A Gallavotti-Cohen Type Symmetry in the Large Deviation Functional for Stochastic Dynamics

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Abstract. We extend the work of Kurchan on the Gallavotti-Cohen fluctuation theorem, which yields a symmetry property of the large deviation function, to general Markov processes. These include jump processes describing the evolution of stochastic lattice gases driven in the bulk or through particle reservoirs, general diffusive processes in physical and/or velocity space, as well as Hamiltonian systems with stochastic boundary conditions. For dynamics satisfying local detailed balance we establish a link between the action functional of the fluctuation theorem and the entropy production. This gives, in the linear regime, an alternative derivation of the Green-Kubo formula and the Onsager reciprocity relations. In the nonlinear regime consequences of the new symmetry are harder to come by and the large derivation functional difficult to compute. For the asymmetric simple exclusion process the latter is determined explicitly using the Bethe ansatz in the limit of large N.

1 Introduction

The study of stationary nonequilibrium states (SNS) of macroscopic systems evolving according to classical (or even quantum) mechanics, which are kept out of equilibrium by contact with thermal reservoirs has a long history. The interactions of the system with the reservoirs are usually modeled by the addition of stochastic boundary terms to the deterministic evolution equations describing the isolated system [1]–[7]. Fully deterministic evolutions of systems coupled to infinitely extended reservoirs have also been investigated [8]–[10], as have fully stochastic models [11]–[14]. A more recent development has been the study of SNS of systems evolving via deterministic "thermostatted" dynamics [15, 16, 17]. In this scheme the SNS is maintained by deterministic external driving forces which are balanced by a "friction term" suitably chosen so that the system evolves on a compact surface (generally one of constant energy) in phase space. The resulting dynamics no longer conserves phase space volume, which is contracted on the average [19]. Consequently, the SNS is singular with respect to the Liouville (volume) measure induced on the surface.

While the jury is still out on what has or can be achieved by such a dynamical systems approach, there are some intriguing theoretical results which have emerged [20, 21]. In particular Gallavotti and Cohen [22] motivated by results of computer simulations [23] discovered that under suitable assumptions these SNS satisfy a certain symmetry, which they doobed a "fluctuation theorem". Assuming that the dynamics satisfies *time reversal invariance* and is sufficiently chaotic, so that the SNS is given by an SRB measure, they prove that the probability distribution for the phase space contraction averaged along a trajectory over the time span τ has, for large τ, a highly non-obvious symmetry, whose specific form will be given below. Near equilibrium the fluctuation theorem implies Onsager reciprocity and the Einstein relations. We refer to [24] for an exhaustive discussion of the theorem and of the "chaotic hypothesis", which implies the validity of the theorem for more general SNS.

In a recent work Kurchan showed that, with proper definitions, the fluctuation theorem is valid also for certain diffusion processes [25]. In the present work we extend Kurchan's results and show that for Markov processes the fluctuation theorem holds in great generality. Our proof is based on the Perron-Frobenius theorem and goes much beyond the cases considered in [25]. While the assumed stochasticity of the dynamics should provide "for free" a suitable modification of the chaotic hypothesis it is far from obvious how to find the quantity that plays the role of the phase space contraction. In analogy to the thermostatted case it is reasonable to expect that it will have some relation to the production of Gibbs entropy. In fact, this comes out from our general construction under the additional assumption of local detailed balance. This condition seems to play, in stochastic dynamics, the same role as time reversal invariance in deterministic thermostatted dynamics. When local detailed balance is satisfied, then the action functional is proportional to the current of the conserved quantity, e.g. in the case of bulk driven lattice gases it is the bulk particle current. If local detailed balance is not satisfied, then the action functional can still be defined but it does not allow for such a direct physical interpretation.

Near equilibrium the fluctuation theorem, generalized to systems with several currents, yields the Onsager symmetry and the usual Kubo formulae for the linear transport coefficients. These give a relation between linear response and current fluctuations in equilibrium. In this sense the fluctuation theorem, which holds also far from equilibrium, can be thought of as a natural extension, in the spirit of GC, of the fluctuation-dissipation theorem which holds for systems close to (local) equilibrium. In fact, when the large deviation functional is approximately quadratic over a sufficiently large range of the driving field, the fluctuation theorem does indeed yield such an approximate extension. We do not, however, have a quantitative criteria of when this approximation is valid. Even aside from this extension it would be of great interest to have an experimentally verifiable consequence of the novel symmetry predicted by the fluctuation theorem for the distribution of large deviations in current carrying systems. This seems difficult to obtain for macroscopic systems since the time required for observing a large deviation in such a system far exceeds any observation time.

The physical meaning of the fluctuation theorem can be understood best through the application to simple models. We therefore determine here the action functional for which such a fluctuation theorem holds in various examples: bulk and/or boundary driven lattice gases, the Fokker-Planck equation with driving forces and a spatially varying temperature, and Hamiltonian particle systems driven by boundary reservoirs. In general, the rate function appearing in the fluctuation theorem cannot be computed explicitly and one has to rely on numerical simulations [23, 26]. In stochastic models the task is easier as long as we stick to noninteracting particles. We discuss one example of interacting particles, where the rate function can be computed via the Bethe ansatz. When the size of the system goes to infinity the rate function becomes singular. This is analogous to the behavior of thermodynamic potentials at a phase transition. This is done in the Appendix which may be read independently of the rest of the paper.

Our analysis extends directly to discrete time stochastic processes, i.e. to probabilistic cellular automata. In this situation it is natural to think of the GC fluctuation theorem as a symmetry of discrete space–time Gibbs measures, as has been pointed out by C. Maes [27]. In fact, the framework of space–time Gibbs measures contains as special cases both the stochastic dynamics studied here and the thermostatted systems satisfying the chaotic hypothesis. In the latter case the space–time Gibbs measure is constructed through a Markov partition of phase space.

2 The fluctuation theorem for jump processes

We start with the fluctuation theorem for a stochastic time evolution governed by a master equation on a state space with a finite number of points. This minimizes technical complications and at the same time provides a blue-print for stochastic systems with Langevin type dynamics. In this section we investigate the abstract structure, specific examples and applications will be discussed in later sections.

2.1 Action functional, large deviations

We consider a continuous time Markov jump process with finite state space $\mathcal{S}$. Points in $\mathcal{S}$ are denoted by σ. The jump process is determined by the rates, $k(\sigma,\sigma') \geq 0$, for jumping from σ to σ'. More precisely, if the system is in the state σ it waits a random time $t \geq 0$ distributed according to the exponential law $r(\sigma)e^{-r(\sigma)t}dt$, $r(\sigma) = \sum_{\sigma'} k(\sigma,\sigma')$, and then jumps to σ' with probability $r(\sigma)^{-1}k(\sigma,\sigma')$, etc.. The generator acting on functions $f : \mathcal{S} \to \mathbb{R}$ is given by

$$Lf(\sigma) = \sum_{\sigma'} k(\sigma,\sigma')[f(\sigma') - f(\sigma)]\,. \tag{2.1}$$

This means, if $\mu(\sigma,t)$ is the probability distribution of σ at time t, then the rate of change of the average of f, $\langle f\rangle_{\mu(t)} = \sum_\sigma \mu(\sigma,t)f(\sigma)$, is given by

$$\frac{d}{dt}\langle f\rangle_{\mu(t)} = \langle Lf\rangle_{\mu(t)}\,. \tag{2.2}$$

Taking f to be a Kronecker delta at σ (2.2) corresponds to the master equation

$$\frac{\partial\mu(\sigma,t)}{\partial t} = \sum_{\sigma'} k(\sigma',\sigma)\mu(\sigma',t) - r(\sigma)\mu(\sigma,t) = L^*\mu(\sigma,t) \tag{2.3}$$

for the evolution of $\mu(\sigma,t)$, where L^* denotes the adjoint of L.

We assume that if $k(\sigma,\sigma') > 0$, then also $k(\sigma',\sigma) > 0$, and that from every σ all other $\sigma' \in \mathcal{S}$ can be reached by a succession of steps with nonzero rates. It follows then from the general theory of finite state Markov processes that there exists a unique stationary measure, μ_s, which satisfies $L^*\mu_s(\sigma) = 0$ and is strictly positive, $\mu_s(\sigma) > 0$. Starting from any initial state σ_0, μ_s is approached exponentially fast in time.

We could as well take the state space $\mathcal{S}$ to be countable or replace $\mathcal{S}$ by $\mathbb{R}^n$. In the latter case one prescribes the rates $k(x,x')dx'$ for a jump from x to the volume element $x'+dx'$. Setting $r(x) = \int k(x,x')dx'$, the waiting time at x is exponential with rate $r(x)$ and the jump probability to $x'+dx'$ is $r(x)^{-1}k(x,x')dx'$. Formally the difference is only in notation. However, now one has to make sure that the jump process has a unique invariant measure.

Let $s \to \sigma_s$ be a trajectory (or history) of the jump process and define for it the quantity

$$W(t, \{\sigma_s, 0 \leq s \leq t\}) = \int_0^t \sum_{\sigma,\sigma'} w_{\sigma,\sigma'}(s) ds \tag{2.4}$$

with $w_{\sigma,\sigma'}(s)$ a sequence of δ-functions, located exactly at those times s when σ_s jumps from σ to σ', with weight

$$w(\sigma, \sigma') = \log k(\sigma, \sigma') - \log k(\sigma', \sigma) . \tag{2.5}$$

This means, if the trajectory σ_s, $0 \leq s \leq t$, visits in succession the states $\sigma_0, \sigma_1, ..., \sigma_n$, where σ_0 is the state at time 0 and σ_n the one at time t, then

$$W(t, \{\sigma_s, 0 \leq s \leq t\}) = \log \left[\frac{k(\sigma_0, \sigma_1)}{k(\sigma_1, \sigma_0)} \cdots \frac{k(\sigma_{n-1}, \sigma_n)}{k(\sigma_n, \sigma_{n-1})} \right] . \tag{2.6}$$

(Note that at an allowed transition $k(\sigma, \sigma') > 0$ and, by assumption, also $k(\sigma', \sigma) > 0$).

For lack of a better name we call $W(t)$, and the similar quantities to be defined below, an *action functional.* (We will generally not indicate explicitly the dependence of $W(t)$ on the stochastic trajectory $\{\sigma_s, 0 \leq s \leq t\}$).

Let $\langle \cdot \rangle$ denote the expectation over all trajectories in the stationary process, i.e. starting in the steady state $\mu_s(\sigma)$. We consider the generating function $\langle \exp[-\lambda W(t)] \rangle$ of $W(t)$ and define

$$\lim_{t \to \infty} -\frac{1}{t} \log \langle e^{-\lambda W(t)} \rangle = e(\lambda) . \tag{2.7}$$

The *fluctuation theorem* we shall prove states that the limit (2.7) exists with $e(\lambda)$ convex downwards, and that

$$e(\lambda) = e(1 - \lambda) . \tag{2.8}$$

By a general result, analogous to the equivalence of ensembles in equilibrium statistical mechanics, (2.7) implies a large deviation property for the probability distribution $p_t(w)$ of $W(t)/t$, i.e. for large t

$$p_t(w) \cong e^{-t\hat{e}(w)} , \tag{2.9}$$

where $\hat{e}$ is the Legendre transform of e. $\hat{e}(w)$ is convex up, $\hat{e}(w) \geq 0$, $\hat{e}(w_0) = 0$ for $w_0 = lim_{t \to \infty} \langle \frac{1}{t} W(t) \rangle$, and by (2.8) $\hat{e}$ satisfies

$$\hat{e}(w) - \hat{e}(-w) = -w , \tag{2.10}$$

i.e. the odd part of $\hat{e}$ is linear with slope $-1/2$.

To be more precise, from (2.7) one concludes that for every interval I

$$\lim_{t\to\infty} -\frac{1}{t}\log \mathrm{Prob}(\frac{1}{t}W(t)\in I) = \min_{w\in I}\hat{e}(w) \tag{2.11}$$

with

$$\begin{aligned}\hat{e}(w) &= \max_{\lambda}\{e(\lambda)-\lambda w\}\\ &= \max_{\lambda}\{e(1-\lambda)-\lambda w\} = \max_{\lambda}\{e(\lambda)-(1-\lambda)w\}\\ &= \hat{e}(-w)-w\,.\end{aligned} \tag{2.12}$$

Eq. (2.10) is of the same form as the GC fluctuation theorem, with the phase space contraction integrated along an orbit of the thermostatted dynamics in GC replaced by (2.5) summed over the jumps along the stochastic trajectory. We note that the convexity of $e(\lambda)$ and (2.8) imply that $\langle w_0\rangle = (de(\lambda)/d\lambda)_{|\lambda=0} \geq 0$. This is analogous to the result [19] that the mean phase space volume contraction in the stationary state is nonnegative.

To prove (2.8) we first define

$$g(\sigma,t) = \mathbb{E}_\sigma[e^{-\lambda W(t)}] \tag{2.13}$$

as the expectation value of $e^{-\lambda W(t)}$ conditioned on the system being in state σ at time $t=0$. We then have

$$\begin{aligned}\frac{d}{dt}g(\sigma,t) &= \sum_{\sigma'} k(\sigma,\sigma')e^{-\lambda w(\sigma,\sigma')}g(\sigma',t) - r(\sigma)g(\sigma,t)\\ &= \sum_{\sigma'} k(\sigma,\sigma')^{1-\lambda}k(\sigma',\sigma)^{\lambda}g(\sigma',t) - r(\sigma)g(\sigma,t)\\ &= L_\lambda g(\sigma,t)\,.\end{aligned} \tag{2.14}$$

Eq. (2.14) is to be solved subject to the initial condition $g(\sigma,0)=1$. Therefore

$$\langle e^{-\lambda W(t)}\rangle = \sum_{\sigma}\mu_s(\sigma)g(\sigma,t) = \sum_{\sigma,\sigma'}\mu_s(\sigma)(e^{L_\lambda t})_{\sigma\sigma'}\,. \tag{2.15}$$

Clearly $(e^{L_\lambda t})_{\sigma\sigma'} > 0$ by our assumption on $k(\sigma,\sigma')$ above. The Perron-Frobenius theorem states that L_λ has a unique maximal eigenvector f_λ which is characterized by $f_\lambda(\sigma)>0$ and satisfies $L_\lambda f_\lambda(\sigma) = -e(\lambda)f_\lambda(\sigma)$ with real maximal $-e(\lambda)$. This implies the existence of the limit in (2.7). Furthermore L_λ and L_λ^* have the same maximal eigenvalue. Using now the definition (2.16) we see that

$$L_\lambda^* = L_{1-\lambda}\,. \tag{2.16}$$

Hence the maximal eigenvector $\bar{f}_\lambda$ of L_λ^* satisfies

$$L_\lambda^*\bar{f}_\lambda(\sigma) = -e(\lambda)\bar{f}_\lambda(\sigma) = L_{1-\lambda}\bar{f}_\lambda(\sigma)\,. \tag{2.17}$$

Since $L_{1-\lambda} f_{1-\lambda}(\sigma) = -e(1-\lambda) f_{1-\lambda}(\sigma)$ and since $\bar{f}_\lambda > 0$, we conclude by uniqueness that $\bar{f}_\lambda = f_{1-\lambda}$ and $e(\lambda) = e(1-\lambda)$.

2.2 Time Reversal

For a Markov chain with transition probability $p(\sigma, \sigma')$ from σ to σ' the history $\{\sigma\} = \{\sigma_0, \ldots, \sigma_n\}$ has the probability

$$P(\{\sigma\}) = \mu_s(\sigma_0) p(\sigma_0, \sigma_1) ... p(\sigma_{n-1}, \sigma_n) \tag{2.18}$$

when starting in the stationary measure μ_s. In analogy to (2.6) we define the action functional as

$$W(n, \{\sigma\}) = -\sum_{j=1}^{n} \log[p(\sigma_j, \sigma_{j-1})/p(\sigma_{j-1}, \sigma_j)] \,. \tag{2.19}$$

If we now denote the time reversed history of $\{\sigma\}$ by $R\{\sigma\} = \{\sigma_n, ..., \sigma_0\}$, then (2.19) can be rewritten as

$$\begin{aligned} W(n, \{\sigma\}) &= -\log[P(R\{\sigma\})/P(\{\sigma\})] + \log[\mu_s(\sigma_n)/\mu_s(\sigma_0)] \\ &= \bar{W}(n, \{\sigma\}) + \log[\mu_s(\sigma_n)/\mu_s(\sigma_0)] \,. \end{aligned} \tag{2.20}$$

One now immediately verifies that $\langle e^{-\lambda \bar{W}(n)} \rangle = \langle e^{-(1-\lambda)\bar{W}(n)} \rangle$, where the average is with respect to $P(\{\sigma\})$. Thus for $\bar{W}(n)$ the fluctuation theorem holds even for finite n.

The form (2.20) is analogous to the form which the GC functional takes for thermostatted systems when the latter deterministic dynamical evolution is described via Markov partitions and it shows explicitly the role of time reversal in the original GC theorem. This observation forms the basis of the analysis of C. Maes in [27], where he studies the fluctuation theorem for space-time Gibbs measures and also discusses symmetry transformations different from time reversal.

For the time continuous jump process a path $\{\sigma_s, 0 \le s \le t\}$ is time reversed as $\{\sigma_{t-s}, 0 \le s \le t\}$. The time reversed process has the jump rates $k^R(\sigma, \sigma') = k(\sigma', \sigma)\mu_s(\sigma')/\mu_s(\sigma)$ whereas the inverse waiting times, $r(\sigma)$, and the steady state, $\mu_s(\sigma)$, remain unmodified. If $P_{[0,t]}$ denotes the path measure of the stationary process in the time window $[0, t]$ and $P^R_{[0,t]}$ the one of the corresponding time reversed process, then $P^R_{[0,t]}$ has a density relative to $P_{[0,t]}$ and

$$P^R_{[0,t]} = e^{-W(t)} (\mu_s(\sigma_t)/\mu_s(\sigma_0)) P_{[0,t]} \tag{2.21}$$

with $W(t)$ from (2.4). Thus, up to boundary terms, the action functional equals $-\log(dP^R_{[0,t]}/dP_{[0,t]})$ with dP^R/dP denoting the Radon-Nikodym derivative.

(2.21) remains meaningful for a stochastic dynamics which is *not Markov* and it can thus be used as a definition of the action functional in such a more general context.

One may wonder whether time-reversal could be replaced by some other transformation on path space. An obvious candidate is an internal symmetry $S : \mathcal{S} \to \mathcal{S}$ such that $S \circ S = 1$. Using this transformation in (2.21) the GC action functional becomes

$$W(t) = -\int_0^t ds \log[r(S\sigma_s)/r(\sigma_s)] \tag{2.22}$$

up to boundary terms. From the examples we have studied it seems that only time-reversal leads to an action functional which has a simple physical interpretation.

2.3 Sum of several generators

We can generalize the above analysis to the case where the generator in (2.1) is the sum of several generators: $L = \sum_{j=1}^m L^{(j)}$ with

$$L^{(j)} f(\sigma) = \sum_{\sigma'} k^{(j)}(\sigma, \sigma')[f(\sigma') - f(\sigma)] \,. \tag{2.23}$$

We require that for transitions between a given pair σ, σ' at most one of the rates $k^{(j)}$ is different from zero. It follows then from our assumptions on $k(\sigma, \sigma')$ that if $k^{(j)}(\sigma, \sigma') > 0$, then also $k^{(j)}(\sigma', \sigma) > 0$. With this decomposition we define, in complete analogy with (2.4)–(2.6), the j-th action functional

$$W^{(j)}(t, \{\sigma_s, 0 \le s \le t\}) = \int_0^t \sum_{\sigma,\sigma'} w^{(j)}_{\sigma,\sigma'}(s) ds \tag{2.24}$$

and the logarithm of the generating function

$$e(\lambda_1, \ldots, \lambda_m) = \lim_{t\to\infty} -\frac{1}{t} \log\langle \exp[-\sum_{j=1}^m \lambda_j W^{(j)}(t)]\rangle \,. \tag{2.25}$$

Repeating the arguments of Section 2.1 we conclude that the fluctuation theorem now takes the form

$$e(\lambda_1, \ldots, \lambda_m) = e(1-\lambda_1, \ldots, 1-\lambda_m) \,. \tag{2.26}$$

The corresponding analog of (2.10) is

$$\hat{e}(w_1, \ldots, w_n) - \hat{e}(-w_1, \ldots, -w_m) = -\sum_{j=1}^m w_j \tag{2.27}$$

We shall use the general form (2.26) in Section 8 to prove the Onsager relations but note here that there are many ways of splitting L into a sum of $L^{(j)}$'s. In fact we can choose a different $L^{(j)}$ for every pair of points (σ, σ') for which $k(\sigma, \sigma') \neq 0$. In all cases setting $\lambda_j = \lambda$ for all j we recover (2.8) and (2.10) for $W = \sum_{j=1}^m W^{(j)}$. We do not expect in general that the distribution of $(1/t)W^{(j)}(t)$ separately satisfies any fluctuation theorem. On the other hand we can consider, as a degenerate case of (2.23), a situation in which our system is composed of several independent systems with generators $L^{(j)}$. In that case, of course, each $L^{(j)}$ satisfies the symmetry relation, $e_j(\lambda_j) = e_j(1-\lambda_j)$, $\hat{e}_j(w_j) - \hat{e}_j(-w_j) = -w_j$, and $e(\lambda_1, \dots \lambda_m) = \sum_{j=1}^m e_j(\lambda_j)$, $\hat{e}(w_1, \dots, w_m) = \sum_{j=1}^m \hat{e}_j(w_j)$.

2.4 Entropy production

For the probability distribution $\mu(\sigma, t)$ at time t the Gibbs entropy is, as usual, given by

$$S_G(\mu(t)) = -\sum_{\sigma} \mu(\sigma, t) \log \mu(\sigma, t)\,. \tag{2.28}$$

Using (2.3) the rate of change of S_G can be written in the form

$$\frac{d}{dt} S_G(\mu(t)) = R(\mu(t)) - A(\mu(t))\,, \tag{2.29}$$

where

$$R(\mu(t)) = \frac{1}{2}\sum_{\sigma,\sigma'} [k(\sigma, \sigma')\mu(\sigma, t) - k(\sigma', \sigma)\mu(\sigma', t)] \log[\frac{\mu(\sigma, t)k(\sigma, \sigma')}{\mu(\sigma', t)k(\sigma', \sigma)}] \geq 0 \tag{2.30}$$

and

$$A(\mu(t)) = \langle I \rangle_{\mu(t)}, \quad I(\sigma) = \sum_{\sigma'} k(\sigma, \sigma') \log[\frac{k(\sigma, \sigma')}{k(\sigma', \sigma)}]\,. \tag{2.31}$$

(When the generator is a sum, $L = \sum_{j=1}^m L^{(j)}$, as in the previous section, then the rate of change in Gibbs entropy is also a sum over j and consequently $R = \sum_{j=1}^m R^{(j)}$, $A = \sum_{j=1}^m A^{(j)}$).

The breakup in (2.30) has the property that R is non-negative, while A is linear in μ. This suggests that we identify R as the entropy produced by the stochastic jumps and A with the entropy flow which can have either sign. Defining now the "integrand" in A, $I(\sigma)$, as a "microscopic" entropy flux we note that the expectation value of $W(t)$, starting with some initial distribution $\mu(\sigma, 0)$, is given by

$$\langle W(t) \rangle_{\mu(0)} = \int_0^t ds \langle I \rangle_{\mu(s)}\,. \tag{2.32}$$

We can therefore say that the average action equals the entropy flow integrated over the time span t. There is of course some arbitrariness in this identification. We could for example add some positive linear term to R and subtract it from A. Our choice of splitting is however quite natural in the examples discussed below.

When the system is in the steady state μ_s, $\frac{d}{dt}S_G(\mu_s) = 0$ and the entropy flow balances the entropy production, i.e.

$$R(\mu_s) = A(\mu_s). \tag{2.33}$$

Thus

$$\langle t^{-1}W(t)\rangle = R(\mu_s) = A(\mu_s) \tag{2.34}$$

and hence the average action equals the rate of entropy production in the steady state. This suggests to identify W with the microscopic production of Gibbs entropy, a role played by the phase space contraction in the context of thermostatted systems; see also Section 7.

We remark that $R(\mu_s) = A(\mu_s) = 0$ in case $k(\sigma, \sigma')$ satisfies detailed balance with respect to the invariant measure $\mu_s(\sigma) \sim e^{-V(\sigma)}$, i.e.

$$e^{-V(\sigma)}k(\sigma, \sigma') = e^{-V(\sigma')}k(\sigma', \sigma)\,. \tag{2.35}$$

Then each term in the sum defining $R(\mu_s)$ in (2.30) vanishes. This implies by (2.29) that $A(\mu_s) = \langle I\rangle_{\mu_s} = 0$. The action functional (2.6) now becomes a telescoping sum with

$$W(t) = V(\sigma_0) - V(\sigma_t)\,. \tag{2.36}$$

It then follows from (2.7) that $e(\lambda) = 0$ and the fluctuation theorem becomes empty. More generally if

$$k(\sigma, \sigma') = k_0(\sigma, \sigma')k_1(\sigma, \sigma') \tag{2.37}$$

and $k_0(\sigma, \sigma')$ satisfies detailed balance while k_1 is a nonequilibrium driving "force", then the $\log k_0$ terms of $W(t)$ sum to a boundary value as before and only the weight corresponding to k_1 contributes in $W(t)$. We will encounter such a situation for driven lattice gases.

3 Bulk driven lattice gases

An important example of an SNS with spatial structure is a stochastic lattice gas where particles jump at random to neighboring lattice sites. We envisage two mechanisms for how the conserved particle density is driven away from equilibrium. The first one, studied in this section, is a global driving force which corresponds to driven diffusive systems (DDS). In the second one, considered in the next section, particles are injected/removed at the boundaries whereas the bulk is governed by reversible dynamics satisfying detailed balance with respect to an equilibrium stationary measure. In both cases the full dynamics does not satisfy detailed balance with respect to the stationary measure μ_s.

We consider particles with exclusion hopping on a regular lattice $\mathbb{Z}^d$. The configuration is specified by the occupation variables η_x, $x \in \mathbb{Z}^d$, taking the values

0 (empty) and 1 (occupied). Particles on different sites may interact by making the jump rate of a given particle depend on the configurations on nearby sites. As explained in Section 2, the fluctuation theorem holds in general. For notational simplicity we restrict ourselves however to the one-dimensional lattice, $d = 1$.

We first study particles subject to a uniform drive. This will set up a steady state current in a finite system of particles jumping on a ring, $x = 1, \ldots, \ell$, with $x = \ell + 1$ identified with $x = 1$. A particle configuration is denoted by $\eta = (\eta_1, \ldots, \eta_\ell)$. We denote by $c_{xx+1}(\eta)$ the exchange rate for the pair of sites $(x, x+1)$, i.e., if $\eta_x = 1$ (0) and $\eta_{x+1} = 0$ (1), then $c_{xx+1}(\eta)$ is the rate at which the particle at x ($x+1$) jumps to the empty site at $x+1$ (x).

In equilibrium the distribution of particles is determined by the Gibbs measure $\mu_{eq} \sim \exp[-\beta H]$ where β is the inverse temperature and $H(\eta)$ is the energy function. The rates c_{xx+1} satisfy the condition of detailed balance, with respect to μ_{eq} whenever

$$e^{-\beta H(\eta)} c_{xx+1}(\eta) = e^{-\beta H(\eta^{xx+1})} c_{xx+1}(\eta^{xx+1}) \,. \tag{3.1}$$

Here η^{xx+1} denotes the configuration η with the occupations at $x, x+1$ interchanged. A simple example of $H(\eta)$ is the energy of a system with nearest neighbor interactions

$$H(\eta) = -J \sum_{x=1}^{\ell} \eta_x \eta_{x+1} \,, \tag{3.2}$$

but such an explicit form is not used here. Rates satisfying (3.1) lead the system to equilibrium. In order to drive the lattice gas by a uniform external force field of strength F we add to $H(\eta)$ the linear term $-\sum_x F x \eta_x$. While this term does not respect the boundary conditions, energy differences always do. Therefore the rates for a uniform drive are assumed to satisfy

$$c^F_{xx+1}(\eta) = c^F_{xx+1}(\eta^{xx+1}) \exp[-\beta(H(\eta^{xx+1}) - H(\eta) - F(\eta_x - \eta_{x+1}))] \,. \tag{3.3}$$

We have called this condition local detailed balance [11, 13], because locally a particle feels a linear potential. It is only through the periodic boundary condition, that the steady state becomes a nonequilibrium one. For a closed system the particles would pile up at the right (for $F > 0$).

To state the fluctuation theorem we merely have to apply the results of Section 2. The logarithmic ratio in (2.5) is

$$-\beta(H(\eta^{xx+1}) - H(\eta)) + \beta F(\eta_x - \eta_{x+1}) \tag{3.4}$$

with η the configuration before and η^{xx+1} the configuration after the jump. The energy difference summed over the jumps is telescoping and yields a pure surface term as in (2.36). Therefore the relevant part of the action functional is given by

$$W(t) = \beta F \int_0^t \sum_{x=1}^{\ell} J_{x,x+1}(s) ds \,. \tag{3.5}$$

$J_{x,x+1}(s)$ is the actual particle current across the bond $(x, x+1)$, i.e. for a given history $\{\eta(s), 0 \leq s \leq t\}$, $J_{x,x+1}(s)$ is a sequence of δ-functions located at the times of jump through the bond $(x, x+1)$ with weight $+1$ (-1) if the jump is from x $(x+1)$ to $x+1$ (x). The action functional is βF times the the total current integrated over the time span t, which equals the signed number of all jumps up to time t.

The entropy production $R(\mu)$ can be read off from (2.30). If we set $\mu(\eta) = g(\eta) Z^{-1} e^{-\beta H(\eta)}$ and denote by $\langle \cdot \rangle_{eq}$ the average over $Z^{-1} e^{-\beta H(\eta)}$, then

$$\begin{aligned} R(\mu) \;&=\; \frac{1}{2} \sum_{x=1}^{\ell} \langle c^F_{xx+1}(\eta) [e^{-\beta F(\eta_x - \eta_{x+1})} g(\eta^{xx+1}) - g(\eta)] \\ &\qquad [\log e^{-\beta F(\eta_x - \eta_{x+1})} g(\eta^{xx+1}) - \log g(\eta)] \rangle_{eq} \,. \end{aligned} \tag{3.6}$$

We clearly have $R(\mu) > 0$ unless $F = 0$ [28]. The identification of $R(\mu)$ as entropy production is further supported by taking μ to be a state of local equilibrium. In the limit of slow density variations R coincides with the phenomenological entropy production based on the nonlinear diffusion equation as a macroscopic equation for the density [28].

We emphasize that the action functional is equal to the total current only if the condition (3.3) of local detailed balance holds. To illustrate this point we consider nearest and next nearest neighbor jumps. Local detailed balance for next nearest neighbor jumps means

$$c^F_{xx+2}(\eta) = c^F_{xx+2}(\eta^{xx+2}) \exp[-\beta(H(\eta^{xx+2}) - H(\eta) - 2F(\eta_x - \eta_{x+2}))] \,. \tag{3.7}$$

As before, $W(t)$ constructed according to the rule (2.5) equals the total current. There are many ways to violate (3.7). Just as an example, if in (3.7) we replace $2F$ by αF, then the action functional is $W(t) = \beta F \int dt \sum_x (J_{x,x+1}(t) + \alpha J_{x,x+2}(t))$ which equals the particle current only if $\alpha = 2$. Thus, while the fluctuation theorem holds in great generality, the specific physical interpretation is linked to local detailed balance. We could also in this case consider the generator as the sum of two generators, one for nearest and one for next nearest neighbor jumps, and have more general fluctuation theorems as in Section 2.3. The physical interpretation would however remain obscure.

4 Boundary driven lattice gases

We use the same set-up as in the previous section. Only now the box consisting of sites $\{1, 2, \ldots, \ell\}$ is not periodic, and there is no driving force. Instead particles are injected and removed at the left ($x = 1$) and right ($x = \ell$) boundary. The generator, L, for the full dynamics is naturally decomposed as a sum of three pieces,

$$L = L_b + L_1 + L_\ell \,. \tag{4.1}$$

L_b is the dynamics inside the box satisfying detailed balance with respect to $e^{-\beta H}$, cf. (3.1) with $x = 1, \ldots, \ell - 1$. L_b conserves the number of particles. L_i models the particle source/sink at the right and left boundaries and has the form

$$L_i f(\eta) = c_i(\eta)[f(\eta^i) - f(\eta)]\,, \quad i = 1, \ell \,. \tag{4.2}$$

$c_i(\eta)$ is the rate for the transition η_i to $1 - \eta_i$ while the remaining configuration is untouched. The configuration after this transition is denoted by η^i. As before we will require the rate $c_i(\eta)$ to satisfy local detailed balance in the form [13]

$$c_i(\eta) = c_i(\eta^i)\exp[-\beta(H(\eta^i) - H(\eta)) + \beta\gamma_i(1 - 2\eta_i)]\,, \tag{4.3}$$

where local refers now to the boundary points which are coupled to reservoirs with chemical potentials γ_1 and γ_ℓ. Thus if we consider the dynamics generated only by $L_b + L_i$, then the dynamics will satisfy detailed balance with respect to the stationary distribution $Z^{-1}\exp[-\beta H(\eta) + \beta\gamma_i N(\eta)]$ (achieved in the long time limit) with $N(\eta) = \sum_{x=1}^{\ell} \eta_x$ the number of particles. The same will be true for the full L in (4.1), if $\gamma_1 = \gamma_\ell$. If on the other hand $\gamma_1 \neq \gamma_\ell$, then the sources are unbalanced and there will be in the steady state a net flux of particles through the system going from the reservoir with high to the reservoir with low chemical potential, i.e. from left to right if $\gamma_1 > \gamma_\ell$.

We now apply the results of Section 2 (with $\lambda_j = \lambda$). The logarithmic ratio (2.5) reads

$$-\beta(H(\eta^{xx+1}) - H(\eta)) - \beta\sum_{i=1,\ell}(H(\eta^i) - H(\eta)) + \sum_{i=1,\ell}\beta\gamma_i(N(\eta^i) - N(\eta)), \tag{4.4}$$

where η is the configuration before and η^{xx+1}, resp. η^i, the configuration after the jump. Again the energy differences sum to a surface term. Let $J_i(t)$ be the boundary current, $i = 1, \ell$. It is a sequence of delta functions located at times when η_i jumps to $1 - \eta_i$ with weight 1 (-1) for the transition from 0 to 1 (from 1 to 0). When the boundary current J_1 is positive there is a net flux of particles from the ith reservoir into the system. Then

$$W(t) = \beta\int_0^t (\gamma_1 J_1(s) + \gamma_\ell J_\ell(s))ds\,. \tag{4.5}$$

Because of particle conservation there are many equivalent expressions for $W(t)$ in the sense that they differ only by surface terms and have therefore the same rate function. Let us denote by $N_{[x,y]}(t)$, $x \leq y$, the number of particles in the interval $[x, y]$ at time t. By the conservation law for the number of particles we have

$$N_{[x,y]}(t) - N_{[x,y]}(0) = \int_0^t (J_{x-1,x}(s) - J_{y,y+1}(s))ds\,. \tag{4.6}$$

Since $N_{[x,y]}(t) \leq |y - x| + 1$, $\int_0^t J_{x-1,x}(s)ds$ and $\int_0^t J_{y,y+1}(s)ds$ must have the same large deviations. If we include in the mass balance also the boundary currents, then we can replace in (4.5) $J_1(t)$ by any $J_{x,x+1}(t)$ and $J_\ell(t)$ by any $-J_{x,x+1}(t)$ without modifying the rate function $\hat{e}(w)$. While this gives many equivalent choices, the simplest one is perhaps

$$W_x(t) = \beta(\gamma_1 - \gamma_\ell) \int_0^t J_{x,x+1}(s)ds = \beta(\gamma_1 - \gamma_\ell)\tilde{W}_x(t)\,. \tag{4.7}$$

$W_x(t)$ differs from $W(t)$ only by a surface term. The action functional $\tilde{W}_x(t)$ is the time integrated particle current across the bond $(x, x + 1)$. The generating function for $\tilde{W}_x(t)$ satisfies the fluctuation theorem in the form $\tilde{e}(\lambda) = \tilde{e}(\beta(\gamma_1 - \gamma_\ell) - \lambda)$, with $\tilde{e}$ independent of the choice of x.

The conservation law (4.6) can be used also in the driven lattice gas of the previous section to produce equivalent action functionals. For example $W(t)$ of (3.5) is equivalent to

$$\bar{W}(t) = \ell\beta F \int_0^t J_{x,x+1}(s)ds\,. \tag{4.8}$$

However the symmetric form (3.5) seems to be more accessible to analytic computations, as can be seen from the examples described in the Appendix.

5 Fluctuation theorem for diffusion processes

We consider next a general diffusion process $x_t \in \mathbb{R}^n$. It is specified by a drift vector $c(x)$ (a vector field on $\mathbb{R}^n$) and a positive definite diffusion matrix $a(x) > 0$ (an $n \times n$ matrix valued function on $\mathbb{R}^n$). For later convenience we write the generator as

$$L = \frac{1}{2}\nabla \cdot (a\nabla) + c \cdot \nabla \tag{5.1}$$

with ∇ representing differentiation with respect to x. x_t is the solution of the stochastic differential equation

$$dx_t = (c + \frac{1}{2}(\nabla \cdot a))(x_t)dt + \sqrt{a}(x_t)db(t) \tag{5.2}$$

with $db(t)/dt$ standard white noise. We use Ito's convention for stochastic differentials.

We claim that for diffusion processes the action functional $W(t)$ is given by

$$W(t) = 2\int_0^t (a^{-1}c(x_s)) \cdot dx_s + \int_0^t a\nabla(a^{-1}c)(x_s)ds\,. \tag{5.3}$$

We may think of $W(t)$ as the limit of the symmetrized (Stratonovich) approximation,

$$W(t) = \lim_{\epsilon\to 0} \epsilon \sum_{j=0}^{t/\epsilon} (a^{-1}c(x_{(j+1)\epsilon}) + a^{-1}c(x_{j\epsilon})) \cdot (x_{(j+1)\epsilon} - x_{j\epsilon})\,. \tag{5.4}$$

If a is diagonal and independent of x, then $a_{ii}/2$ corresponds physically to the temperature β^{-1}. In this case $W(t)/\beta$ equals the work done by the force c on the system during the time span t, in accordance with the physical meaning of the action functional for lattice gases.

As before, we expect that the equilibrium forces do not show up in the large deviations of $W(t)$. For diffusion processes detailed balance with respect to $e^{-U(x)}$ means that

$$c = -\frac{1}{2}a\nabla U\,. \tag{5.5}$$

Inserting into (5.3), by Ito's lemma [29],

$$-\int_0^t \nabla U(x_s)\cdot dx_s - \frac{1}{2}\int_0^t a\nabla\nabla U(x_s)ds = U(x_0) - U(x_t)\,, \tag{5.6}$$

which is indeed a pure surface term. Only driving forces make a contribution to $W(t)$ proportional to t.

Since $a > 0$ by assumption, we are in the uniformly elliptic case, where the transition probability, e^{Lt}, has a density and $(e^{Lt})_{x,x'} > 0$ for $t > 0$. We require that the drift c is sufficiently confining. Then x_t has a unique stationary measure with density $\mu_s(x) > 0$, satisfying $\mu_s e^{Lt} = \mu_s$.

Let us denote by $\langle\cdot\rangle$ expectation with respect to the stationary process x_t (starting in the invariant measure μ_s). Then

$$\lim_{t\to\infty} -\frac{1}{t}\log\langle e^{-\lambda W(t)}\rangle = e(\lambda) \tag{5.7}$$

and the fluctuation theorem

$$e(\lambda) = e(1-\lambda) \tag{5.8}$$

should hold.

To prove (5.8), as for jump processes, we first define the function $g(x,t) = \mathbb{E}_x(\exp[-\lambda W(t)])$ as the expectation with respect to the stationary diffusion process x_t conditioned to start at x. Then $g(x,t)$ satisfies

$$\frac{\partial}{\partial t}g(x,t) = L_\lambda g(x,t) \tag{5.9}$$

with

$$L_\lambda = \frac{1}{2}\nabla\cdot(a\cdot\nabla) + c\cdot\nabla - 2\lambda c\cdot\nabla - \lambda(\nabla\cdot c) - 2\lambda(1-\lambda)c\cdot a^{-1}c\,, \tag{5.10}$$

where the last two terms act as multiplication operators. We conclude that

$$\langle e^{-\lambda W(t)}\rangle = \int\int \mu_s(x)(e^{L_\lambda t})_{x,x'}dxdx'. \tag{5.11}$$

On the other hand, from (5.10),

$$L_\lambda^* = L_{1-\lambda}\,, \tag{5.12}$$

which implies (5.8) by Perron-Frobenius.

Eqs. (5.10) and (5.11) can also be viewed as an application of the Cameron-Martin-Girsanov formula [29]. The path measure of the process generated by L_λ has a density relative to the path measure of the process generated by L. We write this density as $\exp[R]$. Then, according to [29], Section 6.4,

$$\begin{aligned} R &= -2\lambda\int a^{-1}c(x_t)\cdot dx_t + 2\lambda\int(a^{-1}c)\cdot(c+\frac{1}{2}\nabla a)(x_t)dt \\ &\quad -2\lambda^2\int c\cdot a^{-1}c(x_t)dt - 2\lambda(1-\lambda)\int c\cdot a^{-1}c(x_t)dt - \lambda\int\nabla\cdot c(x_t)dt \\ &= -2\lambda\int a^{-1}c(x_t)\cdot dx_t - \lambda\int a\nabla(a^{-1}c)(x_t)dt \\ &= -\lambda W(t)\,, \end{aligned} \tag{5.13}$$

where we used the identity

$$a(\alpha)\frac{d}{d\alpha}a^{-1}(\alpha) = -\left(\frac{d}{d\alpha}a(\alpha)\right)a^{-1}(\alpha) \tag{5.14}$$

valid for a parameter-dependent matrix $a(\alpha)$.

From the argument of Section 2, we conclude that $W(t)/t$ has large deviations as stated in (2.11) with a rate function satisfying the symmetry (2.10).

6 Particle under mechanical and thermal drive

In the stochastic differential equations of Section 5 the diffusion acts everywhere on the configuration space $\mathbb{R}^n$. This is appropriate for strongly overdamped stochastic systems such as those considered in time-dependent Ginzburg-Landau theories. In many physical situations, however, stochasticity is assumed to act only in velocity space. Then the matrix a in (5.1) has zero eigenvalues and, the results of Section 5 are not directly applicable. To understand the required modifications we consider, as an example, a mechanical particle of mass m with position x in the d-dimensional torus T^d and velocity v in $\mathbb{R}^d$ subject to noise and friction. The particle has the mechanical energy $H = \frac{1}{2}mv^2 + U(x)$, where U is some periodic potential. In equilibrium the stationary distribution is given by $\exp[-\beta H(x,v)]$ with β^{-1} the temperature. We envision two mechanisms to drive the system out of equilibrium: (i) There is a mechanical driving force $F(x)$. The standard example is a constant electric field E, i.e. $F(x) = E$. If F has a periodic potential part, it may be added to U but as we will see this has no effect on the large deviation of the action functional. (ii) There is a nonuniform temperature $\beta(x)^{-1}$. The case of a periodic variation in β (and constant friction) has been studied recently in the context of Brownian motors [30, 31] with the at first sight surprising result that the steady state maintains a nonzero current. The dynamics of the particle is governed by the stochastic differential equation

$$m\frac{d^2}{dt^2}x_t = -\nabla U(x_t) + F(x_t) - m\gamma(x_t)v_t + (2m\gamma(x_t)/\beta(x_t))^{\frac{1}{2}}\xi(t)\,. \tag{6.1}$$

Here $\gamma(x) > 0$ is the friction coefficient, $\beta(x) > 0$ the inverse temperature and $\xi(t)$ standard white noise. The generator of the corresponding Fokker-Planck equation reads

$$L = v\cdot\nabla_x + \left(-\frac{1}{m}\nabla U + \frac{1}{m}F - \gamma(x)v\right)\cdot\nabla_v + (\gamma(x)/m\beta(x))\nabla_v^2\,. \tag{6.2}$$

We claim that the action functional for the fluctuation theorem is given by

$$W(t) = \int_0^t \beta(x_s)F(x_s)\cdot dx_s + \int_0^t H(x_s,v_s)d\beta(x_s) \tag{6.3}$$

for x_s, v_s a solution to (6.1). The first term is $\beta\times$(work done by F) and the second term represents $\beta\times$(work due to thermal gradients) integrated along the trajectory x_s, $0 \le s \le t$. If $F = -\nabla V$, then up to a surface term $\int_0^t \beta(x_s)F(x_s)\cdot dx_s = \int_0^t V(x_s)d\beta(x_s)$ which, in (6.3), should be added to the energy $H(x,v)$.

Let $\langle\cdot\rangle$ denote the stationary average for (6.1). Then

$$\lim_{t\to\infty} -\frac{1}{t}\log\langle e^{-\lambda W(t)}\rangle = e(\lambda) \tag{6.4}$$

and $-e(\lambda)$ is the maximal eigenvalue of

$$L_\lambda = L - \lambda(\beta(x)F(x)\cdot v + H(x,v)v\cdot\nabla_x\beta(x))\,, \tag{6.5}$$

the last two terms being considered as multiplication operators. The corresponding maximal eigenvector is denoted by $f_\lambda(x,v) > 0$. Let R be the velocity reversal operator, $Rf(x,v) = f(x,-v)$. Then

$$Re^{-\beta(x)H}L_\lambda e^{\beta(x)H}R^{-1}Re^{-\beta(x)H}f_\lambda(x,v) = -e(\lambda)Re^{-\beta(x)H}f_\lambda(x,v)\,. \tag{6.6}$$

By a straightforward computation

$$Re^{-\beta(x)H} L_\lambda e^{\beta(x)H} R^{-1} = L^*_{1-\lambda} . \tag{6.7}$$

Therefore

$$L^*_{1-\lambda} Re^{-\beta H} f_\lambda = -e(\lambda) Re^{-\beta H} f_\lambda = -e(1-\lambda) Re^{-\beta H} f_\lambda \tag{6.8}$$

by Perron-Frobenius, since $Re^{-\beta(x)H} f_\lambda(x,v) > 0$. We conclude that the fluctuation theorem holds and $e(\lambda) = e(1-\lambda)$.

As for lattice gases, we expect that the action functional $W(t)$ is linked to the entropy balance. To spell out the details we consider the time-dependent probability density $\rho_t(x,v)$ of (x_t, v_t). It satisfies $\frac{\partial}{\partial t}\rho_t = L^*\rho_t$. As usual the Gibbs entropy is given by $S_G(\rho_t) = -\int \rho_t \log \rho_t dxdv$ and changes in time as

$$\frac{d}{dt} S_G(\rho_t) = \sigma(\rho_t) + j_s(\rho_t) . \tag{6.9}$$

The first term

$$\sigma(\rho_t) = \int \gamma \frac{1}{\rho_t} [\sqrt{m\beta} v \rho_t + \frac{1}{\sqrt{m\beta}} \nabla_v \rho_t]^2 dxdv \tag{6.10}$$

is positive definite. We identify it as the entropy production in the system. The remainder reads

$$j_s(\rho_t) = \frac{d}{dt} \int \rho_t \beta H dxdv - \int \rho_t \beta F \cdot v dxdv - \int \rho_t H v \cdot \nabla_x \beta dxdv . \tag{6.11}$$

We regard it as the entropy flow from the system to the mechanical and heat reservoirs.

According to the rules used before, we construct $W(t)$ by integrating the linear functional defining the entropy flow along a stochastic trajectory. Using (6.11) this yields

$$\int_0^t \left\{ -\frac{d}{ds} \beta H(x_s, v_s) + \beta F(x_s) \cdot v_s + H(x_s, v_s) v_s \cdot \nabla \beta(x_s) \right\} ds . \tag{6.12}$$

Since the first summand is a surface term, we recover (6.3).

7 Stochastic and thermostatting heat reservoirs

Physical systems with stationary flows of heat, momentum, etc., are usually modeled by coupling the system to thermal reservoirs represented by stochastic forces acting near the boundaries [1]–[7]. Away from the boundary the time evolution obeys the same laws as an isolated system. To be specific, let us consider one such model of heat flow through a classical system of N particles of mass m with position q_j, momentum $p_j, j = 1, \ldots, N$, inside the slab $\Lambda = [-\ell - a, \ell + a] \times [0, \ell]^2$. Let the boxes $\Lambda_- = [-\ell - a, -\ell] \times [0, \ell]^2$, $\Lambda_+ = [\ell, \ell + a] \times [0, \ell]^2$ be the left and right boundary zones. The indicator functions of these sets are denoted by $\chi_\pm$. The particles interact through a short range pair potential V and are confined to the slab by the wall potential V_w. The equations of motion are

$$\begin{aligned}
\frac{d}{dt} q_j &= \frac{1}{m} p_j \,, \\
\frac{d}{dt} p_j &= F_j + F_w(q_j) + \sum_{\delta = \pm} \chi_\delta(q_j)(-\gamma p_j + (2m\gamma/\beta_\delta)^{1/2} \xi_j(t)) \,,
\end{aligned} \tag{7.1}$$

where $q_j \in \Lambda, p_j \in \mathbb{R}^3$, F_j is the force acting on the j-th particle, $F_j = -\sum_{i \neq j = 1}^N \nabla V(q_j - q_i), F_w = -\nabla V_w$ is the force from the wall. $\{\xi_j(t)\}$ are a collection of independent white noises. The friction and the stochastic forces operate only when the particle is in the boundary layers acting there like thermal reservoirs at inverse temperature β_δ. If $\beta_+ = \beta = \beta_-$, then the steady state is $Z^{-1} \exp[-\beta H]$, $H = \sum_{j=1}^N (\frac{1}{2m} p_j^2 + V_w(q_j)) + \frac{1}{2} \sum_{i,j=1}^N V(q_i - q_j)$. If $\beta_+ \neq \beta_-$, there is, in the steady state, a constant heat flux from the higher to the lower temperature reservoir. (This is a variation of the model used to describe heat flow in a crystal where the Langevin forces act on the particles in the end layers [3], [10]).

We now follow the method explained in Section 6. For the similarity transformation we use

$$\exp \left[-\sum_{j=1}^N \beta(q_j) \left\{ \frac{1}{2m} p_j^2 + V_w(q_j) + \frac{1}{2} \sum_{i=1}^N V(q_i - q_j) \right\} \right] . \tag{7.2}$$

The local inverse temperature $\beta(q) = \beta_\delta$ for $q \in \Lambda_\delta$ and $\beta(q)$ interpolates smoothly otherwise. For each choice of $\beta(q)$ we obtain a distinct action functional $W(t)$. By local conservation of energy, these differ only through boundary terms. For later purposes it is convenient to choose a step interpolation as $\beta(q) = \beta_-$ for $q_1 < 0$ and $\beta(q) = \beta_+$ for $q_1 \geq 0$. Then the action functional is

$$W(t) = (\beta_+ - \beta_-) \int_0^t ds J_0(s) \tag{7.3}$$

with J_0 the energy current through the plane $\{q_1 = 0\}$,

$$\begin{aligned}
J_0 &= \sum_{j=1}^N \frac{1}{m} p_j \left\{ \frac{1}{2m} p_j^2 + \frac{1}{2} \sum_{i \neq j = 1}^N V(q_i - q_j) \right\} \delta(q_{j1}) \\
&+ \frac{1}{2} \sum_{i,j=1}^N \frac{1}{2m} [((p_j + p_i) \cdot F(q_j - q_i))(q_j - q_i) \int_0^1 d\lambda \delta(\lambda q_{j1} + (1 - \lambda) q_{i1}) \,,
\end{aligned} \tag{7.4}$$

where q_{j_1} is the x-component of the jth particle position vector.

As an advantageous numerical alternative deterministic thermostatting reservoirs have been developed [16]. We mention here the proposal of Gallavot-ti and Cohen [22] for thermal reservoirs. The equations of motions are Newtonian in the bulk. At the boundary layers Λ_+ and Λ_- additional friction terms are added which are constructed in such a way that the total kinetic energy of the particles in Λ_+, resp. Λ_-, is kept constant. The particular boundary temperature is then fixed through the initial conditions. The equations of motion read

$$\begin{aligned} \frac{d}{dt} q_j &= \frac{1}{m} p_j \,, \\ \frac{d}{dt} p_j &= F_j + F_w(q_j) + \sum_{\delta=\pm} \chi_\delta(q_j) \alpha_\delta p_j \,. \end{aligned} \tag{7.5}$$

The 'friction' coefficients α_+, α_- are given by

$$\begin{aligned} \alpha_\delta &= \left[\sum_{j=1}^N \chi_\delta(q_j) p_j^2 \right]^{-1} \sum_{j=1}^N \left\{ \frac{1}{m} p_j \cdot \nabla \chi_\delta(q_j) \frac{1}{2m} p_j^2 \right. \\ &\quad \left. + \frac{1}{m} \chi_\delta(q_j)(F_j + F_w) \cdot p_j \right\} \,, \quad \delta = \pm 1 \,. \end{aligned} \tag{7.6}$$

For thermostatted systems the action functional is the phase space contraction integrated along a trajectory of the dynamical system, which in our case equals

$$3N\sigma = 3N_+\alpha_+ + 3N_-\alpha_- + \mathcal{O}(1) \tag{7.7}$$

with $N_\pm$ the number of particles in $\Lambda_\pm$. The fluctuation theorem holds provided the dynamics is sufficiently hyperbolic for the SNS to be described by an SRB measure. This is not expected to be true in general. It is then an assumption, embodied in the chaotic hypothesis [24], that the fluctuation theorem remain valid for realistic physical systems. The numerical simulation in [32] gives strong support for the validity of the fluctuation theorem in one such model. There the two heat reservoirs are linked through an anharmonic chain, rather than a fluid. Further numerical support comes from a study of shear flow for hard disks in a box [33] where momentum but no energy is transferred to the system at opposite boundaries. The fluctuation theorem is well verified [34], although it seems to be difficult to get beyond the quadratic approximation.

The action functional defined with the phase space contraction (7.7) appears to be rather different than the one of (7.3). However the conservation law can be used again to transform a boundary flux to an interior flux. Let H_1 be the total energy of particles in the left half box $[-a-\ell, 0] \times [0, \ell]^2$. We have

$$\frac{d}{dt} H_1(t) = -J_0(t) - \left[\sum_{j=1}^N \chi_-(q_j) p_j^2 \right] \alpha_-$$

$$= \quad -J_0(t) - \frac{1}{\beta_-}3N_-\alpha_- \,, \tag{7.8}$$

since $\sum_{j=1}^{N} \chi_-(q_j)p_j^2$ is a constant of motion and initially fixed to $3N_-/\beta_-$. We conclude that

$$\int_0^t ds 3N\sigma(s) = -H(t) + H(0) + (\beta_+ - \beta_-)\int_0^t ds J_0(s) \,. \tag{7.9}$$

Up to a boundary term the phase space contraction is just the energy flux across the plane $\{q_1 = 0\}$, the same quantity which has been obtained for stochastic reservoirs, compare with (4.7).

It is tempting to assume that for stochastic and thermostatted boundaries, the rate functions of the fluctuation theorem are identical. This requires however a very strong form of equivalence of ensembles, in the sense that in the interior of the system even the large deviations of the current are in the steady state independent of the mechanism by which the boundaries are cooled/heated. This appears to be the case for the model studied in [32]. On the other hand recent simulations [36] suggest that this equivalence fails for the model described in [33]–[34].

8 Green-Kubo formula, Onsager reciprocity

As observed in [24] the fluctuation theorem yields the Green-Kubo formula at equilibrium. We give an alternate derivation in the spirit of [25]. For the sake of concreteness we consider a k-species lattice gas on a d-dimensional lattice. The lattice gas is driven by an external field, cf. Section 3, and satisfies local detailed balance. For each species the driving field is a d-component vector. It is convenient to regard the driving field as the m-component vector $\vec{F} = (F_1, \ldots, F_m)$, $m = d \times k$. There are m different types of jump, labeled by the species and lattice directions. Therefore the generator of the lattice gas is the sum

$$L = \sum_{j=1}^{m} L^{(j)} \,, \tag{8.1}$$

where each $L^{(j)}$ satisfies the conditions of Section 2.3, compare with (2.23). To each $L^{(j)}$ there is associated the current $J_j(t)$.

We define

$$e(\vec{F}; \lambda_1, \ldots, \lambda_m) = \lim_{t\to\infty} -\frac{1}{t}\log\langle\exp[-\beta\sum_{j=1}^{m}\int_0^t \lambda_j J_j(s)ds]\rangle_{\vec{F}} \,, \tag{8.2}$$

where we have, in the action, absorbed F_j into the λ_j's and indicated explicitly the dependence of the stationary state and the dynamics on $\vec{F}$. The fluctuation theorem now takes the form

$$e(\vec{F}*;\lambda_1,\ldots,\lambda_m)=e(\vec{F}*;F_1-\lambda_1,\ldots,F_m-\lambda_m)\,. \tag{8.3}$$

We have $\langle J_j(t)\rangle_0=0$, since $\vec{F}=0$ corresponds to equilibrium. Differentiating (8.2) at $\lambda=0$, we obtain

$$\frac{\partial}{\partial\lambda_j}e(\vec{F}*;0)=\beta\langle J_j(t)\rangle_{\vec{F}}\,, \tag{8.4}$$

the average j-th current.

Now the linear response in the average current to a small driving field is given by

$$\frac{\partial}{\partial F_j}\frac{1}{\beta}\frac{\partial}{\partial\lambda_i}e(0;0)=\sigma_{ij}\,. \tag{8.5}$$

Differentiating (8.3) with respect to $\vec{F}$ and $\vec{\lambda}$ at $\vec{F}=\vec{\lambda}=0$ we conclude that

$$\beta\sigma_{ij}=-\beta\sigma_{ij}+\beta^2\hat{\sigma}_{ij} \tag{8.6}$$

and therefore

$$\sigma_{ij}=\frac{1}{2}\beta\hat{\sigma}_{ij}\,, \tag{8.7}$$

where

$$\hat{\sigma}_{ij}=-\frac{1}{\beta^2}\frac{\partial}{\partial\lambda_i}\frac{\partial}{\partial\lambda_j}e(0;0)=\int_{-\infty}^{\infty}dt\langle J_i(t)J_j(0)\rangle_0\,. \tag{8.8}$$

This is the standard Einstein-Green-Kubo relation between linear response in the current and the time–integrated current–current correlation, which satisfies the Onsager relation $\hat{\sigma}_{ij}=\hat{\sigma}_{ji}$.

We remark that the derivation of (8.7) differs considerably from the standard computation, we refer to [28] for an exposition of the latter. There one differentiates, at finite volume, the steady state current $\langle j_{\vec{F}}\rangle_{\vec{F}}$ at $\vec{F}=0$, which by definition equals σ_{ij}. This gives two terms: one from differentiating the current function $j_{\vec{F}}$ and one from differentiating the steady state $\langle\cdot\rangle_{\vec{F}}$. Their sum is then (8.8), because $\langle J_i(t)J_j(0)\rangle_0$ has a δ-peak at $t=0$, whose weight is the first term, and a smooth piece, whose time integral equals the second term.

9 Conclusions

Within the framework of stochastic dynamics the fluctuation theorem holds in great generality. For finite state spaces, like stochastic lattice gases, we have given a proof. For the nondegenerate diffusion processes of Section 5 we could provide sufficient conditions on the driving forces and the diffusion matrix which ensure the validity of (5.8). The situation is more delicate for degenerate diffusion processes, in particular for deterministic bulk systems driven by stochastic boundaries. Since the noise vanishes on large parts of the phase space, even the convergence to the steady state is not obvious. To our knowledge there are only a few rigorous investigations of SNS of this type [3, 4, 5, 7, 10]. In [5, 7] classical point particles are considered. At a collision with the wall they are reflected with a Maxwellian distribution at the local temperature of the wall. Existence and uniqueness of the invariant measure is established provided the forces are repulsive and have a range of the size of the box. This latter property prevents pockets in phase space which never see the wall. In [3] explicit SNS measures are obtained for a harmonic chain coupled to stochastic reservoirs specified by Langevin forces at the ends of the chain. While in [10] an anharmonic chain is coupled to a free field leading to similar boundary conditions. For this system existence and uniqueness of the invariant measure is established in under a Hörmander condition. We expect that for these systems the GC fluctuation theorem can be proved. Thermostatted boundaries are beyond our mathematical abilities at the present time.

Viewed from the physics point of view the fluctuation theorem is a consequence of time-reversal. For a given stationary stochastic process one considers the density of the path measure of the time-reversed process relative to the original one. The logarithm of this density is the action functional which satisfies the fluctuation theorem. At this level of generality it is somewhat unexpected that in concrete models, which satisfy the condition of local detailed balance, the action functional has a direct physical interpretation. By separating the rate of change of Gibbs entropy into a production and flow term we identify the observable whose average defines the entropy flow. The action functional is then this observable integrated along a stochastic trajectory. Generically it is the current, multiplied by the driving force, corresponding to the conserved field. The GC fluctuation theorem is then a symmetry property for the large deviations in the current. Such large deviations are not readily observed in physical systems, because they refer to exponentially small probabilities. Also in numerical experiments special efforts are needed [23], [34], [35]. Even worse, the action functional is extensive and the probabilities are exponentially small also in N. *Thus it would be desirable to have a local quantity satisfying (at least approximately) the fluctuation theorem but this does not appear to be the case for the systems investigated numerically thus far [34], [36].

There is one prediction of the fluctuation theorem which is worthwhile to emphasize. We use the convention of the previous section where the symmetry reads $e(\lambda) = e(F-\lambda)$, i.e. e is even relative to $\lambda = F/2$, and we may expand as $e(\lambda) = e_0 + \frac{1}{2}e_2\lambda(F-\lambda)+\ldots$. Assuming that in the interval $-\delta < \lambda < F+\delta$ with some small $\delta > 0$ the quadratic approximation is valid, then by differentiating at $\lambda = 0$ we obtain $\langle j\rangle_F = e_2 F/2$, where $e_2 = \int_{-\infty}^{\infty} dt(\langle J(t)J(0)\rangle_F - \langle J(t)\rangle_F\langle J(0)\rangle_F)$ will generally depend on F. The nonlinear response in the current is then linked to the time-integral over the current-current correlation. The knowledge of $e(\lambda)$ thus provides information about the range of validity of the Einstein relation and linear response theory.

A Appendix: Large deviation function for the asymmetric exclusion process

To determine the large deviation function in any of the models we have discussed is like computing a free energy in equilibrium statistical mechanics. Therefore it is not surprising that even in the stochastic framework explicit results are available only for a few models. We discuss here the large deviation function for the asymmetric simple exclusion process in one dimension where particles random walk with an average drift and interact through the constraint that there can be at most one particle per lattice site. As a warm up we consider this model without constraint, i.e. independent biased random walks on a lattice. It would be of interest to have also an example for the boundary driven lattice gases of Section 4. Besides independent particles, the simplest model is symmetric exclusion in the bulk and boundary reservoirs as discussed in Section 4. Its large deviaiton function, for $\tilde{W}_x(t)$, satisfies then $e(\lambda) = e(\beta(\gamma_1 - \gamma_\ell) - \lambda)$, cf. (4.7). Thus in the limit $\gamma_1 \to \infty$, i.e. at the left boundary particles are only injected, the GC fluctuation theorem predicts $\lim_{t\to\infty}(-1/t)\log \mathrm{Prob}(\{\tilde{W}_x < at\}) = 0$ for $a < 0$.

We first consider N independent particles, i.e. no exclusion, on a ring of size ℓ driven by a uniform force of strength F. Since particles are independent, it suffices to study the one-particle problem. For N particles we merely have to multiply by N at the end. It is convenient to set $\beta F/2 = E$. The generator for the dynamics reads

$$L_E f(x) = (e^E/2\cosh E) f(x+1) + (e^{-E}/2\cosh E) f(x-1) - f(x)\,. \qquad \text{(A.1)}$$

The elementary jump time is normalized such that for $E \to \infty$ the jump rate to the right is one. $W(t)$ is now the total number of signed jumps up to time t. To compute the generating function $\langle e^{-\lambda W(t)}\rangle$ for large t we need the maximal eigenvalue of

$$L_{E,\lambda} f(x) = (e^{E-\lambda}/2\cosh E) f(x+1) + (e^{-E+\lambda}/2\cosh E) f(x-1) - f(x)\,. \qquad \text{(A.2)}$$

Clearly $f = 1$ solves $L_{F,\lambda} f = -e(\lambda) f$ with

$$e(\lambda) = 1 - (\cosh(E-\lambda)/\cosh E)\,. \qquad \text{(A.3)}$$

Its Legendre transform is given by

$$\hat{e}(w) = -Ew + 1 + w\mathrm{argsinh}(w\cosh E) - \sqrt{w^2 + (\cosh E)^{-2}}\,. \qquad \text{(A.4)}$$

$\hat{e}$ vanishes at the average current $j = \tanh E$. On general grounds we know that $e(\lambda)$ is convex down, $e(0) = 0, e'(0) = -j$, the average current, $e(\lambda) = e(2E - \lambda)$

and that $\hat{e}(w)$ is convex up, $\hat{e}(w) \geq 0$, $\hat{e}(w_0) = 0$ for $w_0 = j = \frac{1}{t}\langle W(t)\rangle$, $\hat{e}(w) - \hat{e}(-w) = -2Ew$.

Note that in the limit $E \to \infty$, $\hat{e}$ degenerates to $\hat{e}(w) = 1 - w + w\log w$ for $w \geq 0$ and $\hat{e}(w) = \infty$ for $w < 0$, which merely reflects that left jumps have probability zero for $E = \infty$.

We expect more structure for particles interacting through hard core exclusion. This corresponds to $H(\eta) = 0$ in the notation of Section 3. The jump rates with a uniform driving field are then

$$c^E_{xx+1}(\eta) = (e^E/2\cosh E)\eta_x(1-\eta_{x+1}) + (e^{-E}/2\cosh E)(1-\eta_x)\eta_{x+1}\,. \qquad \text{(A.5)}$$

We normalized the rates such that for $E \to \infty$ a particle jumps with unit rate to the right. (A.5) are the jump rates of the asymmetric simple exclusion process (ASEP).

The action functional $W(t)$ is the total current integrated over the time span t. Expectations, $\langle\cdot\rangle$, are taken in the stationary process at a given number of particles N, $1 \leq N \leq \ell - 1$. For the ASEP this means that at time $t = 0$ all allowed configurations have equal weight. Then

$$\lim_{t\to\infty} -\frac{1}{t}\log\langle e^{-\lambda W(t)}\rangle = e_E(\lambda, \ell, N) \qquad \text{(A.6)}$$

and $-e_E$ is the maximal eigenvalue of L_λ with

$$L_\lambda f(\eta) = (2\cosh E)^{-1}\sum_{x=1}^{\ell}\big\{(e^{E-\lambda}\eta_x(1-\eta_{x+1}) + e^{-(E-\lambda)}(1-\eta_x)\eta_{x+1}) \\ f(\eta^{xx+1}) - (e^E\eta_x(1-\eta_{x+1}) + e^{-E}(1-\eta_x)\eta_{x+1})f(\eta)\big\}\,. \qquad \text{(A.7)}$$

The fluctuation theorem reads

$$e_E(\lambda) = e_E(2E - \lambda)\,, \qquad \text{(A.8)}$$

which can be seen also directly from (A.7).

L_λ is a linear operator with a structure which is similar to that of the hamiltonian for a quantum spin chain. To make contact with that model we rewrite L_λ in terms of the Pauli spin $\frac{1}{2}$ matrices $\vec{\sigma}_x = (\sigma^1_x, \sigma^2_x, \sigma^3_x)$ associated to every lattice site x. We identify $\eta_x = 1$ with spin up, $\sigma^3_x = 1$, and $\eta_x = 0$ with spin down, $\sigma^3_x = -1$. Then

$$-L_\lambda = H_\lambda = \sum_{x=1}^{\ell}\big\{(1/4)(1-\sigma^3_x\sigma^3_{x+1}) - (e^{E-\lambda}/2\cosh E)\sigma^+_x\sigma^-_{x+1} \\ -(e^{-E+\lambda}/2\cosh E)\sigma^-_x\sigma^+_{x+1}\big\}\,, \qquad \text{(A.9)}$$

where $\sigma^\pm_x = \frac{1}{2}(\sigma^1_x \pm i\sigma^2_x)$ are the spin raising and lowering operators. We note that $H^*_\lambda \neq H_\lambda$, unless $E = \lambda$, and H_λ does not have directly a quantum mechanical interpretation, except through analytic continuation in λ.

To determine the ground state energy of H_λ, the only technique available is the Bethe ansatz. Fortunately, H_λ is covered by the famous paper of Sutherland and Yang [37]. However, the analysis of the nonlinear Bethe equations still require a considerable effort, which in our section of parameter space has been carried out only recently. We use the results by D.Kim [38]. He is in fact interested in the energy gap, but also gives $e_E(\lambda,\ell,N)$ to leading order in N in the limit $\ell\to\infty$, $N\to\infty$, $\rho=N/\ell$ fixed. We expect that also order 1 terms could be obtained, but such an analysis is certainly beyond the scope of our paper. In the limiting case $E\to\infty$, the Bethe equations simplify. This has been exploited recently by Derrida et al. [39, 40]. They determine $e_\infty(\lambda,\ell,N)$ fairly explicitly and discuss the order 1 corrections to the infinite volume limit.

To leading order in N, $N/\ell=\rho$, we have

$$e_E(\lambda,\ell,N)\cong \ell\bar{e}_E(\lambda,\rho)\,, \tag{A.10}$$

i.e. e_E is extensive. $\bar{e}_E$ has a flat piece, $\bar{e}_E(\lambda,\rho)=0$ for $0\le\lambda\le 2E$. At $\lambda=0$, $\bar{e}_E$ has the slope $\rho(1-\rho)\tanh E$ and the asymptotics [38]

$$\begin{aligned}\bar{e}_E(\lambda,\rho) &= \rho(1-\rho)(\tanh E)\lambda \\ &- \frac{1}{20}\left(\frac{3\pi}{2}\right)^{2/3}(4\rho(1-\rho))^{4/3}(\tanh E)|\lambda|^{5/3}(1+\mathcal{O}(|\lambda|^{2/3}))\end{aligned} \tag{A.11}$$

for $\lambda<0$. By symmetry $\bar{e}_E$ has the same asymptotics at $\lambda=2E$. For $E\to\infty$, the right zero $e_E(\lambda,\ell,N)$ moves to ∞ and the flat piece of $e_E(\lambda,\ell,N)$ never levels off, in agreement with [39, 40].

$\bar{e}'(0)$ is just the average current which is $\rho(1-\rho)\tanh E$. $\bar{e}''(0)$ is formally the integral over the total current-current correlation and therefore the mobility of the lattice gas [28]. In our case $\bar{e}''(0)=\infty$, which reflects the fact that in the ASEP density fluctuations propagate superdiffusively [41].

At $E=0$ (A.6) gives the large deviations in the total current at equilibrium, i.e. for the symmetric simple exclusion process. The fluctuation theorem reduces then to $e_{0,\ell,N}(\lambda)=e_{0,\ell,N}(-\lambda)$, which also follows from time reversibility. $\bar{e}_0(\lambda,\rho)$ has no longer a flat piece. For small $\lambda, \bar{e}_0(\lambda,\rho)=-\frac{1}{2}\lambda^2\rho(1-\rho)$. Thus the mobility $\sigma(\rho)=\rho(1-\rho)$ and the diffusion constant, which is σ divided by the compressibility, $D(\rho)=1$, independent of the density in agreement with the known bulk diffusion of the symmetric simple exclusion process. The more precise asymptotics [38] is given by

$$\bar{e}_0(\lambda,\rho)=-\frac{1}{2}\rho(1-\rho)\lambda^2-\frac{1}{20}2^{1/3}(2\pi)^{2/3}(\rho(1-\rho))^{4/3}|\lambda|^{8/3}(1+\mathcal{O}(|\lambda|^{4/3}). \tag{A.12}$$

On a formal level the "Burnett coefficients" correspond to higher derivatives of $\bar{e}_E(\lambda)$ at $\lambda=0$ [42]. (A.12) shows that for the symmetric simple exclusion process the Burnett coefficients are infinite.

Just as free energies, the large deviation function may become singular in the infinite volume limit and this happens already for the first nontrivial example. To understand the origin of this behavior, it is necessary to analyze those configurations which give the main contribution to $\langle e^{-\lambda W(t)}\rangle$. If $\lambda \to \infty$ only left jumps are permitted and similarly for $\lambda \to -\infty$ only right jumps are permitted, essentially independent of the driving field E, $E > 0$ for the sake of discussion. However, in the intermediate regime $0 \le \lambda \le 2E$, the particles have two opposing instructions. Should they follow E or λ? In fact, neither. As can be inferrred from the maximal eigenvector, they just stick and form one big cluster [43]. The clustering is seen most easily at $\lambda = E$, where H_λ is the ferromagnetic, anisotropic Heisenberg model and the maximal eigenvector its ground state. At our parameters, H_λ is in the ferromagnetic phase. Since the magnetization is fixed, typical configurations condense into one large cluster. In our units the corresponding ground state energy is of order 1 independent of ℓ.

It is instructive to reconsider our result from the point of view of the probability distribution of $W(t)/t$, which is obtained from the Legendre transform of $\bar{e}_E(\lambda)$. To make it well defined, we note that, for large N, $e_E(\lambda)$ smoothly interpolates between $e_E(0) = 0 = e_E(2E)$, such that $e'_E(0) = Nj(\rho), e'_E(2E) = -Nj(\rho), j(\rho) = \rho(1-\rho)\tanh E$, and $e_E(E) = \mathcal{O}(1)$. Thereby we obtain, for $E \ge 0$,

$$\hat{\bar{e}}_E(w,\rho) = \begin{cases} 0 & \text{for} \quad 0 \le w \le j(\rho)\,, \\ -2Ew & \text{for} \quad -j(\rho) \le w \le 0\,. \end{cases} \tag{A.13}$$

For w slightly larger than $j(\rho)$ we have $\hat{\bar{e}}_E(w,\rho) \simeq (w - j(\rho))^{5/2}$ and $\hat{\bar{e}}_E(w,\rho) \simeq w \log w$ in the limit of large w. For $w < -j(\rho)$ the values of $\hat{\bar{e}}_E$ are fixed by the fluctuation theorem.

To understand the N-dependence of $\hat{e}_E(w,\ell,N)/\ell$, we note that for $W(t)/Nt$ to have a value larger than $j(\rho)$ we have to speed up all N particles. For it to have a value smaller than $j(\rho)$ it suffices to slow down a single particle, since the other particles pile up behind. Typical configurations consist of essentially a single cluster. The large deviation rate is $\mathcal{O}(1/N)$ which on our scale corresponds to $\hat{\bar{e}}_E = 0$. Such a mechanism works only for $(W(t)/Nt) \ge 0$. To have a negative total current, again all N particles are forced to move, now opposite to E. The linear decrease of $\hat{e}_E(w < N, \ell)/\ell$ with corrections of $\mathcal{O}(1/N)$ for $-j(\rho) \le w \le 0$ follows from the fluctuation theorem. In the limit $E \to \infty$, $\hat{e}_E(w,\ell,N) = \infty$ for $w < 0$. This just reflects the fact that the underlying process does not allow for histories with negative currents.

From our discussion of $\hat{\bar{e}}$ we conclude that the non-smooth behavior of $\bar{e}(\lambda)$ for large N comes from blocking through slow particles, which suggests that, if we go to higher spatial dimension or soften the hard core, a smooth large deviation function may be recovered. But this remains to be seen. The symmetric case, $E = 0$, warns against too fast a conjecture.

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References

[1] P.G. Bergmann, J.L. Lebowitz, *New approach to nonequlibrium processes*, Phys. Rev. **99**, 578 (1955)

[2] J.L. Lebowitz, P.G. Bergmann, *Irreversible Gibbsian ensembles*, Annals of Physics **1**, 1 (1957)

[3] Z. Rieder, J.L. Lebowitz and E. Lieb, *Properties of a harmonic crystal in a stationary nonequilibrium state*, Journ. Math. Phys. **8**, 1073 (1967)

[4] A.J. O'Conner, J.L. Lebowitz, *Heat conduction and sound transmission in isotopically disordered harmonic crystals*, Journ. Math. Phys. **15**, 629 (1974)

[5] S. Goldstein, J.L. Lebowitz, E. Presutti, *Mechanical system with stochastic boundaries*. In: Random Fields, ed. J.Fritz, J.L.Lebowitz, D.Szász, Vol.I. North-Holland, Amsterdam 1979

[6] J.L. Lebowitz, *Exact results in nonequilibrium statistical mechanics: where do we stand?*, Prog. Theor. Physics, Supplement **64**, 35 (1978)

[7] S. Goldstein, C. Kipnis, N. Ianiro, *Stationary states for a mechanical system with stochastic boundary conditions*, J. Stat. Phys. **41**, 915 (1985)

[8] J.L. Lebowitz, H. Spohn, *Stationary nonequilibrium states of infinite harmonic systems*, Comm. Math. Phys. **54**, 97 (1977)

[9] S. Goldstein, J.L. Lebowitz, K. Ravishankar, *Approach to equilibrium in models of a system in contact with a heat bath*, J. Stat. Phys. **43**, 303 (1986)

[10] J.-P. Eckmann, C.-A. Pillet, L. Rey-Bellet, *Non-equilibrium statistical mechanics of anharmonic chains coupled to two heat baths at different temperatures*, preprint 1998, Texas Archive for Mathematical Physics

[11] S. Katz, J.L. Lebowitz, H. Spohn, *Stationary nonequilibrium states for stochastic lattice gas models of ionic superconductors*, J. Stat. Phys. **34**, 497 (1984)

[12] H. Spohn, *Long range correlations for stochastic lattice gases in a nonequilibrium steady state*, J. Phys. **A16**, 4275 (1983)

[13] G. Eyink, J.L. Lebowitz, H. Spohn, *Microscopic origin of hydrodynamic behavior: entropy production and the steady state*, in: 'Chaos, Soviet-American Perspectives in Nonlinear Science', Hg. D.K Campbell, p. 367. American Institute of Physics, 1990

[14] G. Eyink, J.L. Lebowitz, H. Spohn, *Hydrodynamics, fluctuations, and large deviations outside local equilibrium*, J. Stat. Phys. **83**, 385 (1996)

[15] W.G. Hoover, *Molecular Dynamics*. Lecture Notes in Physics 258. Springer, Heidelberg, 1986

[16] D.J. Evans, G.P. Morriss, *Statistical Mechanics of Nonequilibrium Fluids*. Acamdemic Press, London 1990

[17] N.J. Chernov, G.L. Eyink, J.L. Lebowitz, Ya.G. Sinai, *Derivation of Ohm's law in a determinisitic mechanical model*, Phys. Rev. Lett. **70**, 2209 (1993)

[18] N.J. Chernov, G.L. Eyink, J.L. Lebowitz, Ya.G. Sinai, *Steady-state electrical conduction in the periodic Lorentz gas*, Comm. Math. Phys. **154**, 569 (1993)

[19] D. Ruelle, *Positivity of entropy production in nonequilibrium statistical mechanics*, J. Stat. Phys. **85**, 1 (1996)

[20] G. Gallavotti, *Chaotic dynamics, fluctuations, nonequilibrium ensembles*, preprint, Texas Archive for Mathematical Physics No.97-266

[21] D. Ruelle, *New theoretical ideas in nonequilibrum statistical mechanics*. Lecture Notes, Rutgers University, fall 1997

[22] G. Gallavotti, E.G.D. Cohen, *Dynamical ensembles in stationary states*, J. Stat. Phys. **80**, 931 (1995)

[23] D.J. Evans, E.G.D. Cohen, G.P. Morriss, *Probability of second law violations in steady flows*, Phys. Rev. Lett. **71**, 2401 (1993)

[24] G. Gallavotti, *Chaotic hypothesis: Onsager reciprocity and fluctuation dissipation theorem*, J. Stat. Phys. **84**, 899 (1996)

[25] J. Kurchan, *Fluctuation theorem for stochastic dynamics*, J. Phys. A.: Math. Gen. **31**, 3719 (1998)

[26] F. Bonetto, G. Gallavotti, P. Garrido, *Chaotic principle: an experimental test*, Physica D **105**, 226 (1997)

[27] C. Maes, *The fluctuation theorem as a Gibbs property*, preprint, 1998

[28] H. Spohn, Large Scale Dynamics of Interacting Particles. Springer, Heidelberg 1991

[29] D. Stroock, S.R.S. Varadhan, Multidimensional Diffusion Processes. Springer, Berlin 1979

[30] M. Büttiker, *Transport as a consequence of state-dependent diffusion*, Z. Physik **68**, 161 (1987)

[31] Ya.M. Blanter, M. Büttiker, *Rectification of fluctuations in an underdamped ratchet*, preprint 1998

[32] S. Lipri, R. Livi, A. Politi, *Energy transport in anharmonic lattice close and far from equlibrium*, preprint, archived in xxx.lanl.gov.cond-mat ♯9709195

[33] N.I. Chernov, J.L. Lebowitz, *Stationary nonequilibrium states in boundary-driven Hamiltonian systems: shear flow*, J. Stat. Phys. **86**, 953 (1997)

[34] F. Bonetto, N.I. Chernov, J.L. Lebowitz, *(Global and local) fluctuations of phase space contraction in deterministic stationary non-equilibrium*, Chaos, 1998 (to appear)

[35] F. Bonetto, G. Gallavotti, P. Garrido, *Chaotic principle: an experimental test*, Physica D **105**, 226 (1997)

[36] F. Bonetto and J.L. Lebowitz (work in progress)

[37] B. Sutherland, C.N. Yang, C.P. Yang, *Exact solution of a model of two-dimensional ferroelectric in an arbitrary external electric field*, Phys. Rev. Lett. **19**, 588 (1967)

[38] D. Kim, *Bethe ansatz solution for crossover scaling functions of the asymmetric XXZ chain and the KPZ-type growth model*, Phys. Rev. **E 52**, 3512 (1995)

[39] B. Derrida, J.L. Lebowitz, *Exact large deviation function in the asymmetric exclusion process*, Phys. Rev. Lett. **80**, 209 (1998)

[40] B. Derrida, C. Appert *Universal large deviation function of the Kardar-Parisi-Zhang equation in one dimension*, preprint, 1998

[41] H. van Beijeren, R. Kutner, H. Spohn, *Excess noise for driven diffusive systems*, Phys. Rev. Lett. **54**, 2026 (1985)

[42] H. van Beijeren, *Transport properties of stochastic Lorentz models*, Rev. Mod. Phys. **54**, 195 (1982)

[43] C.N. Yang, C.P. Yang, *Ground state energy of a Heisenberg-Ising lattice*, Phys. Rev. **147**, 303 (1966)