# **Positivity of Entropy Production**<sup>1</sup>

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We discuss the positivity of the mean entropy production for stochastic systems driven from equilibrium, as it was defined in refs. 7 and 8. Non-zero entropy production is closely linked with violation of the detailed balance condition. This connection is rigorously obtained for spinflip dynamics. We remark that the positivity of entropy production depends on the choice of time-reversal transformation, hence on the choice of the dynamical variables in the system of interest.

KEY WORDS: Entropy production; nonequilibrium Gibbs states.

# 1. MOTIVATION

Boltzmann's famous formula  $S = \log W$  relates the Clausius thermodynamic entropy S with the configurational entropy  $\log W$ ; W denotes the "thermodynamic probability" obtained by "counting the number of microstates compatible with the values of a given set of macro-variables" for a system containing a huge amount of degrees of freedom (we ignored additive and multiplicative constants).

Going to open systems which are driven away from equilibrium by external forces (Clausius–Duhem processes) it is often no longer clear what are the "natural" macro-variables. This makes it difficult to apply the Gibbs formalism as method of statistical inference and to understand what nonequilibrium entropy can possibly mean.

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To start a statistical mechanics for non-equilibrium thermodynamics, a natural first step would be to consider the currents appearing in hydrodynamical (continuity) equations together with their microscopic expressions. These currents mostly correspond to the macroscopic variables (e.g., conserved quantities) one is used to work with in equilibrium. Driving the equilibrium system means applying gradients (via reservoirs) in chemical potential, pressure, temperature and the like. The non-equilibrium state is in the first place a current-carrying state and vice versa. From this point of view, the logical continuation must be to describe the open system in its steady state on a space-time level. By their very nature, currents consist of quantities passing a region in a given time. It is thus rather natural to attempt a space-time description in which given values of the currents determine the "action functional" governing the pathspace measure. The word "action-functional" stands for the analogue of the Hamiltonian generating the distribution of an equilibrium system but now our functional will contain both spatial and temporal integration. The space-time distribution is thus seen as a Gibbs measure in the traditional sense but with, for equilibrium, unusual constraints or ensembles. This is the Gibbsian hypothesis that was put forward in ref. 7 to be compared with the Chaoticity hypothesis of Gallavotti-Cohen, see refs. 2 and 3. The true (space-like) stationary state is then just the "projection" or "restriction" of this space-time steady state to a hypersurface (consisting of all space-time points which have the same time-coordinate).

Under the Gibbsian hypothesis, we now have a natural candidate for entropy production. The crucial point about currents is that they allow to break the time-reversal invariance that was present under equilibrium conditions. The equilibrium dynamics will give rise to a space-time steady state which is invariant under time-reversal. Imposing gradients adds however time-reversal symmetry breaking terms to the action functional (generating currents) and the time-reversed state is no longer equal to the original one. For almost all spacetime configurations, the mean entropy production (that we will define below) can be thought of as measuring the distance (in the sense of relative entropy) between the original space-time state and the time-reversed space-time state. The fluctuations of the entropy production (as a random variable) around that value are negligibly small in the spatiotemporal size of the observation window and they satisfy the same symmetry as in the Gallavotti–Cohen theorem, see refs. 1–3, 5, 7, 8, and 11.

In the present paper we are mostly concerned with the relation between positivity of entropy production and detailed balance. This relation becomes nontrivial only when dealing with systems in the thermodynamic limit. We prove the equivalence between zero entropy production and detailed balance only for spinflip processes. We wish to restrict us

here to that mathematically simplest case while it appears evident that the proof can be extended to for example diffusive systems which physically, for the purpose of studies of entropy production, are more interesting by the presence of conserved quantities.

# 2. ENTROPY PRODUCTION

### 2.1. Heuristics

Suppose we have obtained by some procedure a probability distribution  $P^J$  on the (microscopic) trajectories in phase space of our system which is consistent with the values of space-time macroscopic variables J. This distribution  $P^J$  represents the plausibilities that we attach within a model to certain time-series of microscopic states given certain macroscopic information. That time-series is produced by the dynamics but our probabilities are certainly not "created by nature" or by some "truly random or chaotic" dynamics.

One way to construct  $P^J$  is to start from an equilibrium dynamics and to add to the basic equations driving terms and reservoirs to generate currents. Starting from such a non-equilibrium dynamics one constructs the pathspace measure  $P^J$  with respect to some natural stationary measure. Macroscopic information is here contained in the choice of the amplitude by which the non-equilibrium condition is maintained. This amplitude may for example consist of the value of the temperature gradient between two reservoirs with which the system is brought into contact and in this case it is conjugate to the heat current. Or it may be the value of an external (electric) field (measuring the gradient in chemical or electric potential at the ends of the system) in which case it is conjugate to the particle or charge current.

A second way to obtain  $P^J$  is physically more pragmatic. There one starts with the choice of a reference pathspace measure  $P^0$  which is supposed to describe the unperturbed equilibrium steady state via a time-reversal invariant space-time action functional  $A^0$  ( $P^0 \simeq \exp(-A^0)$ ). It could correspond to a classical (or quantum) KMS state which is time-reversal invariant, see ref. 1 for a quantum example. Macroscopic information is contained in a choice of values for currents J and, in the spirit of the maximum entropy principle for equilibrium states, one simply expects  $P^J \sim$  $\exp - [A^0 + E \cdot J]$  as the space-time Gibbs state corresponding to the new action  $A^J = A^0 + E \cdot J$ . The product  $E \cdot J$  is responsible for breaking timereversal invariance and possibly includes a sum over different types of currents as well as a space-time integration.

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Whatever the case, we take it as part of our Gibbsian hypothesis that we have found the distribution  $P^J$  which, for the purpose at hand, correctly describes the plausibility of microscopic trajectories and for which it is possible to identify an action functional  $A^J$  on space-time.

In fact, for the definition of entropy production, not all details of the distribution  $P^J$  must be taken in consideration. The main point is that we wish to give meaning to the quantity

$$\dot{S}(\omega) = \log \frac{P^{J}(\omega)}{P^{J}(\theta\omega)} = A^{J}(\theta\omega) - A^{J}(\omega) = 2E \cdot J$$
(2.1)

where  $\theta$  is the time-reversal operation on space-time trajectories  $\omega$ , defined from  $(\theta\omega)(t) = \pi(\omega(-t))$ , where  $\pi$  is an involution (also sometimes called, time-reversal) on phase space, and where we used the antisymmetry of the currents under time-reversal:  $J(\theta\omega) = -J(\omega)$ . The relation (2.1) "defines" what we call the entropy production for a microscopic trajectory  $\omega$  when the relative weight  $P^J(\omega)/P^J(\theta\omega)$  is well-defined. This last condition must allow us to compare the plausibility of every trajectory with its time-reversed motion. It is clear that one needs to have that  $P^J(\theta\omega) = 0$  implies  $P^J(\omega) = 0$ . In other words, time-reversed trajectories must remain possible trajectories for the system (with perhaps a much smaller or a much larger plausibility) at least for the overwhelming majority of trajectories as measured by  $P^J$ . We call this property dynamical reversibility (as in ref. 12) but it should not be confused with microscopic reversibility (which is more or less the same as detailed balance).

Clearly, and on the same formal level, if we take the expectation of  $\dot{S}$  over  $P^{J}$ , that is in the non-equilibrium steady state (NESS), then the mean entropy production is obtained and, by concavity of the logarithmic function, it is clearly non-negative:

$$P^{J}(\dot{S}) = \left\langle \log \frac{P^{J}(\omega)}{P^{J}(\theta\omega)} \right\rangle_{\text{NESS}} \ge 0$$
(2.2)

with equality only if the pathspace action  $A^{J}$  is time-reversal invariant.

### 2.2. Definition

The above discussion and definition (2.1) have remained mathematically naive and physically vague. The main mathematical question is here to develop a sufficiently general theory of space-time Gibbs measures. For simplicity however, we merely repeat here the definition of entropy production for a Markov process with a finite state space. For more complicated

models the story is very similar. Let X be a finite set, the phase space, and let K be a finite set for the values of parameters. For every parameter value  $a \in K$  there is a stationary Markov process  $x_t, t \in \mathbb{R}$ , with positive transition rates  $p_a(x, y)$  for jumps  $x \to y$  and a stationary density  $\rho_a$  on X. We are given time-reversal transformations  $\pi_X$  on X and  $\pi_K$  on K, i.e., an involution leaving invariant the counting measure. For a trajectory  $\omega =$  $(x_1, x_2, ..., x_n)$  in X and a value  $a \in K$  for the parameters, the entropy production corresponding to the time-reversal  $\pi$  is

$$\dot{S}_a(\omega) = \ln \frac{p_a(x_1, x_2) \cdots p_a(x_{n-1}, x_n)}{\tilde{p}_a(x_n, x_{n-1}) \cdots \tilde{p}_a(x_2, x_1)}$$

where  $\tilde{p}_a(u, v) = p_{\pi_K(a)}(\pi_X(u), \pi_X(v))$ . The mean entropy production (MEP) in the stationary state  $\rho_a$  is the expectation value of  $\dot{S}_a(\omega)$  in the Markov process. It equals

$$MEP_{\pi}(\rho_{a}) = \sum_{x, y \in X} \rho_{a}(x) p_{a}(x, y) \ln \frac{p_{a}(x, y)}{\tilde{p}_{a}(y, x)}$$
(2.3)

A more general set-up with various examples also of calculations in specific models can be found in refs. 7 and 8; we just take (2.3) as our definition in the present simplest case.

### 2.3. Positivity

For the mean entropy production we are interested in conditions under which it is positive or when it is zero. For systems with a finite phase space, we have the following easy proposition:

**Proposition 2.1.** The mean entropy production defined in (2.3) satisfies

$$\operatorname{MEP}_{\pi}(\rho_a) \ge 0 \tag{2.4}$$

with equality if and only if

$$p_a(x, y) \rho_a(x) = \tilde{p}_a(y, x) \rho_a(y), \qquad x, y \in X$$
 (2.5)

The condition (2.5) is sometimes called generalized detailed balance. It will reappear as the equality in (4.24).

# 3. ENTROPY PRODUCTION FOR SPINFLIP PROCESSES

Spinflip dynamics are Markov (jump) processes for Ising spin configurations  $\sigma$  on an infinite lattice whereby the elementary transitions are spin flips  $\sigma \to \sigma^i$  governed by (spinflip) rates  $c(i, \sigma)$  at the sites *i* of the lattice. For simplicity we take the *d*-dimensional cubic lattice  $\mathbb{Z}^d$  to the sites of which we have assigned Ising spins  $\sigma(i) = \pm 1$ ,  $i \in \mathbb{Z}^d$ . The dynamics is defined via rates  $c(i, \sigma)$ : they give the probability per unit time that the spin at site *i* will flip when the current configuration is  $\sigma$ . After flipping at lattice site *i* the new configuration is denoted by  $\sigma^i$ . We make the standard assumptions that the rates are translation invariant, finite range and positive. This means that the process is spatially homogeneous, that the spinflip rates  $c(i, \sigma)$  only depend on the configuration  $\sigma$  restricted to a finite neighborhood of the site *i* and that there exists a constant  $\delta > 0$  so that  $c(i, \sigma) \ge \delta$ . We refer to ref. 6 for a mathematically precise definition and for more details.

To start we recall the notion of a potential for lattice spin systems. A potential is a family of local functions  $V_A$  on the spin configurations  $\sigma$  parametrized by the finite subsets A of  $\mathbb{Z}^d$  with

$$V_{A}(\sigma) = V_{A}(\sigma(i), i \in A)$$

and such that

$$\sum_{A \ni i} \sup_{\sigma} |V_A(\sigma)| < +\infty, \qquad i \in \mathbb{Z}^d$$
(3.6)

We say that the spinflip dynamics is a stochastic Ising model for the potential  $(V_A)$ , or shorter, satisfies the condition of detailed balance, when

$$\frac{c(i,\sigma)}{c(i,\sigma^{i})} = \exp\left(-\sum_{A\ni i} \left[V_{A}(\sigma^{i}) - V_{A}(\sigma)\right]\right)$$
(3.7)

A standard example is the Glauber dynamics for the Ising model in which case  $V_A(\sigma) = 0$  except when  $A = \{i, j\}$  is a pair of nearest neighbor sites *i*, *j* and then  $V_A = -\beta J\sigma(i) \sigma(j)$  for some inverse temperature  $\beta$  and coupling coefficient *J*.

Suppose now that we have a translation-invariant stationary probability distribution  $\rho$  for our spinflip dynamics. Stationarity of a probability measure  $\rho$  is expressed by condition

$$\int \rho(d\sigma) \sum_{i \in \mathbb{Z}^d} c(i, \sigma) [f(\sigma^i) - f(\sigma)] = 0$$
(3.8)

for all local functions f on the spin configurations. From  $\rho$  we can define its local spinflip transform  $\rho^i$ ,  $i \in \mathbb{Z}^d$ , via

$$\int \rho(d\sigma) f(\sigma^i) = \int \rho^i(d\sigma) f(\sigma)$$

for all local functions f. We say that  $\rho^i$  is absolutely continuous with respect to  $\rho$  if there exists an  $L^1(d\rho)$ -function  $r_i$ ,  $\int \rho(d\sigma) |r_i(\sigma)| < +\infty$ , for which

$$\int \rho^{i}(d\sigma) f(\sigma) = \int \rho(d\sigma) r_{i}(d\sigma) f(\sigma),$$

for all local f. We say that  $\rho$  is a Gibbs distribution for the potential  $(V_A)$  if

$$\int \rho(d\sigma) f(\sigma^{i}) = \int \rho(d\sigma) f(\sigma) \exp\left(-\sum_{A \ni i} \left[V_{A}(\sigma^{i}) - V_{A}(\sigma)\right]\right) \quad (3.9)$$

for all  $i \in \mathbb{Z}^d$  and for all local functions f. In this case we have

$$r_i(\sigma) = \frac{d\rho^i}{d\rho}(\sigma) = \exp\left(-\sum_{A \ni i} \left[V_A(\sigma^i) - V_A(\sigma)\right]\right)$$

In ref. 8 we obtained the following expression for the mean entropy production (MEP) in the stationary state  $\rho$ :

$$\operatorname{MEP}(\rho) = \int \rho(d\sigma) \ c(0,\sigma) \ln \frac{c(0,\sigma)}{c(0,\sigma^0)}$$
(3.10)

Here we used the standard time-reversal  $\theta(\sigma_t) = \sigma_{-t}$ , with  $\pi$  the identity. It is easy to see that when the spinflip dynamics satisfies detailed balance, as in (3.7), then MEP( $\rho$ ) = 0 for all translation invariant stationary distributions  $\rho$ .

**Proposition 3.1.** Suppose that the spinflip rates satisfy (3.7) for some potential  $(V_A)$  and that  $\rho$  is a translation invariant stationary distribution as in (3.8). Then,

# $MEP(\rho) = 0.$

*Proof.* Using translation invariance, we can substitute (3.7) in (3.10) to obtain that

$$\text{MEP}(\rho) = -\frac{1}{|\mathcal{A}|} \sum_{i \in \mathcal{A}} \int \rho(d\sigma) c(i, \sigma) \sum_{\mathcal{A} \ni i} \left[ V_{\mathcal{A}}(\sigma^{i}) - V_{\mathcal{A}}(\sigma) \right]$$

for all finite  $A \subset \mathbb{Z}^d$ . We now split the sum over  $A \ni i$  in two parts:  $A \subset \Lambda$ and  $A \cap \Lambda^c \neq \emptyset$ . For the first part we get

$$-\frac{1}{|\Lambda|} \sum_{i \in \Lambda} \int \rho(d\sigma) \, c(i,\sigma) [H_{\Lambda}(\sigma^{i}) - H_{\Lambda}(\sigma)]$$

with  $H_A(\sigma) = \sum_{A \subset A} V_A(\sigma)$  only depending on the spin configuration  $\sigma$  in  $\Lambda$ . Therefore, and by the stationarity (3.8) of  $\rho$ , this first part is equal to

$$\frac{1}{|\Lambda|} \int \rho(d\sigma) \sum_{i \in \Lambda^c} c(i, \sigma) [H_{\Lambda}(\sigma^i) - H_{\Lambda}(\sigma)] = 0$$

For the second part we get

$$-\frac{1}{|\Lambda|}\sum_{i\in\Lambda}\int\rho(d\sigma)\,c(i,\sigma)\sum_{\Lambda\ni i,\,A\cap\Lambda^c\neq\varnothing}\left[V_A(\sigma^i)-V_A(\sigma)\right]$$

But since the potential  $(V_A)$  is by definition uniformly and absolutely summable by (3.6), it easily follows that this second part goes to zero as  $\Lambda \uparrow \mathbb{Z}^d$  along a sequence of cubes.

**Remark.** When the potential  $V_A$  satisfies

$$\sum_{A \ge 0} |A| \sup_{\sigma} |V_A(\sigma)| < \infty$$
(3.11)

Proposition 3.1 can also be obtained as an application of Corollary 4.2 in ref. 4.

We see from the previous Proposition that the condition of detailed balance (3.7) implies that the MEP is zero for all translation invariant stationary states. We are now going to show a sort of inverse: if there is a "nice" stationary distribution  $\rho$  such that  $MEP(\rho) = 0$ , then the spinflip dynamics satisfies detailed balance. In particular,  $\rho$  is then necessarily a reversible Gibbs measure!

**Proposition 3.2.** Suppose  $\sup_{\sigma} c(0, \sigma) = M < \infty$ . Suppose  $\rho$  is a translation invariant probability measure such that  $d\rho^0/d\rho$  exists and is bounded from below:

$$\frac{d\rho^{0}}{d\rho} \ge c > 0 \tag{3.12}$$

Then we have MEP( $\rho$ ) = 0 iff  $\bar{c}(0, \sigma) = c(0, \sigma)$ ,  $\rho$ -a.s., where

$$\bar{c}(0,\sigma) = \frac{d\rho^0}{d\rho}(\sigma) c(0,\sigma^0)$$
(3.13)

**Proof.** Let  $\mathscr{F}_A$  denote the  $\sigma$ -field generated by  $\sigma(x), x \in A$ . Denote by  $\rho_A$ , resp.,  $\rho_A^0$  the restriction of  $\rho$ , resp.,  $\rho^0$  to the  $\sigma$ -field  $\mathscr{F}_A$ . We obviously have

$$\frac{d\rho_{A}^{0}}{d\rho_{A}} = \mathbb{E}\left[\left.\frac{d\rho^{0}}{d\rho}\right| \mathscr{F}_{A}\right]$$
(3.14)

Since  $d\rho^0/d\rho \in L^1(d\rho)$  we conclude from the martingale convergence theorem that

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{d\rho_{\Lambda}^0}{d\rho_{\Lambda}} = \frac{d\rho^0}{d\rho}$$
(3.15)

in  $L^1(d\rho)$ . Denote by  $v_A$  the Bernoulli measure with  $v(\sigma(0) = +1) = 1/2$ , restricted to  $\mathscr{F}_A$ . Then, by stationarity of  $\rho$  we have, with  $f_A = d\rho_A/dv_A$ ,

$$0 = \sum_{i \in A} \int \rho(d\sigma) c(i, \sigma) [\ln f_A(\sigma^i) - \ln f_A(\sigma)]$$
  

$$= \sum_{i \in A} \int \rho(d\sigma) c(i, \sigma) \ln \frac{d\rho_A^i}{d\rho_A}(\sigma)$$
  

$$= \sum_{i \in A} \int \rho(d\sigma) c(i, \sigma) \ln \frac{d\rho^i}{d\rho}$$
  

$$+ \sum_{i \in A} \int \rho(d\sigma) c(i, \sigma) \left[ \ln \frac{d\rho_A^i}{d\rho_A}(\sigma) - \ln \frac{d\rho^i}{d\rho}(\sigma) \right]$$
  

$$= |A| \int \rho(d\sigma) c(0, \sigma) \ln \frac{d\rho^0}{d\rho}(\sigma)$$
  

$$+ \sum_{i \in A} \int \rho(d\sigma) c(i, \sigma) F_A^i(\sigma)$$
(3.16)

Here we abbreviated

$$F_{A}^{i}(\sigma) = \left(\ln\frac{d\rho_{A}^{i}}{d\rho_{A}} - \ln\frac{d\rho^{i}}{d\rho}\right)$$
(3.17)

and used the translation invariance of  $\rho$  in the last step. From (3.16) we obtain:

$$\left| \int \rho(d\sigma) c(0,\sigma) \ln \frac{d\rho^{0}}{d\rho}(\sigma) \right| \leq \frac{1}{|\Lambda|} \sum_{i \in \Lambda} \left| \int \rho(d\sigma) c(i,\sigma) F_{\Lambda}^{i}(\sigma) \right|$$
$$\leq M \frac{1}{|\Lambda|} \sum_{i \in \Lambda} \int d\rho |F_{\Lambda-i}^{0}|$$
(3.18)

where in the last step we used translation invariance of  $\rho$  once again. Now from the elementary inequality  $|\ln a - \ln b| \leq |(a-b)|/a \wedge b$  we can deduce the following: if  $f_n$  converges to f in  $L^1(d\rho)$  and if  $f_n$ , f are bounded from below by some constant c > 0, then  $\ln f_n$  converges to  $\ln f$  in  $L^1(d\rho)$ . This fact implies that for given  $\varepsilon > 0$ , we can choose  $\Delta \subset \mathbb{Z}^d$  such that for all  $\Delta' \supset \Delta$ 

$$\int d\rho \ |F^{0}_{\ A'}| \leqslant \frac{\varepsilon}{2M} \tag{3.19}$$

Next we can choose  $\Lambda \subset \mathbb{Z}^d$  such that

$$\frac{|\{i: \Delta + i \not\subset \Lambda\}|}{|\Lambda|} \leqslant \frac{\varepsilon}{2M \sup_{\Lambda} \|F_{\Lambda}^{0}\|_{L^{1}(d\rho)}}$$
(3.20)

and we obtain from (3.18):

$$\left| \int \rho(d\sigma) c(0,\sigma) \ln \frac{d\rho^0}{d\rho}(\sigma) \right|$$
  
$$\leqslant \frac{1}{|\Lambda|} \sum_{i \in \Lambda, \ \Delta + i \subset \Lambda} \frac{\varepsilon}{2} + \frac{|\{i : \Delta + i \not\subset \Lambda\}|}{|\Lambda|} \sup_{\Lambda} \|F_{\Lambda}^0\|_{L^1(d\rho)} \leqslant \varepsilon \quad (3.21)$$

Now start from the expression (3.10) for the entropy production. A simple computation shows that

$$\operatorname{MEP}(\rho) = \frac{1}{2} \int \rho(d\sigma)(c(0,\sigma) - \bar{c}(0,\sigma)) \ln \frac{c(0,\sigma)}{\bar{c}(0,\sigma)} + \int \rho(d\sigma) c(0,\sigma) \ln \frac{d\rho^0}{d\rho}(\sigma)$$
(3.22)

But (3.21) shows that the second term in (3.22) is equal to zero, and the first term is zero if and only if  $c(0, \Lambda) = \overline{c}(0, \sigma) \rho$ -a.s.

# 4. ENTROPY PRODUCTION AND INFORMATION

We restrict ourselves again to a simple example. Suppose that X is a finite set and consider a Markov process on  $X \times \{-1, +1\}$  with transition rates  $p_a(x, y)$  for the change  $(x, a) \rightarrow (y, a)$  and transition rates  $q_x(a, b) = 1$  for the change  $(x, a) \rightarrow (x, b)$ . No other transitions are allowed. We thus have the Master Equation

$$\frac{\partial P_t(x,a)}{\partial t} = \sum_{y \in X} \left[ p_a(y,x) P_t(y,a) - p_a(x,y) P_t(x,a) \right] + \sum_{b=\pm 1} \left[ P_t(x,b) - P_t(x,a) \right]$$
(4.23)

for a probability distribution  $P_t$  on  $X \times \{-1, +1\}$ . Assuming that  $p_a$  is double stochastic:

$$\sum_{y} p_a(x, y) = 1 = \sum_{y} p_a(y, x), \quad \text{for} \quad x \in X, \quad a = \pm 1$$

the distribution  $\rho$  defined by  $\rho(x, a) = 1/(2 |X|)$ ,  $x \in X$ ,  $a = \pm 1$  is stationary for the Markov process (4.23).

Assume furthermore that

$$p_a(x, y) = p_{-a}(y, x) \neq p_a(y, x)$$
 (4.24)

We now define two mean entropy productions that differ only by the choice of time-reversal transformation. For the first choice we define

$$\theta(x_t, a_t) = (x_{-t}, a_{-t})$$

and the corresponding mean entropy production is

$$\text{MEP}(\rho) = \frac{1}{2|X|} \sum_{x, y \in X} \left[ p_{-1}(x, y) - p_{+1}(x, y) \right] \ln \frac{p_{-1}(x, y)}{p_{+1}(x, y)}$$

which is clearly strictly positive as a consequence of the assumption  $p_{-a}(x, y) \neq p_{a}(x, y)$  in (4.24). For the second choice, we define the involution  $\pi(x, a) = (x, -a)$  on  $X \times \{-1, +1\}$  and the corresponding time-reversal

$$\theta'(x_t, a_t) = (x_{-t}, -a_{-t}) = \theta \circ \pi(x_t, a_t)$$

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In that case, by (4.24), the corresponding mean entropy production  $MEP_{\pi}$ is easily found to be zero! As an obvious conclusion: the mean entropy production in a stationary state depends on the choice of time-reversal transformation used to define it. More physically relevant however is that this example reminds us of the significant difference between entropy and functions directly defined on the microscopic phase space. In contrast to e.g., the energy, which is obtained by evaluating the microscopic phase point, a definition of entropy should start by specifying the macroscopic or thermodynamic variables which determine the macroscopic state. In other words, what are the control parameters and what variables are considered part of the dynamics. In the previous example, we can think of particles performing a random walk (on the set X) with a local bias defined in terms of a spin variable  $a = \pm 1$ . In the first definition of the entropy production above, this bias is considered as an *external* field that breaks detailed balance. In the second definition however, this field appears as another dynamical variable which, under time-reversal, must be reflected. In this case microscopic reversibility is restored (the field has become part of the-now-equilibrium dynamics) and the mean entropy production is zero.

Other, physically more realistic, examples of this same phenomenon can easily be given. In this way, one can argue, positivity of entropy production cannot be reduced to a dynamical property alone (as is done in refs. 9 and 10). Just as for the equilibrium entropy: its definition and its increase for isolated systems depends (also) on the choice of variables reflecting the observational set-up. More generally, one would say that questions on the positivity of transport coefficients cannot be answered without specifying experimental conditions and control; referring to microscopic chaos or ergodic-theoretic considerations can never provide a complete explanation. Remark nevertheless that the traditional definition of transport coefficients (as used within linear response theory) relies on a good space-time decay of current correlations which is both a static and a dynamic issue.

# REFERENCES

- T. Antal, Z. Rácz, and L. Sasvári, Nonequilibrium steady state in a quantum system: onedimensional transverse Ising model with energy current, *Phys. Rev. Lett.* 78:167 (1997).
- G. Gallavotti, Chaotic hypothesis: Onsager reciprocity and fluctuation-dissipation theorem, J. Stat. Phys. 84:899–926 (1996).
- 3. G. Gallavotti and E. G. D. Cohen, Dynamical ensembles in stationary states, J. Stat. Phys. 80:931-970 (1995).
- H. Künsch, Non reversible stationary measures for infinite interacting particle systems, Z. Wahrsch. Verw. Gebiete 66:407 (1984).

- J. L. Lebowitz and H. Spohn, A Gallavotti–Cohen type symmetry in the large deviation functional for stochastic dynamics, J. Stat. Phys. 95:333–365 (1999).
- 6. T. M. Liggett, *Interacting Particle Systems* (Springer, Berlin, Heidelberg, New York, 1985).
- 7. C. Maes, The Fluctuation Theorem as a Gibbs Property, J. Stat. Phys. 95:367-392 (1999).
- C. Maes, F. Redig, and A. Van Moffaert, On the definition of entropy production, via examples, J. Math. Phys. 41:1528 (2000).
- D. Ruelle, Positivity of entropy production in nonequilibrium statistical mechanics, J. Stat. Phys. 85:1–25 (1997).
- D. Ruelle, Entropy production in nonequilibrium statistical mechanics, Commun. Math. Phys. 189:365–371 (1997).
- 11. D. Ruelle, Smooth dynamics and new theoretical ideas in nonequilibrium statistical mechanics, J. Stat. Phys. 95:393–468 (1999).
- 12. R. C. Tolman, *The Principles of Statistical Mechanics* (Oxford at the Clarendon Press, 1938), p. 102.