Entropy production of nonequilibrium steady states with irreversible transitions

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Abstract. In Nature, stationary nonequilibrium systems cannot exist on their own, rather they need to be driven from outside in order to keep them away from equilibrium. While the internal mean entropy of such stationary systems is constant, the external drive will on average increase the entropy in the environment. This external entropy production is usually quantified by a simple formula, stating that each microscopic transition of the system between two configurations $c \rightarrow c'$ with rate $w_{c \rightarrow c'}$ changes the entropy in the environment by $\Delta S_{\text{env}} = \ln w_{c \rightarrow c'} - \ln w_{c' \rightarrow c}$. According to this formula irreversible transitions $c \rightarrow c'$ with a vanishing backward rate $w_{c' \rightarrow c} = 0$ would produce an infinite amount of entropy. However, in experiments designed to mimic such processes, a divergent entropy production, which would cause an infinite increase of heat in the environment, is not seen. The reason is that in an experimental realization the backward process can be suppressed but its rate always remains slightly positive, resulting in a finite entropy production. This letter discusses how this entropy production can be estimated and specifies a lower bound depending on the observation time.
Entropy production of irreversible transitions

**Keywords:** driven diffusive systems (theory), exact results, stochastic particle dynamics (theory), large deviations in non-equilibrium systems

### Contents

1. Introduction  
2. The lower bound on the entropy production of micro-irreversible transitions  
3. Examples  
4. Conclusions  

References 9

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1. Introduction

In classical statistical physics, complex systems are often modeled as continuous-time Markov processes in a discrete configuration space. Such systems evolve by spontaneous random transitions from configuration $c$ to configuration $c'$ according to certain transition rates $w_{c \to c'}$. For isolated systems these rates are symmetric so that the model evolves into an equilibrium state with maximal entropy. For open systems, which interact with the surrounding environment, the transition rates are generally asymmetric. In this case the dynamical evolution changes not only the system’s entropy but also the entropy in the environment. The entropy change in the environment is referred to as the *entropy production* of the system.

As shown by Schnakenberg, Andrieux, Gaspard and Seifert [1]–[4], the entropy in the environment $S_{\text{env}}$ changes discontinuously by

$$
\Delta S_{\text{env}} = \ln \frac{w_{c \to c'}}{w_{c' \to c}}
$$

whenever the system jumps from $c$ to $c'$ (note that we set $k_B = 1$ for simplicity). This simple formula is independent of the specific composition and structure of the environment, provided that it equilibrates almost instantaneously between successive transitions of the Markov process [5] (see the supplemental material available at stacks.iop.org/JSTAT/2012/L12001/mmedia).

The entropy production formula (1) requires that for any transition $c \to c'$ with a non-vanishing forward rate $w_{c \to c'} > 0$, the corresponding backward rate $w_{c' \to c}$ has to be nonzero as well since otherwise the entropy production would diverge. This means that the definition of entropy production is only meaningful in models with microscopically reversible transitions. Usually it is argued that in realistic physical systems the effective backward rate is always nonzero since the classical description results from a coarse graining of the underlying quantum-mechanical processes which are intrinsically time reversible.
However, in statistical physics a large variety of models investigated in the literature involve microscopically irreversible transitions. For some of these models experiments have been suggested or performed. A simple example is the totally asymmetric simple exclusion process, where particles hop only in one direction, which is studied experimentally by optical tweezers [6]–[8]. Another example is directed percolation [9], the standard model of a phase transition from a fluctuating phase into a frozen state, which was recently realized experimentally for the first time [10]. However, a divergent entropy production, which would manifest itself in the form of a divergent increase of heat in the environment, has not been reported in these experiments. This suggests that this divergence is a theoretical artifact and needs to be regularized in a meaningful way.

To the best of our knowledge ben-Avraham et al [11] were the first to address this problem in detail. As a possible solution they suggested coarse graining the stochastic evolution by interval sampling: instead of monitoring each transition event separately, they proposed to read off the configuration at regular temporal intervals and to use the resulting configuration sequence to define effective transition rates. Even if the backward rate \( w_{c' \to c} \) is zero, meaning that direct transitions from \( c' \) to \( c \) are forbidden, the sampling allows the system to evolve from \( c' \) to \( c \) through a loop of other intermediate configurations between two consecutive readings. This gives rise to a small but finite effective backward rate in the sampled data, regularizing the entropy production depending on the sampling rate.

In this letter we propose an alternative regularization method which is more closely related to the question of how micro-irreversibility can be implemented in experiments. We start with the assertion that equation (1) is indeed correct and that the preceding argument about the fundamental impossibility of vanishing backward rates in Nature remains valid. This means that it is in principle impossible to realize micro-irreversible processes experimentally. However, in practice one can approximate irreversible processes very well by designing the experiment in such a way that the backward transition is strongly suppressed. In such an experiment the actual backward rate is positive but so small that the reverse transition practically never takes place during data taking. Nevertheless, the positivity of this rate ensures that the entropy produced by the corresponding forward process is still finite.

The aim of this work is to specify a lower bound on the entropy production of a physical system which is designed to approximate an irreversible process over a finite time span \( T \). We find that the entropy production rate of such a system can be split into two parts, namely, a conventional constant part stemming from the reversible transitions, and a second part coming from the approximated irreversible transitions which grows logarithmically with \( T \).

### 2. The lower bound on the entropy production of micro-irreversible transitions

The starting point is a continuous-time Markov process defined by a certain set of configurations \( c \in \Omega \). The model evolves by random transitions \( c \to c' \) with rates \( w_{c \to c'} > 0 \), where some of the allowed transitions are microscopically irreversible, i.e. \( w_{c' \to c} = 0 \). Suppose that we are able to design an experiment with an identical set of possible configurations that approximately reproduces the Markovian dynamics of the model. In what follows let us distinguish between
• the defining rates $w_{c\rightarrow c'}$ of the original model, and
• the corresponding actual rates $\tilde{w}_{c\rightarrow c'}$ realized in the experiment.

However, the actual rates in the experiment are usually not directly accessible, rather they have to be estimated from the observed number of transitions $n_{c\rightarrow c'}$ during a finite time span $T$ of data taking. If the system is found in the configuration $c'$ with probability $P_{c'}$, the expectation value of this number is given by $P_{c'}\tilde{w}_{c\rightarrow c'}T$. Observing a vanishing number $n_{c'\rightarrow c}=0$ in a single experiment does not necessarily imply that the corresponding actual rate $\tilde{w}_{c'\rightarrow c}$ is zero, it only means that this rate is sufficiently smaller than $(P_{c'}T)^{-1}$ so that this transition did not occur during data taking.

In the following we use this framework to specify a lower bound for the entropy production caused by irreversible transitions in experiments with a finite observation time. The idea is to estimate the actual rate $\tilde{w}$ of a transition $c \rightarrow c'$ in the experiment for a given defining rate $w$ on the basis of the expected count numbers $n_{c\rightarrow c'}$ within a given observation time $T$. In this way we want to find a physically motivated conditional probability distribution $P(\tilde{w}|w)$ of the actual rate $\tilde{w}$ for a given defining rate $w$.

To determine $P(\tilde{w}|w)$ let us assume that the transition $c \rightarrow c'$ occurs $n$ times during the observation time $T$. As these events are spontaneous and uncorrelated, $n$ is randomly distributed according to a Poisson distribution

$$P(n|w) = \frac{(\tau w)^n e^{-\tau w}}{n!},$$

where $\tau = P_{c'}T$ is the expected time that the system spends in the configuration $c$. This allows us to express $P(\tilde{w}|w)$ as

$$P(\tilde{w}|w) = \sum_{n=0}^{\infty} P(\tilde{w}|n)P(n|w),$$

where $P(\tilde{w}|n)$ is the likelihood for the distribution of the actual rate $\tilde{w}$ for a given number of transitions $n$. According to Bayes’ rule [12] this likelihood is given by

$$P(\tilde{w}|n) = \frac{P(n|\tilde{w})P(\tilde{w})}{P(n)},$$

where $P(\tilde{w})$ is the prior distribution and

$$P(n) = \int_{0}^{\infty} d\tilde{w} P(n|\tilde{w})P(\tilde{w})$$

is the normalizing marginal likelihood. The prior $P(\tilde{w})$ expresses our belief on how the rates are typically distributed and therefore introduces a certain degree of ambiguity in the derivation. However, if no specific information about this distribution is available, it is customary to use the so-called conjugate prior which ensures that the posterior $P(\tilde{w}|n)$ and the prior $P(\tilde{w})$ belong to the same family of distributions. The conjugate prior of a Poisson likelihood distribution $P(n|\tilde{w})$ is the Gamma distribution

$$P(\tilde{w}) = \frac{\tilde{\beta}^{\tilde{\alpha}} \tilde{w}^{\tilde{\alpha}-1} e^{-\tilde{\beta} \tilde{w}}}{\Gamma(\tilde{\alpha})},$$

which depends on two hyperparameters $\tilde{\alpha}$ and $\tilde{\beta}$ (the tilde is used to avoid confusion with the rates $\alpha, \beta$ for various models used in the literature). With this prior the posterior is

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4
Entropy production of irreversible transitions

given by

\[ P(\tilde{\omega}|n) = \frac{\tilde{\omega}^{\tilde{\alpha}+n-1}e^{-(\tilde{\beta}+\tau)\tilde{\omega}}}{\Gamma(n + \tilde{\alpha})}, \]  

(7)

which allows one to compute the expectation value of the actual rate for the transition \( c \rightarrow c' \)

\[ \langle \tilde{\omega} \rangle = \int d\tilde{\omega} \tilde{\omega} P(\tilde{\omega}|\omega) = \frac{\tau w + \tilde{\alpha}}{\tau + \tilde{\beta}}. \]  

(8)

As can be seen, this formula maps a vanishing defining rate \( w = 0 \) onto a non-vanishing actual rate \( \langle \tilde{\omega} \rangle \propto \frac{1}{\tau} \). By defining \( \tau' = P_c T \) and inserting this expectation value into the entropy production formula (1) and taking the limit \( T \gg 1 \) the entropy production for reversible transitions

\[ \Delta S_{\text{rev}}^{\text{env}}(c \rightarrow c') = \ln \frac{\langle \tilde{\omega}_{c \rightarrow c'} \rangle}{\langle \tilde{\omega}_{c' \rightarrow c} \rangle} = \ln \frac{(\tau w_{c \rightarrow c'} + \tilde{\alpha})/(\tau + \tilde{\beta})}{(\tau' w_{c' \rightarrow c} + \tilde{\alpha})/(\tau' + \tilde{\beta})} \approx \ln \frac{w_{c \rightarrow c'}}{w_{c' \rightarrow c}} \]  

(9)

reproduces the known result in equation (1). As our main result, for irreversible transitions we obtain a finite entropy production which grows logarithmically with the observation time

\[ \Delta S_{\text{irr}}^{\text{env}}(c \rightarrow c') = \ln \frac{\langle \tilde{\omega}_{c \rightarrow c'} \rangle}{\tilde{\alpha}/(\tau + \tilde{\beta})} = \ln \frac{(\tau w_{c \rightarrow c'} + \tilde{\alpha})/(\tau + \tilde{\beta})}{\tilde{\alpha}/(\tau' + \tilde{\beta})} \approx \ln \frac{\tau' w_{c \rightarrow c'}}{\tilde{\alpha}}. \]  

(10)

Note that we have simplified the derivation by replacing \( \langle \ln \tilde{\omega} \rangle \rightarrow \ln \langle \tilde{\omega} \rangle \). However, as shown in section 3 of the supplemental material (available at stacks.iop.org/JSTAT/2012/L12001/mmedia), apart from a redefinition of \( \tilde{\alpha} \), a correct derivation to lowest order leads to the same result.

The prior distribution (6) depends on two hyperparameters \( \tilde{\alpha} \) and \( \tilde{\beta} \) which determine its shape and scale. Since the entropy production depends on a ratio of rates, the scale hyperparameter \( \tilde{\beta} \) drops out. However, the shape hyperparameter \( \tilde{\alpha} \) appears in the final result and thus it has to be defined in a physically meaningful way. In this regard note that the Gamma distribution (6) evaluated at the origin is finite for \( \tilde{\alpha} = 1 \), infinite for \( \tilde{\alpha} < 1 \) and zero for \( \tilde{\alpha} > 1 \). Therefore, in experiments on models with irreversible transitions, where the likelihood of a vanishing defining rate is expected to be finite, the most natural choice, which we will use from now on, is \( \tilde{\alpha} = 1 \).

3. Examples

In what follows we study the entropy production in three exemplary nonequilibrium systems with micro-irreversible transitions in their steady states (further examples can be found in the supplemental material available at stacks.iop.org/JSTAT/2012/L12001/mmedia). To this end we first determine the stationary probability distribution \( P_c \) to find
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the system in configuration $c$. The average entropy production is then given by

$$
\langle \dot{S}_{\text{env}} \rangle = \sum_{c \neq c'} P_c \Delta S_{\text{env}}(c \rightarrow c'),
$$

where one has to sum over $\Delta S_{\text{env}}^{\text{rev}}(c \rightarrow c')$ or $\Delta S_{\text{env}}^{\text{irr}}(c \rightarrow c')$ depending on whether the transition $c \rightarrow c'$ is reversible or irreversible. For lattice models with $L$ sites, we define the average entropy production per site as

$$
\dot{s}_{\text{env}} := \frac{1}{L} \langle \dot{S}_{\text{env}} \rangle.
$$

**TASEP.** The first example is the totally asymmetric simple exclusion process (TASEP) on a finite lattice with $L$ sites, where particles are added at the left boundary (removed from the right boundary) with rate $\alpha$ ($\beta$) if the first (last) lattice site is empty (occupied). Since particles hop exclusively to the right, all microscopic transitions are irreversible. The stationary probability distribution of the TASEP can be calculated exactly using the matrix product method [13], where the stationary weight of each configuration is determined by a product of noncommuting operators corresponding to the actual configuration. Using the exact results of [13] in formulas (12) and (10) it turns out that, to leading order in $T$, the large-$L$ limit of the average entropy production rate

$$
\dot{s}_{\text{env}} \approx J(\alpha, \beta) \ln T
$$

is proportional to the particle current $J(\alpha, \beta)$ in the steady state. Depending on the values of $\alpha$ and $\beta$ the current is equal to $J(\alpha, \beta) = \frac{1}{4}$ for $\alpha, \beta \geq \frac{1}{2}$, $J(\alpha, \beta) = \alpha(1-\alpha)$ for $\alpha < \beta$ and $\alpha < \frac{1}{2}$, and $J(\alpha, \beta) = \beta(1-\beta)$ for $\beta < \alpha$ and $\beta < \frac{1}{2}$. Thus, the average entropy production changes continuously in the parameter space and attains its maximum for $\alpha, \beta \geq \frac{1}{2}$, where the particle current is maximal.

**BCP.** The second example is the branching–coalescing process (BCP) on a one-dimensional lattice with $L$ lattice sites and open boundaries. Each lattice site is either empty ($\emptyset$) or occupied by at most one particle (1). In the bulk the BCP evolves by the dynamical rules

$$
\begin{align*}
\emptyset 1 & \rightarrow 11 \text{ with rate } w, \\
11 & \rightarrow \emptyset 1 \text{ with rate } w, \\
11 & \rightarrow 1 \emptyset \text{ with rate } 1, \\
1 \emptyset & \rightarrow 11 \text{ with rate } 1, \\
1 \emptyset & \rightarrow \emptyset 1 \text{ with rate } 1.
\end{align*}
$$

In addition, particles are added at (removed from) the left boundary with rate $\alpha$ ($\gamma$) while at the right boundary particles are removed with rate $\beta$.

It is known that the steady state of the BCP can be written as a linear superposition of Bernoulli shock measures provided that $\gamma = \alpha + w/2 - 1$ [14]. Moreover, under the same constraint it turns out that the model has a matrix product steady state [15]. Varying $w$, the process undergoes a phase transition between a high- and a low-density phase at $w_c = 4$. Applying the matrix product method with the two-dimensional representation introduced in [15], it is straightforward to calculate the average entropy production rate...
Figure 1. The branching–coalescing process (BCP) at the critical point, exhibiting a diffusing Bernoulli shock. Particles are represented by black pixels while the integrated entropy production at each site is visualized by a periodically changing color scale.

per site in the steady state. To leading order in $T$ and in the large-$L$ limit one finds

$$\dot{s}_{\text{env}} \approx \begin{cases} \frac{1}{4} \ln T & \text{for } 2(1 - \alpha) < w < w_c, \\ 0 & \text{for } w > w_c. \end{cases}$$

(15)

As can be seen, the average entropy production of the BCP changes discontinuously at the transition point. The nonzero part of the entropy production in (15) comes from both reversible and irreversible processes in (14) (see the supplemental material available at stacks.iop.org/JSTAT/2012/L12001/mmedia). In figure 1 the time evolution of the entropy production at each lattice site is plotted at the critical point $w = w_c$. In this case the last particle in the system (the last black pixel from the left) performs an unbiased random walk on the lattice. It can be seen that only occupied lattice sites contribute to the entropy production.

AKGP. The third example is the one-dimensional asymmetric Kawasaki–Glauber process (AKGP) with the dynamical rules

$$\begin{align*}
1 \emptyset \to \emptyset \emptyset & \text{ with rate } w_1, \\
1 \emptyset \to 1 1 & \text{ with rate } w_2, \\
\emptyset 1 \to \emptyset \emptyset & \text{ with rate } w_3, \\
\emptyset 1 \to 1 \emptyset & \text{ with rate } w_4, \\
\emptyset 1 \to 1 0 & \text{ with rate } w_5.
\end{align*}$$

(16)

In addition, particles are added at (removed from) the left (right) boundary with rate $\alpha$ ($\beta$). In this model all transitions are irreversible. It is known that the AKGP has a matrix product steady state, which can also be written as a linear superposition of Bernoulli shock measures [14], and that it exhibits a phase transition at $w_1 = w_2$ from a low-density to a high-density phase. Using the two-dimensional matrix representation introduced in [15], one can calculate the average entropy production rate in the limit.
Entropy production of irreversible transitions

Figure 2. Average irreversible entropy production in the AKGP as a function of $w_2$ for $w_1 = 0.4$, $\alpha = 0.3$, $\beta = 0.1$, $L = 10^6$ and $T = 10^6$. The phase transition occurs at $w_2 = 0.4$.

$L \to \infty$ and to leading order in $T$, obtaining

$$\langle \dot{S}_{\text{env}} \rangle \approx \begin{cases} 
2\alpha w_1 & \text{for } w_1 > w_2, \\
\frac{\alpha + w_1 - w_2}{2\beta w_2} \ln T & \text{for } w_2 > w_1.
\end{cases}$$

(17)

Since the probability of a given configuration consisting of a particle in front of an empty lattice site is zero in the steady state, the last three processes in (16) do not contribute to the average entropy production, explaining why the parameters $\omega_3$, $\omega_4$, $\omega_5$ do not appear in the result. In figure 2 the average entropy production rate is plotted as a function of $w_2$. In contrast to the BCP, it changes continuously at the transition point.

4. Conclusions

In this letter we have addressed the problem of entropy production in systems with irreversible transitions. For such systems the Schankenber formula (1) predicts an infinite entropy production which is not seen in experiments. We suggest that the finite amount of entropy produced in experiments is related to the fact that vanishing reverse rates are impossible in Nature; it is only possible to keep such rates very small. By introducing the concept of a ‘defining rate’ and an ‘actual rate’ and estimating the latter by Bayesian inference, we could specify a lower bound on the entropy production which splits up into a constant contribution for reversible transitions and an additional contribution for irreversible transitions which grows logarithmically with the observation time $T$.

Using the modified entropy production formula, we have calculated the average entropy production rate for three exactly solvable reaction–diffusion models in the steady state (further examples are discussed in the supplemental material available at stacks.iop.org/JSTAT/2012/L12001/mmedia). The steady states of the BCP and AKGP are very similar in the sense that they can both be written as a linear superposition of Bernoulli shock measures, where the shock performs a simple random walk [14]. However, the average entropy production behaves quite differently, namely, discontinuously in the BCP.
and continuously in the AKGP. This suggests that the irreversible entropy production may be used as an additional tool for the classification of nonequilibrium phase transitions.

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