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Entropy bound for time reversal markers

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We derive a bound for entropy production in terms of the mean of normalizable path-antisymmetric observables. The optimal observable for this bound is shown to be the signum of entropy production, which is often easier determined or estimated than entropy production itself. It can be preserved under coarse graining by the use of a simple path grouping algorithm. We demonstrate this relation and its properties using a driven network on a ring, for which the bound saturates for short times for any driving strength. This work can open a way to systematic coarse graining of entropy production.

1 Introduction

A common way of analyzing complex systems is observation of particle trajectories, e.g., via microscopy [1–3] in biological systems [4–8] or complex fluids [9, 10]. Detecting and quantifying the deviation from equilibrium, i.e., the violation of detailed balance, based on trajectories is, however, a challenging task, especially if relevant degrees of freedom are hidden, and non-equilibrium processes are random [11–17]. Several methods for such detection have been developed.

The fluctuation dissipation theorem (FDT) connects fluctuations and response functions [18], and it is violated out of equilibrium [19–21]. How far away from equilibrium a system is, e.g., has been quantified by using the so-called effective temperatures or effective energies [22–27].

Another way of detecting broken detailed balance is via entropy production, which has been found to obey a variety of theorems including the fluctuation theorems [28–31]. A number of important relations have been found that bound entropy production, such as the thermodynamic uncertainty relation (TUR) [32–38]. The TUR bounds mean and variance of currents by entropy production or *vice versa*. It has been extended and refined, including path antisymmetric observables (FTUR) or to more general path weights [39–42] and has been applied to experiments and numerical data [43–46]. Little is, however, known about how bounds behave under coarse graining.

In this paper, we derive an entropy bound in terms of the mean of path-antisymmetric observables, based on an integrated fluctuation theorem. In contrast to the TUR and FTUR, it does not involve the variance of the observable. We determine the optimal observable, i.e., the observable that maximizes the bound, to be the signum of entropy production so that a relation between entropy production and its sign appears. As this relation saturates for a binary process at short times, we argue that no better relation between entropy production and its sign can exist with the same range of validity. The sign of entropy production, and hence the bound for entropy production,

can be preserved under coarse graining with a simple path grouping rule. We apply these results for a discrete network on a ring. For this network, the signum of entropy production is coarse-grained under preservation to the signum of the traveled distance, demonstrating how a bound for microscopic entropy production is obtained from a macroscopic observable. Under such coarse graining, entropy production can at most reduce to the original bound.

2 Setup and fluctuation theorem

A path observable $O[\omega]$ is considered, with path ω in the phase space, with path probability $p[\omega]$, and the average is formally given by the sum over paths [47] $\langle O \rangle = \int \mathcal{D}\omega\, O[\omega] p[\omega]$. To construct a marker for path reversal, the sum is reordered [48]

$$2\langle O \rangle = \int \mathcal{D}\omega \left\{ O[\omega] p[\omega] + O[\theta\omega] p[\theta\omega] \right\}. \tag{1}$$

We introduced notation for path reversal, $\theta\omega$, including reversal of time and of kinematic reversal of momenta [49]. Validity of Eq. 1 requires the sum of paths to include $\theta\omega$ for any included ω. Adding a zero yields

$$2\langle O \rangle = \int \mathcal{D}\omega \{ (O[\omega] + O[\theta\omega]) p[\theta\omega] \\ + O[\omega] (p[\omega] - p[\theta\omega]) \}, \tag{2}$$

where the term $O[\omega] + O[\theta\omega]$ in the first line of Eq. 2 is the path symmetric part of O:

$$O[\omega] + O[\theta\omega] \equiv 2O_+[\omega]. \tag{3}$$

With detailed balance obeyed, i.e., $p[\omega] = p[\theta\omega]$, antisymmetric observables average to zero, and

$$\langle O \rangle \overset{\text{d.b.}}{=} \langle O_+ \rangle. \tag{4}$$

Violations of Eq. 4, thus, indicate the breakage of detailed balance [50, 51]. Although the symmetric part O_+ does not appear in the final result, Eq. 12 below, for the derivation, it is useful to start with O_+ finite.

To quantify the path reversal properties of cases that break detailed balance, we introduce the stochastic change in entropy defined as the log ratio of path probabilities ($k_B = 1$) [52–54].

$$s = \log \frac{p[\omega]}{p[\theta\omega]}. \tag{5}$$

For simplicity, we will, in the following, refer to s as the entropy production despite some caveats regarding this term[1]. The thermodynamic relevance of s is a topic of its own, which has been discussed in various works [52–54]. Substituting s into Eq. 2 yields

$$2\langle O \rangle = 2\langle O_+ \rangle + \int \mathcal{D}\omega\, O[\omega](1 - e^{-s}) p[\omega]. \tag{6}$$

Reordering the terms yields a fluctuation theorem including O:

$$\langle O(1 + e^{-s}) \rangle = 2\langle O_+ \rangle. \tag{7}$$

Equation 7 may be found equivalently from the so-called strong detailed fluctuation theorem [48] and has been stated in the similar form [50].

3 Entropy bound

Equation 7 can be used to find bounds for s, and we, therefore, restrict to positive observables, $O[\omega] \geq 0$. This allows Jensen's inequality [55, 56] to be applied for the average $\langle O \dots \rangle / \langle O \rangle$, to obtain from Eq. 7,

$$\frac{2\langle O_+ \rangle - \langle O \rangle}{\langle O \rangle} = \frac{\langle Oe^{-s} \rangle}{\langle O \rangle} \geq e^{-\frac{\langle Os \rangle}{\langle O \rangle}}. \tag{8}$$

As expected from Jensen's inequality, Eq. 8 saturates for small s, as seen by expanding it in this limit,

$$\frac{\langle Oe^{-s} \rangle}{\langle O \rangle} = 1 - \frac{\langle Os \rangle}{\langle O \rangle} + \mathcal{O}(s^2) = e^{-\frac{\langle Os \rangle}{\langle O \rangle}} + \mathcal{O}(s^2). \tag{9}$$

Taking the logarithm of Eq. 8 yields a lower bound for the correlation $\langle Os \rangle$:[2]

$$\log\left(\frac{\langle O \rangle}{2\langle O_+ \rangle - \langle O \rangle}\right) \leq \frac{\langle Os \rangle}{\langle O \rangle}. \tag{10}$$

Because the conjugate observable $O^*[\omega] = O[\theta\omega]$ is non-negative if O is non-negative, Eq. 10 is also valid for O^*. The bounds for $\langle Os \rangle$ and $\langle O^*s \rangle$ may, thus, be added to arrive at a bound for $\langle sO_+ \rangle$, the correlation of s, and the symmetric part O_+:

$$2\langle sO_+ \rangle \geq (\langle O \rangle - \langle O^* \rangle)\log\left(\frac{\langle O \rangle}{\langle O^* \rangle}\right). \tag{11}$$

Notably, when adding Eq. 10 for $\langle Os \rangle$ and $\langle O^*s \rangle$, the linear term in Eq. 9 drops out so that Eq. 11 does, in general, not saturate for small s. As will be discussed below, it saturates for a binary process for short times, for any value of s.

A direct way to extract a bound for $\langle s \rangle$ from Eq. 11 is by considering $O_+ = 1$, i.e., path-independent. In order for O to be positive, the antisymmetric part, $2O_-[\omega] = O[\omega] - O[\theta\omega]$, must be normalized to $|O_-[\omega]| \leq 1$. This yields the following equation:

$$\langle s \rangle \geq \langle O_- \rangle\log\left(\frac{1 + \langle O_- \rangle}{1 - \langle O_- \rangle}\right) \geq 0. \tag{12}$$

Equation 12 is a main result of this paper, a bound for entropy production $\langle s \rangle$ in terms of the average of the antisymmetric observable O_-. This relation is, thus, fundamentally different from uncertainty relations, which bound entropy production in terms of mean and variance [40].

The condition of $|O_-[\omega]| \leq 1$ may seem to be a strong restriction of validity of Eq. 12. However, a bound between $\langle s \rangle$ and $\langle O_- \rangle$ can

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1 The entropy defined in Eq. 5 corresponds to the total change in entropy in overdamped stationary systems. In underdamped or non-stationary systems, the boundary terms differ [54].

2 A similar relation was derived in [57], however, with the left hand side always negative.
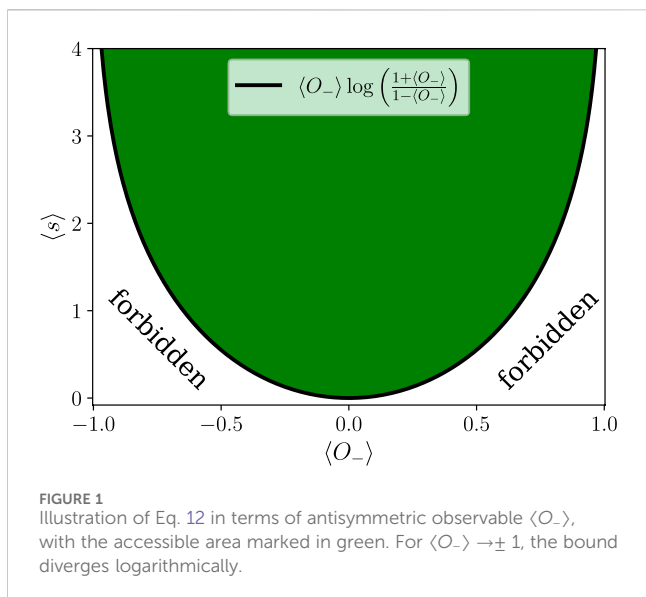
FIGURE 1
Illustration of Eq. 12 in terms of antisymmetric observable $\langle O_- \rangle$, with the accessible area marked in green. For $\langle O_- \rangle \to \pm 1$, the bound diverges logarithmically.

only be useful if O_- is normalizable, i.e., if a maximum value of $\max_\omega |O_-| < \infty$ exists. Whenever this maximum exists, O_- can be normalized to fulfill $|O_-[\omega]| \leq 1$. Eq. 12 is, thus, applicable for any normalizable antisymmetric observable. We also note that the right hand side of Eq. 12 is non-negative so that any non-zero $\langle O_- \rangle$ yields a positive bound for $\langle s \rangle$.

Equation 12 can be read in the following two ways: (i) a given $\langle s \rangle$ yields a bound for how far the mean of (any) O_- can deviate from zero. Using, e.g., a time interval from $-t_0$ to t_0, O_- can be the time-moment at which a certain event occurs, which is then bound by $\langle s \rangle$ via Eq. 12. This will be investigated in future works. (ii) A given non-vanishing value of $\langle O_- \rangle$ yields a lower bound for entropy production. We will analyze this below.

The form of Eq. 12 is illustrated in Figure 1. For small $\langle O_- \rangle$, the bound grows quadratically in $\langle O_- \rangle$, while it diverges logarithmically for $\langle O_- \rangle \to 1$.

4 Optimal observable: signum of entropy

Equation 12, as mentioned, is valid for any normalizable antisymmetric observable, and, naturally, the observable that maximizes the right hand side of it yields the best estimate for $\langle s \rangle$. Which observable is it? Answering this important question has been found non-trivial for entropy bounds [58, 59], while it has a clear answer for Eq. 12. To see this, rewrite[3]

$$\langle O_- \rangle = \sum_\omega O_-[\omega] p[\omega] = \frac{1}{2} \sum_\omega O_-[\omega] \left(p[\omega] - p[\theta\omega] \right) \tag{13}$$
$$\leq \langle \text{sign}(s) \rangle.$$

In the second step, we used the anti-symmetry of O_-. The inequality in the last step of Eq. 13 follows by noting that the

sum is maximized if $O_-[\omega] = 1$ for $p[\omega] > p[\theta\omega]$ and $O_-[\omega] = -1$ for $p[\omega] < p[\theta\omega]$. This is the definition of $O_- = \text{sign}(s)$[4].

As the right hand side of Eq. 12 is a monotonically growing function of $|\langle O_- \rangle|$ (compare Figure 1), $O_- = \text{sign}(s)$ yields the optimal bound for $\langle s \rangle$ from Eq. 12. To emphasize this, we write explicitly

$$\langle s \rangle \geq \langle \text{sign}(s) \rangle \log\left(\frac{1 + \langle \text{sign}(s) \rangle}{1 - \langle \text{sign}(s) \rangle} \right)$$
$$\geq \langle O_- \rangle \log\left(\frac{1 + \langle O_- \rangle}{1 - \langle O_- \rangle} \right). \tag{14}$$

The first inequality of Eq. 14 bounds $\langle s \rangle$ by $\langle \text{sign}(s) \rangle$. Writing $\langle \text{sign}(s) \rangle = \frac{1}{2} \sum_\omega \text{sign}(p[\omega] - p[\theta\omega])(p[\omega] - p[\theta\omega])$ shows that $\langle \text{sign}(s) \rangle \geq 0$ and that $\langle \text{sign}(s) \rangle = 0$ only if $\langle s \rangle = 0$, i.e., Eq. 14 yields a finite bound for any finite $\langle s \rangle$. The second inequality of Eq. 14 restates that $O_- = \text{sign}(s)$ yields the optimal bound so that any other O_- lies below it.

5 Coarse graining

A bound of $\langle s \rangle$ in terms of $\langle \text{sign}(s) \rangle$ is fundamentally interesting, and it is also useful, as, e.g., $\langle \text{sign}(s) \rangle$ has beneficial properties under coarse graining. Therefore, consider coarse-grained paths Ω with probabilities $P(\Omega) = \sum_{\omega \in \Omega} p(\omega)$ and coarse-grained entropy production $S = \log \frac{P[\Omega]}{P[\theta\Omega]}$. Naturally, $O_- = \text{sign}(S)$ fulfills Eq. 13 so that for any grouping of paths,

$$0 \leq \langle \text{sign}(S) \rangle \leq \langle \text{sign}(s) \rangle. \tag{15}$$

Coarse graining, thus, leads, in general, to a decrease in $\langle \text{sign}(s) \rangle$, reminiscent of the finding that $\langle s \rangle$ also decreases under coarse graining [60]. Notably, grouping paths according to the sign of s, i.e., with $\text{sign}(s[\omega]) = \text{sign}(S[\Omega_o])$ *conserves* $\langle \text{sign}(s) \rangle$.

$$\langle \text{sign}(s) \rangle = \frac{1}{2} \sum_{\Omega_o} \text{sign}(P[\Omega_o] - P[\theta\Omega_o]) \times$$
$$\times \sum_{\omega \in \Omega_o} (p[\omega] - p[\theta\omega])$$
$$= \langle \text{sign}(S_o) \rangle. \tag{16}$$

Under this "optimal" (index o) coarse graining, the bound provided by $\text{sign}(s)$ is invariant so that the macroscopic $\langle \text{sign}(S_o) \rangle$ yields the same bound as the microscopic $\langle \text{sign}(s) \rangle$. Furthermore, as the bound must hold for s and S_o alike, coarse-grained entropy production S_o never falls below the original, microscopic bound. This algorithm, thus, provides a controlled coarse graining of entropy production, which is especially useful if the bound from $\text{sign}(s)$ is close to s.

6 Example: network on a ring

To display this in an example, consider a network on a ring, where every state is connected to two neighbors (see inset

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[3] Eq. 13 holds also for $-O_-$ and thus for $|\langle O_- \rangle|$.

[4] The terms with $p[\omega] = p[\theta\omega]$ cancel in the sum in Eq. 13 due to $O_-[\omega] = -O_-[\theta\omega]$, and $O_-[\omega]$ can be chosen arbitrarily in these cases.

FIGURE 2
Network on a ring model: entropy production $\langle s \rangle$ as a function of N, Eq. 17, for $p = 0.57$, *versus* the bound obtained from Eq. 12 for various observables as sign(s), sign(d) and $\tanh(\frac{d}{2})$ using numerical simulations. The gray dotted line is the asymptotic limit of large N. The graph also shows optimally coarse-grained entropy $\langle S_o \rangle$.

FIGURE 3
Network on a ring model, with identical parameters as shown in Figure 2, here focusing on the comparison to FTUR. FTUR is used with two different observables as indicated, sign(s) or s. For large N, Eq. 12 and FTUR for the sign(s) scale linearly in N, while FTUR for s scales with log(N).

sketch of Figure 2). In every discrete time step, a particle jumps to the left (right) with probability p (q). For $q \neq p$, the system violates detailed balance and shows a directed flow. After N steps, the probability of finding a specific path with n_L steps to the left is given by the binomial distribution $p[\omega] = \frac{1}{L} p^{n_L} q^{N-n_L}$, with L the number of states in the network. With it, entropy production after N steps is given by the following equation:

$$\langle s \rangle = N(p-q)\log\left(\frac{p}{q}\right). \qquad (17)$$

Optimal coarse graining can be performed here in a straightforward manner: because $s = d \log(p/q)$, the sign of entropy production equals the sign of $d = n_L - n_R$ (for $p > q$), with n_R being the number of steps to the right, i.e., sign($d[\omega]$) = sign($s[\omega]$). This system, thus, allows coarse graining toward the measurement of the net displacement d, under preservation of the bound. We may expect that d is easier to measure than s.

Having established that Eq. 12 is maximal for $O_- = \text{sign}(d[\omega])$, we can test the quality of the estimate for $\langle s \rangle$ provided by it. For $N = 1$, $\langle \text{sign}(d) \rangle = p - q$ and

$$\langle s \rangle \overset{N=1}{=} \langle \text{sign}(d) \rangle \log\left(\frac{1 + \langle \text{sign}(d) \rangle}{1 - \langle \text{sign}(d) \rangle}\right). \qquad (18)$$

For $N = 1$, the bound of Eq. 12, thus, meets entropy production exactly, for any p and q, i.e., arbitrarily far from equilibrium. This is the abovementioned case of the binary process, where a particle either jumps right or left.

Figure 2 shows $\langle s \rangle$ and the bound of Eq. 12 as a function of N. For $N > 1$, the bound grows sublinear in N for an intermediate range and, thus, falls below the value of s. For $N \gg 1$, it approaches a linear asymptote, which can be found via a large deviation principle. We find for $p > \frac{1}{2}$ and $N \to \infty$ [61],

$$\langle \text{sign}(s) \rangle = \langle \text{sign}(d) \rangle \sim 1 - \frac{2}{1 - \frac{q}{p}} \frac{\left(\frac{1}{4pq}\right)^{-\frac{N}{2}}}{\sqrt{\frac{\pi}{2}N}}, \qquad (19)$$

i.e., $\langle \text{sign}(d) \rangle$ approaches unity exponentially fast with N. Because of this, the bound for s of Eq. 12 grows linear in N, and substituting (19) into Eq. 12 yields $\frac{1}{2}\log\left(\frac{1}{4pq}\right)N$, shown as a gray line in the graph. The ratio between this large N asymptote and $\langle s \rangle$ of Eq. 17 varies between $\frac{1}{2}$ for $p \to 1$ and $\frac{1}{4}$ for $p \to \frac{1}{2}$.

Coarse graining groups paths according to their displacement, i.e., Ω for $d > 0$ and $\theta\Omega$ for $d < 0$. This way, the coarse-grained entropy $\langle S_o \rangle$ can be determined, which is also shown in Figure 2. The curve demonstrates that it, as expected, stays above the bound. As only two coarse grained paths with finite S_o exist, it is obtained from.

$$\langle S_o \rangle = \log\left(\frac{P[\Omega_o]}{P[\theta\Omega_o]}\right)P[\Omega_o],$$
$$+ \log\left(\frac{P[\theta\Omega_o]}{P[\Omega_o]}\right)P[\theta\Omega_o]. \qquad (20)$$

$$\overset{N \text{odd}}{=} \langle \text{sign}(d) \rangle \log\left(\frac{1 + \langle \text{sign}(d) \rangle}{1 - \langle \text{sign}(d) \rangle}\right). \qquad (21)$$

Notably, the bound shown in Eq. 12 is saturated with respect to S_o for odd N, as indicated. For N even, paths with zero entropy production exist, and the second equality shown in Eq. 21 is not valid, and Eq. 12 lies below $\langle S_o \rangle$. For large N, these differences vanish so that the bound of Eq. 12 and $\langle S_o \rangle$ share the same asymptote. In this system, entropy production may, thus, be coarse-grained by a maximal loss of a factor between 2 and 4, depending on p, using the optimal algorithm.

According to Eq. 13, any other normalizable antisymmetric observable should yield a lower bound, which we exemplify by using $O_- = \tanh(d/2)$. Indeed, it lies lower but approaches the optimal bound for large N because then, a typical

trajectory shows $d \gg 1$ so that $\tanh(d/2)$ becomes equivalent to $\text{sign}(d)$.

Although optimal coarse graining is possible in an exact manner in this model, we expect an approximate preservation of $\text{sign}(s)$ to be possible in more complicated systems, which will be investigated in future works.

Can we compare to other relations such as TUR? The original TUR is not applicable to time-discrete dynamics, as used in this example. We, thus, compare to the so-called FTUR [40], as shown in Figure 3. Not knowing the optimal observable for FTUR, we use $\text{sign}(s)$ and s, analytically computing the required variances for these two. Interestingly, for each of the three curves shown in the figure, there exists a regime of N, where it provides the highest estimate. It is also remarkable that FTUR used with $\text{sign}(s)$ can provide a better estimate compared to using s. This shows the advantage of Eq. 17, for which the optimal observable is known, leading to the coarse-graining scheme. It also shows that the comparison between these relations is rich and non-trivial and needs to be studied in future works.

7 Discussion

Entropy production is bound by the mean of normalizable antisymmetric observables. The optimal observable is identified to be the signum of entropy production so that we determine a bound between entropy production and its sign, $\text{sign}(s)$. The latter may often be estimated from simple observables, like here, the displacement on a ring. The network example shows that measuring $\text{sign}(s)$ (did the particle move left or right?) is expected to require a lower experimental resolution compared to measuring s (where did the particle move when?). One can also estimate $\langle \text{sign}(s) \rangle$ by the use of Eq. (13), i.e., by testing various observables O_- and finding the maximum deviation from zero. For the investigated network, $\langle \text{sign}(s) \rangle$ approaches unity exponentially fast with the number of steps so that the bound grows with the expected linear dependence. Grouping paths according to $\text{sign}(s)$ yields a coarse-graining algorithm that preserves $\text{sign}(s)$ and the bound. The presented analysis is not restricted to specific dynamics. Due to this, it is, additionally to the here-discussed discrete system, also valid for fluids and biological systems [27]. Future work may investigate applications to Langevin systems as well, like active Brownian particles, or quantum mechanics [62–65].

Data availability statement

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

Author contributions

GK: writing–original draft. TM: writing–review and editing. TB: writing–review and editing. MK: writing–original draft.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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