D(\bar{\rho})} - \frac{\sigma'(\bar{\rho})}{4\sigma(\bar{\rho})} - \frac{\sigma^{(3)}(\bar{\rho})}{12\sigma''(\bar{\rho})} \right) a_1^2
\tag{63}
$$

where $\mathbb{A}(\bar{\rho})$ is defined in (62). Thus for $\varepsilon < 0$, one finds at the second order

$$
\mathcal{F}(j) = \frac{(Lj_c + \varepsilon - v\sigma(\bar{\rho}))^2}{2\sigma(\bar{\rho})} - \frac{3\sigma''(\bar{\rho})^4 (Lj_c)^2}{\sigma(\bar{\rho})\mathbb{A}(\bar{\rho})} \varepsilon^2 + O(\varepsilon^3).
\tag{64}
$$

Comparing (58) to (64), we see that if $\mathbb{A}(\bar{\rho}) > 0$ the time dependent profile gives lower $\mathcal{F}(j)$ than the flat profile.

As an example, we consider the weakly asymmetric simple exclusion process (WASEP) which follows the same exclusion rule as the SSEP with jump rates biased by $\exp(v/L)$ to the right and $\exp(-v/L)$ to the left. In this case $D(\rho) = 1$ and $\sigma(\rho) = 2\rho(1-\rho)$. Since $\sigma''(\bar{\rho}) = -4$, the threshold of stability of the flat profile is given by

$$
Lj_c = \sqrt{v^2 \sigma(\bar{\rho})^2 - 2\pi^2 \sigma(\bar{\rho})}
$$

For $\varepsilon < 0$, a perturbation of the form (59) leads to the quartic form (60)

$$
\frac{\pi^2 + \frac{3}{4}(v^2 \sigma(\bar{\rho})^2 - 4\pi^2 \sigma(\bar{\rho}))}{\sigma(\bar{\rho})^3} a_1^4 + \frac{3\pi^2 \sigma'(\bar{\rho})}{2\sigma(\bar{\rho})^2} a_1^2 a_2 + \frac{3\pi^2}{\sigma(\bar{\rho})} a_2^2 - \frac{Lj_c}{\sigma(\bar{\rho})^2} a_1^2 + \frac{1}{2\sigma(\bar{\rho})}
\tag{65}
$$

The quartic form (65) is stable so that the amplitudes of the traveling wave (59) are given by

$$
a_1 = \sqrt{\frac{2Lj_c \sigma(\bar{\rho})}{3v^2 \sigma(\bar{\rho})^2 - 6\pi^2 \sigma(\bar{\rho}) + \pi^2}} \quad \text{and} \quad a_2 = -\frac{\sigma'(\bar{\rho})}{4\sigma(\bar{\rho})} a_1^2
\tag{66}
$$

Finally for $\varepsilon < 0$, one finds at the second order

$$\mathcal{F}(j) = \frac{(Lj_c + \varepsilon - \nu\sigma(\bar{\rho}))^2}{2\sigma(\bar{\rho})} - \frac{\nu^2\sigma(\bar{\rho}) - 2\pi^2}{3\nu^2\sigma(\bar{\rho})^2 - 6\pi^2\sigma(\bar{\rho}) + \pi^2}\varepsilon^2 + \mathrm{O}(\varepsilon^3)$$

It is interesting to note that for the WASEP on a ring at density $\bar{\rho} = 1/2$, the optimal velocity is 0, thus the optimal profile remains time independent. This means that the phase transition could have been detected already at the level of the functional F_L.

Finally, let us mention that in the large drift limit $\nu \to \infty$, the asymptotic cost for (50) as well as the asymptotic shape of the optimal traveling waves can be computed [49]. In particular for the WASEP, the current large deviation function (50) converges in the large drift limit $\nu \to \infty$ to the current large deviation function of the totally asymmetric simple exclusion process [50,51]. We refer the reader to [49] for further details and to [52] for a study of the large drift limit in the case of open systems.

7. Conclusion

In this article, we have shown how to generalize the detailed balance relation to take into account the effect of reservoirs. From this generalized detailed balance relation the fluctuation theorem [16,17] can be recovered which characterizes the odd part of the large deviation function of the current. By a simple additivity principle [35], one can predict for diffusive systems the whole large deviation function as well as all the cumulants of the current. These predictions agree with previous exact computations for some stochastic models like the symmetric simple exclusion process [32]. For some models, however, the additivity principle provides only an upper bound of the large deviation function of the current [12]. This fact as well as the occurrence of phase transitions has been discussed in the framework of the macroscopic fluctuation theory [43,49].

A challenging issue would be to characterize precisely the range of validity of the additivity principle in the case of diffusive stochastic models. Here we were only able to address the local stability of the time independent solution of the additivity principle. How to calculate the large deviation function of the heat or particle current in a more general framework (several species of particles, additional conserved or non-conserved quantities) is also an interesting open question.

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