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Unifying thermodynamic uncertainty relations

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Abstract

We introduce a new technique to bound the fluctuations exhibited by a physical system, based on the Euclidean geometry of the space of observables. Through a simple unifying argument, we derive a sweeping generalization of so-called thermodynamic uncertainty relations (TURs). We not only strengthen the bounds but extend their realm of applicability and in many cases prove their optimality, without resorting to large deviation theory or information-theoretic techniques. In particular, we find the best TUR based on entropy production alone. We also derive a periodic uncertainty principle of which previous known bounds for periodic or stationary Markov chains known in the literature appear as limit cases. From it a novel bound for stationary Markov processes is derived, which surpasses previous known bounds. Our results exploit the non-invariance of the system under a symmetry which can be other than time reversal and thus open a wide new spectrum of applications.

1. Introduction

At several levels of complexity, random processes are successfully employed to model natural phenomena, such as open quantum system [1], soft and active matter [2], biochemical reactions [3], and population ecology [4], just to name a few. In recent years, the understanding of their dynamical fluctuations has greatly advanced thanks to exact results of nonequilibrium physics. Most importantly, fluctuation theorems [5, 6] and response relations [7] have been derived that, respectively, constrain the distribution of currents and relate the system's perturbation to its dissipation and dynamical activity. Moreover, stochastic thermodynamics has emerged as a comprehensive framework to rigorously study the energetics and thermodynamics of stochastic processes [8, 9].

   Recently, uncertainty relations appeared as a new powerful tool to investigate dynamical fluctuations. They denote a set of inequalities in which the square-mean-to-variance ratio, or precision $\mathfrak{p}(f)$, of a generic observable f integrated over a time interval t_f is bounded by an f-independent functional[4], which constitutes an upper estimate on the maximum possible precision $\mathfrak{p}_{max}$:

$$\mathfrak{p}(f) := \frac{|\langle f \rangle|^2}{\mathrm{Var} f} \leqslant \mathfrak{p}_{max}. \qquad (1)$$

It was first conjectured in [11] that $\mathfrak{p}$ for a time-integrated current-like (i.e. odd under time reversal) observable f is bounded by half the expected entropy $\langle \sigma \rangle$ produced over the interval t_f, i.e. $\mathfrak{p}_{max} \leqslant \langle \sigma \rangle / 2$. This so-called thermodynamic uncertainty relation, originally proved in the linear response regime and under stationary conditions, triggered an intense activity seeking generalizations or improvements for the largest possible class of out-of-equilibrium conditions. Apart from its conceptual importance, i.e. the existence of an universal upper bound set by dissipation on the precision of any current, (1) has major

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[4] Observable dependent bounds were also studied see, e.g., [10].

Table 1. Summary of the quantities entering the various bounds.

(Normalized) precision	'Dissipation'	Total variation distance	Entropy prod. per period	Entropy prod. rate	Prob. flow
$\mathfrak{np} := \frac{\langle f \rangle^2}{\langle f^2 \rangle}$ $\mathfrak{p} := \frac{\langle f \rangle^2}{\mathrm{Var} f}$	$\sigma := \ln \frac{p}{\bar{p}}$	$d := \frac{1}{2} \sum_\omega |p - \bar{p}|$	$\langle \sigma_i \rangle := \sum_{\omega_i} p_i \ln \frac{p_i}{\bar{p}_i}$	$\langle \dot{\sigma} \rangle := \frac{\langle \sigma_i \rangle}{\Delta t}$	$j_e := \frac{p_e}{\Delta t}$

Table 2. Summary of the various bounds.

Non-Markovian dyn. time-antisymmetric f (section 3)	$\mathfrak{np}_{\max} = \left\langle \tanh \frac{\sigma}{2} \right\rangle \leqslant d \tanh \frac{\langle \sigma \rangle}{2d} \leqslant \tanh \frac{\langle \sigma \rangle}{2}$ $\mathfrak{p}_{\max} \leqslant \frac{e^{\langle \sigma \rangle} - 1}{2}$ tightest asymptotic bound $\mathfrak{p}_{\max} \leqslant e^{\langle \sigma \rangle}/4$ for $\langle \sigma \rangle \gg 1$
Markovian stationary dynamics satisfying (34) (section 4)	$\frac{\mathfrak{p}_{\max}(\Omega)}{N} \leqslant \mathfrak{p}_{\max}(\Omega_i)$
Markovian periodic dynamics time-antisymmetric integrated f (section 4.6)	$\frac{\mathfrak{p}_{\max}(\Omega)}{N} \leqslant \frac{e^{\langle \sigma_i \rangle} - 1}{2}$
Markovian stationary dynamics time-antisymmetric time-summed f (section 5)	$\frac{\mathfrak{p}_{\max}}{t_{\mathrm{f}}} \leqslant \sum_e \frac{(j_e - j_{\bar{e}})^2}{j_e + j_{\bar{e}}} \leqslant \frac{1}{2} \sum_e |j_e - j_{\bar{e}}| \leqslant \frac{1}{2} \sum_e (j_e + j_{\bar{e}})$ $\frac{\mathfrak{p}_{\max}}{t_{\mathrm{f}}} \leqslant \frac{\langle \dot{\sigma} \rangle}{2}$
Markovian stationary dynamics time-summed f (section 4.7)	$\frac{\mathfrak{p}_{\max}}{t_{\mathrm{f}}} \leqslant \frac{1}{2} \sum_e (j_e + j_{\bar{e}})$

practical consequences. Indeed, (1) allows one to bound functions of the system's dissipation which are not directly measurable, e.g. the thermodynamic efficiency of molecular motors [12], or to reveal the existence of hidden nonequilibrium states [13]. A first proof valid beyond the linear regime but restricted to large time intervals t_{f} [16] was soon extended to arbitrary t_{f} [22]. These, and related early results [14, 15, 18–21] were obtained within large deviation theory, by progressively refining the bound on the rate function for empirical currents of jump and diffusion processes. Simultaneously, the same formalism was employed to extend (1) to counting observables of jump processes [17]. In this context it was found that $\mathfrak{p}$ is bounded by the mean of the total number of jumps, or activity, occurring in the time span t_{f}.

A different method to tackle the problem, based on perturbing the generating function of an arbitrary observable f, was designed in [25]. It yields an upper bound for the response of f, which reduces to (1) when the chosen perturbation results in a time rescaling of the dynamics. The entropic [24] as well as the activity bound [35] have thus been extended to both current-like and counting observables. This approach, which makes contact with inequalities originally derived by Kullback [26], has sparked much interest in the application of information theoretic results and concepts.

More recently [27], the exponential bound $\mathfrak{p}_{\max} \leqslant (\exp \langle \sigma \rangle - 1)/2$ has been derived for Langevin dynamics with feedback, under the condition of validity of the detailed (joint) fluctuation theorem for σ and f. The same bound had already been derived in [23] for periodically driven Markovian systems with a time-symmetric protocol, where now $\langle \sigma \rangle$ is computed over one period and $(\exp \langle \sigma \rangle - 1)/2$ bounds the precision divided by the (asymptotically large) number of periods.

Here, we provide an overarching method, based on elementary observations on the Hilbert space structure of observables, to recover and generalize the various bounds obtained so far in the literature. First, we provide an exact expression for $\mathfrak{p}_{\max}$ in the case of arbitrary stochastic processes, possibly non-Markovian, time-varying or non-stationary, and show that the bound $(\exp \langle \sigma \rangle - 1)/2$ can be improved by a factor 2, and no more. In the case of periodic Markovian processes, we derive a periodic uncertainty relation—the deepest result of this article—stating that the precision over a period bounds the precision per period over arbitrary time intervals, which trivializes or extends most asymptotic bounds obtained so far in the periodic Markovian case. In the case of stationary time-invariant Markov processes, it also allows to replace them with simple and tighter bounds, valid over all time intervals, the most revealing being the sum of the absolute values of the currents (tables 1 and 2).

2. The Hilbert uncertainty relation

2.1. General formulation

We first state the most abstract version of our result. We consider a general real or complex Hilbert space $\mathcal{F}$ with some scalar product $\langle . | . \rangle$. To every $f \in \mathcal{F}$ is associated the so-called mean value of f, a scalar quantity $\langle f \rangle$ that is linear and continuous in f, i.e. a one-form in the dual of $\mathcal{F}$. By virtue of the Riesz representation theorem, one can find a special element m in $\mathcal{F}$, so that the mean is expressed as $\langle f \rangle = \langle m | f \rangle$, $\forall f \in \mathcal{F}$. We call m an averaging observable for $\mathcal{F}$. We now consider the following ratio, that we called normalized

precision for reasons that will appear clearly below,

$$\mathfrak{np}(f) := \frac{|\langle f \rangle|^2}{\langle f | f \rangle}. \tag{2}$$

Through Cauchy–Schwarz inequality we get $|\langle f \rangle|^2 = |\langle m | f \rangle|^2 \leqslant \langle m | m \rangle \langle f | f \rangle$, with equality when f is a multiple of m. Thus

$$\mathfrak{np}_{\max} := \max_{f \in \mathcal{F}} \frac{|\langle f \rangle|^2}{\langle f | f \rangle} = \langle m | m \rangle = \langle m \rangle. \tag{3}$$

This constitutes the key observation of this article which we call the Hilbert uncertainty relation.

2.2. Application to random dynamical systems

To be concrete, we focus on classical physical systems described by a configuration space Ω whose elements ω are, for example, trajectories of a random dynamical system. The configuration space is endowed with a probability measure $p(\omega)$. An obvious Hilbert space of interest is the space $\mathcal{L}^2(\Omega)$ of square-summable observables, i.e. functions $f : \Omega \to \mathbb{R}$ such that the mean

$$\langle f \rangle = \sum_{\omega} f(\omega) p(\omega) \tag{4}$$

and the mean square

$$\langle f^2 \rangle = \sum_{\omega} f(\omega)^2 p(\omega) \tag{5}$$

are well-defined and finite. Introducing the scalar product between two observables f and g,

$$\langle g | f \rangle = \sum_{\omega} g(\omega) f(\omega) p(\omega), \tag{6}$$

we can recast (4) and (5) as, respectively,

$$\langle f \rangle = \langle 1 | f \rangle, \quad \langle f^2 \rangle = \langle f | f \rangle. \tag{7}$$

We adopt the discrete summation notations, even though our considerations also apply to continuous cases. For example, ω can be a point in the phase-space of a Hamiltonian system. The normalized precision now ranges between zero and one, and is equivalent to precision via the relation

$$\mathfrak{p}(f) = \mathfrak{np}(f)/(1 - \mathfrak{np}(f)), \tag{8}$$

since $\mathrm{Var}(f) = \langle f | f \rangle - \langle f \rangle^2$. In this situation, the averaging observable m is simply the constant observable 1, so that $\mathfrak{np}_{\max} = 1$, corresponding to zero variance and infinite precision.

However in many situations we are interested in a (closed) linear subspace $\mathcal{F}$ of those observables, sharing some properties of interest, which we call for the sake of convenience the 'legitimate observables'. If this subspace, itself a Hilbert space for the same scalar product, does not contain the constant observables, then there is a non-trivial legitimate averaging observable m, for which $\mathfrak{np}_{\max}$ now caps the normalized precision of all legitimate observables. It is also the orthogonal projection of the constant observable 1 onto the space $\mathcal{F}$ of legitimate observables, as $\langle f \rangle = \langle 1 | f \rangle = \langle m | f \rangle$ implies that $1 - m$ is orthogonal to all legitimate observables. From (3) and (8), it follows that the corresponding $\mathfrak{p}_{\max}$ over $\mathcal{F}$ is $\langle m | m \rangle / (1 - \langle m | m \rangle)$.

2.3. Geometric interpretation

Interestingly the quantity $\langle m | m \rangle / (1 - \langle m | m \rangle)$ has a geometric interpretation. Assume that we find a square-summable observable M—possibly illegitimate, i.e. outside of $\mathcal{F}$—that
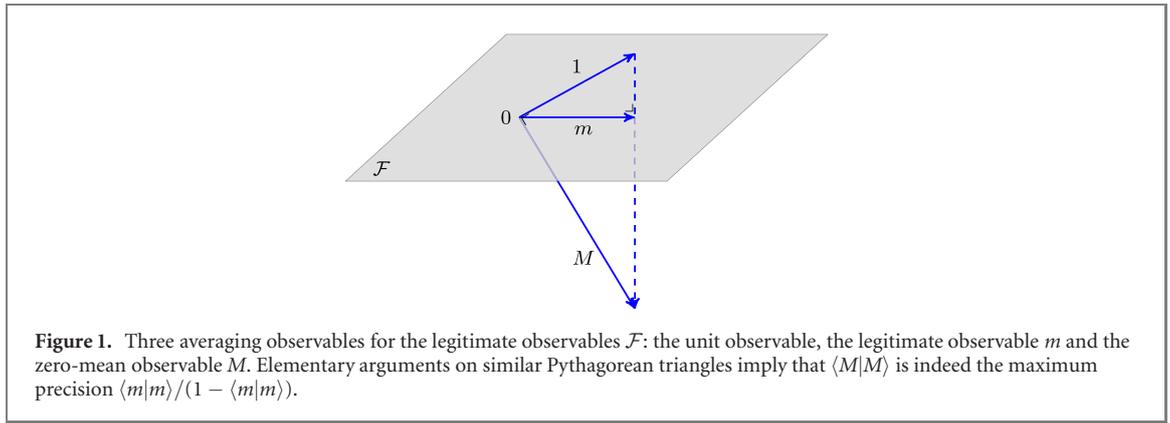
(a) is zero-mean, $\langle M \rangle = \langle 1 | M \rangle = 0$ i.e. it is orthogonal to 1,
(b) is an averaging observable, i.e. $\langle M | f \rangle = \langle f \rangle$ for all legitimate observables f.

Then $\langle M | f \rangle$ is also the covariance of M with f. Indeed,

$$\mathrm{Cov}(M, f) := \langle M | f \rangle - \langle M \rangle \langle f \rangle \overset{(a)}{=} \langle M | f \rangle \overset{(b)}{=} \langle f \rangle. \tag{9}$$

Therefore, Cauchy–Schwarz inequality applied to the covariance,

$$\langle f \rangle^2 = \mathrm{Cov}(M, f)^2 \leqslant \mathrm{Var}(M) \, \mathrm{Var}(f) = \langle M | M \rangle \, \mathrm{Var}(f), \tag{10}$$

Figure 1. Three averaging observables for the legitimate observables $\mathcal{F}$: the unit observable, the legitimate observable m and the zero-mean observable M. Elementary arguments on similar Pythagorean triangles imply that $\langle M|M \rangle$ is indeed the maximum precision $\langle m|m \rangle / (1 - \langle m|m \rangle)$.

yields that $\langle M|M \rangle$ is an upper bound on the maximum precision of legitimate observables. In fact, if M belongs to the span of 1 and m (while being orthogonal to 1), namely,

$$M(\omega) = 1 - \frac{1 - m(\omega)}{1 - \langle m \rangle}, \tag{11}$$

we find that $\langle M|M \rangle$ is exactly the maximum precision $\langle m|m \rangle / (1 - \langle m|m \rangle)$ reachable over $\mathcal{F}$ (see figure 1 for a geometric representation).

3. Time anti-symmetric observables

The TURs are obtained by considering Ω as the set of all possible paths of a random process, endowed with an involution symmetry (i.e. a transformation whose square is the identity) called time-reversal, which maps any path ω in Ω to its time-reversed path $\overline{\omega}$. We consider legitimate the observables that are time-antisymmetric, i.e. satisfying $f(\omega) = -f(\overline{\omega})$. The time-reversal induces another probability measure $\overline{p}(\omega) = p(\overline{\omega})$, attributing to an event the p-probability of the time-reversed event. Then the scalar product of two time-antisymmetric observables g and f can be written as

$$\langle g|f \rangle = \sum_\omega f(\omega)g(\omega)(p(\omega) + \overline{p}(\omega))/2 \tag{12}$$

while the mean of f is written as

$$\langle f \rangle = \sum_\omega f(\omega)(p(\omega) - \overline{p}(\omega))/2. \tag{13}$$

Setting $g = m$ in (12) and equating to (13), we deduce that the mean observable m (satisfying $\langle m|f \rangle = \langle f \rangle$) is the time-antisymmetric observable

$$m = \frac{p - \overline{p}}{p + \overline{p}}. \tag{14}$$

Hence, the maximum normalized precision over all time-antisymmetric observables follows from the Hilbert uncertainty principle (3):

$$\mathfrak{np}_{\max} = \left\langle \frac{p - \overline{p}}{p + \overline{p}} \right\rangle = \frac{1}{2} \sum_\omega \frac{(p - \overline{p})^2}{p + \overline{p}}. \tag{15}$$

This *exact* bound can be written in terms of $\sigma := \ln \frac{p}{\overline{p}}$ as

$$\mathfrak{np}_{\max} = \left\langle \tanh \frac{\sigma}{2} \right\rangle. \tag{16}$$

For a simple example of application, consider a stationary (Markovian or not) diffusive process (on a continuous state space) over an infinitesimal time interval Δt, where σ is itself very small with probability one, due to continuity of trajectories. As a result, (16) yields $\mathfrak{p}_{\max} = \langle \sigma \rangle / 2$, since (8) gives $\mathfrak{np}_{\max} = \mathfrak{p}_{\max}$ plus $O(\Delta t^2)$ corrections. This shows that the celebrated entropy bound is tight in this case, as observed already in [28]. Therefore, if one uses TURs in order to lower-bound entropy production on such a process, the observation interval should be as small as possible [29].

Equation (15) clearly cancels when the probability measure is time-symmetric, $p = \overline{p}$, and can be loosened in terms of two different quantities that capture the gap separating p from $\overline{p}$. First, the total

variation distance, ranging between zero and one, $d := \frac{1}{2}\sum_\omega |p - \overline{p}|$. Second, the Kullback–Leibler (KL) divergence $\langle\sigma\rangle$. Rewriting (15) as $\mathfrak{np}_{\max}/d = \sum_\omega (|p - \overline{p}|/2d) \tanh(|\sigma|/2)$, a convex combination of positive values of the function tanh (concave on the positive values), we obtain the relaxed inequality

$$\mathfrak{np}_{\max} \leqslant d \tanh \frac{\langle\sigma\rangle}{2d}, \tag{17}$$

the main result of this section. As this expression is increasing in d, one can use the coarse bound $d \leqslant 1$ to obtain $\mathfrak{np}_{\max} \leqslant \tanh \frac{\langle\sigma\rangle}{2}$. Using (8), the latter reads in term of square-mean-to-variance ratio

$$\mathfrak{p}_{\max} \leqslant \frac{e^{\langle\sigma\rangle} - 1}{2}, \tag{18}$$

a bound recently proposed under the name of General TUR [27, 31]. We underline that this result is valid for arbitrary dynamics, such as non-Markovian and non-autonomous, for all time intervals T, and all possible time-antisymmetric observables—not necessarily time-integrated ones. It is even valid for set of paths of variable length, e.g., defined by a random stopping time. It is also valid for any notion of 'time-reversal' that is an involution of Ω. For example, if a path is defined as a discrete or continuous list of 'states', then the time-reversed path may be defined as the time-reversed list of the same states, or the time-reversed list of conjugated states. Typically, in a model of an underdamped system we want to include the speed or momentum as part of the state, and flip it as well as reversing the order of states when applying time-reversal. All these choices for the time-reversal involution will yield mathematically valid inequalities, but not all will carry the same physical meaning. For instance, it is only in the circumstances where the detailed fluctuation relation holds [6] that $\langle\sigma\rangle$ is the physical entropy production associated with the process (as discussed in [27]). One such circumstance is when the system is driven by a time-symmetric protocol, and respects local detailed balance at all times. Outside these examples, $\langle\sigma\rangle$ is to be regarded as an observable of interest, accessible in principle to the measurement, bearing no direct connection to thermodynamics, yet useful as a bound on the fluctuations of time-antisymmetric observables such as total displacement, etc. Note that some observables of practical interest, such as work or heat, are dependent on the parameters of the protocol and therefore are time-antisymmetric if the time-varying protocol is itself time-symmetric. Time-symmetric protocol is an assumption requested by [23, 27]. In the case of arbitrary time-varying protocols, another notion of time-reversal is needed, which also reverses the protocol, in order to include those observables of interest in the space of legitimate observables. This was first investigated in [30] with a tailored large deviation argument and later in [31]. In appendix A we provide a formal statement and a proof of the main result in [30] as a direct corollary of (18).

A slightly tighter bound than (18) (whose implicit expression appears in [32]) follows from replacing d in (17) by an upper bound given in terms of $\langle\sigma\rangle$. Here we show how to obtain such bound on d exploiting (17) itself in combination with the legitimate observable $f = \mathrm{sgn}(p - \overline{p})$. For the latter the normalized precision $\mathfrak{np}$ is d^2 and (8) becomes

$$d^2 \leqslant d \tanh \frac{\langle\sigma\rangle}{2d}, \tag{19}$$

or

$$2d \, \mathrm{atanh} \, d \leqslant \langle\sigma\rangle, \tag{20}$$

which allows to find the bound $d \leqslant d^*(\langle\sigma\rangle)$ where the right-hand-side is defined by

$$2d^* \, \mathrm{atanh} \, d^* = \langle\sigma\rangle. \tag{21}$$

Injecting this bound on d into (8), we obtain

$$\mathfrak{np}_{\max} \leqslant d^* \tanh \frac{\langle\sigma\rangle}{2d^*} = d^*(\langle\sigma\rangle)^2, \tag{22}$$

a tighter bound than (18), which was obtained from the trivial bound $d \leqslant 1$ (see figure 2 for a comparison of the two bounds). Remarkably, this is the tightest bound obtainable from the sole knowledge of $\langle\sigma\rangle$ as the following argument proves. We split Ω into Ω_0 and $\overline{\Omega}_0$. On both parts we take a uniform probability distribution, so that the total probability of Ω_0 is $p_0 \geqslant 1/2$. With this choice we obtain $(2p_0 - 1) \ln \frac{p_0}{1 - p_0} = \langle\sigma\rangle$. One sees that the total variation distance is precisely $d = 2p_0 - 1$, so that $d = \tanh(\langle\sigma\rangle/2d)$. Hence, the bound is matched with equality.

As a minimal example of physical system reaching the bound, consider the deterministic, reversible dynamics of a single particle moving in one spatial (linear or angular) dimension in absence of external forces. The probability for the particle to have started with positive (resp. negative) velocity is p_0 (resp. $1 - p_0$). Since the dynamics does not alter this probability, we have that at any time the average velocity is
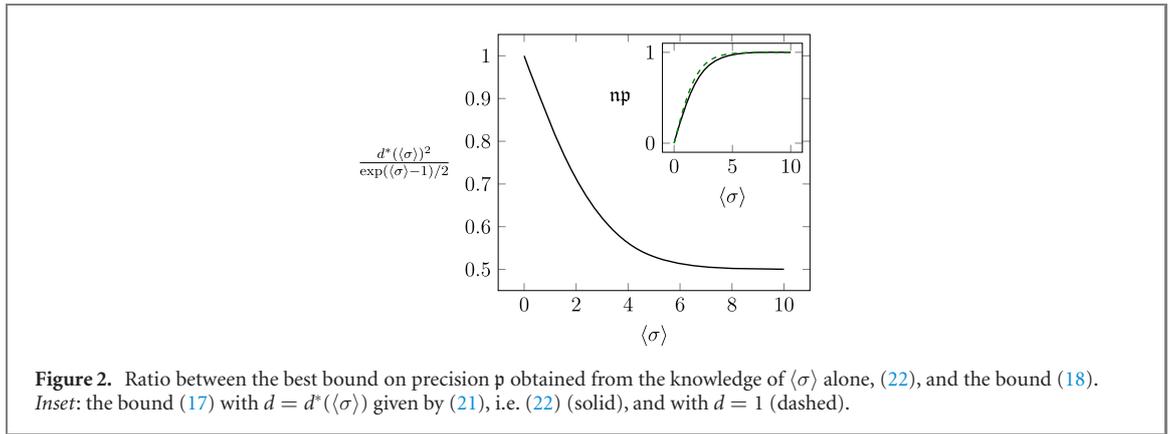
Figure 2. Ratio between the best bound on precision $\mathfrak{p}$ obtained from the knowledge of $\langle\sigma\rangle$ alone, (22), and the bound (18). *Inset*: the bound (17) with $d = d^*(\langle\sigma\rangle)$ given by (21), i.e. (22) (solid), and with $d = 1$ (dashed).

$2p_0 - 1$, the second moment equals 1, so that $\mathfrak{np} = (2p_0 - 1)^2 = d^2$ and the bound (22) is saturated. This is also an example where σ is well-defined but may not coincide with the physical entropy production.

For $\langle\sigma\rangle \gg 1$, or equivalently $1 - d^* \ll 1$, the asymptotic expression of (22) gives the novel bound

$$\mathfrak{p}_{\max} \leqslant e^{\langle\sigma\rangle}/4 \quad \text{for } \langle\sigma\rangle \gg 1. \tag{23}$$

To obtain it we expand $d^* = \tanh\frac{\langle\sigma\rangle}{2d^*} \approx 1 - 2e^{-\frac{\langle\sigma\rangle}{d^*}} \approx 1 - 2e^{-\langle\sigma\rangle}$. The latter step stems from $d^* \approx 1$ but requires some care in the error analysis, in particular it requires to show that $(1 - d^*)\langle\sigma\rangle \ll 1$. Plugging d^* into (22) and using the relation $\mathfrak{p} = \mathfrak{np}/(1 - \mathfrak{np})$, we obtain (10), confirming the numerical observation in figure 2.

Again, (23) is reached for the deterministic one-dimensional system above, with $1 - p_0 \ll 1$.

4. The periodic uncertainty relation

We come back to the general setting of (2.2), i.e. a physical system with stochastic dynamics, for an arbitrary class of legitimate observables f. We introduce progressively the assumptions of Markovianity on the path level, then periodicity, and finally the construction of a state space and state observables (as for now we have only considered path observables). This will lead us to the central result of this paper, the periodic uncertainty relation. Roughly speaking, it states that if the gradient-like observables (obtained as the gradient of a state observable) are legitimate, then the precision reachable over N periods (for any $N > 1$) is less than N times the precision reachable over a single period:

$$\frac{\mathfrak{p}_{\max}(\Omega)}{N} \leqslant \mathfrak{p}_{\max}(\Omega_i). \tag{24}$$

We then show how all the results about periodic continuous-time or discrete-time Markov chains derived in the literature for various classes of observables from various arguments can be immediately derived from our periodic uncertainty relation.

4.1. Time-summed observables

We first set up the most appropriate formalism to describe time-summed observables. We decompose the configuration space Ω as a Cartesian product $\Omega_0 \times \Omega_1 \times \ldots \Omega_{N-1}$, so that a global configuration ω is seen as the concatenation of N 'local' configurations $\omega_0, \omega_1, \ldots, \omega_{N-1}$. Although the formalism applies in principle to any sort of configurations (for instance spin configurations), having in mind the application to the thermodynamic uncertainty relations, from now on we refer to ω_i as the 'local path', of duration Δt, and to ω and as the 'global path' of duration $N\Delta t$.

The global probability measure $p(\omega)$ on Ω naturally projects into marginal probability measures $p_i(\omega_i)$ on each Ω_i, and into marginal pairwise probability measures $p_{ji}(\omega_j, \omega_i)$ on each pair $\Omega_j \times \Omega_i$. The so-called *time-summed observables* on Ω are those of the form $f = \sum_{i=0}^{N-1} f_i$, where $f_i(\omega_i)$ is an observable on Ω_i. We take the legitimate observables on Ω as those time-summed observables f such that each f_i is locally legitimate, i.e. belongs to the space $\mathcal{F}_i$ of legitimate observables on Ω_i. The mean of a time-summed observable is the sum of local means $\langle f\rangle = \sum_i \langle f_i\rangle_i$. The mean product of two such observables $g = \sum_j g_j$ and $f = \sum_i f_i$ can be written in terms of scalar products on each Ω_j,

$$\langle g|f\rangle = \sum_{i,j}\sum_{\omega_i,\omega_j} g_j p_{ji} f_i = \sum_{i,j}\langle g_j|P_{i|j}f_i\rangle_j. \tag{25}$$

Here, we decomposed p_{ji} as $p_j p_{i|j}$, with $p_{i|j}(\omega_j, .)$ the conditional probability measure on Ω_i given ω_j, and wrote $\sum_{\omega_i} p_{i|j} f_i = P_{i|j} f_i$ to emphasize that it maps an observable on Ω_i to an observable on Ω_j through a linear conditional mean operator $P_{i|j}$. If the local paths spaces Ω_i and Ω_j are discrete then we can understand f_i as a column vector indexed by the elements of Ω_i and $P_{i|j}$ as a transition matrix whose entries are $p_{i|j}(\omega_j, \omega_i)$ and rows sum to one; in this intepretation $P_{i|j} f_i$ is a usual matrix-vector multiplication. Note that even if f_i is legitimate, i.e. belongs to $\mathcal{F}_i$, the conditional mean observable $P_{i|j} f_i$ may be an arbitrary square-integrable observable on Ω_j, not necessarily legitimate. Observe that $P_{j|i} = P_{i|j}^*$, where * denotes the adjunction of linear operators between the Hilbert spaces $\mathcal{L}^2(\Omega_i)$ and $\mathcal{L}^2(\Omega_j)$ equipped with their respective scalar products.

4.2. Periodic Markovian processes

We now specialize the computation of (25) introducing first the assumption of Markovian dynamics, and later of periodic dynamics. Assuming that the sequence $\omega_0, \dots, \omega_{N-1}$ is a Markov chain implies that $P_{i|j} = P_{i|k} P_{k|j}$ for any $i < k < j$, and also for any $j < k < i$, which is known as Chapman–Kolmogorov's equation. Moreover, assume that the dynamics is periodic of period Δt, which means that all Ω_i can be taken identical with identical marginals $p_i = p_j$, the joint measures p_{ji} only depend on the difference $i - j$, and the spaces of legitimate observables are identical as well, $\mathcal{F}_i = \mathcal{F}_j$. Then, it is enough to consider $P := P_{j+1|j}$, from which we compute any $P_{i|j}$ as P^{i-j} if $i \geqslant j$, and $(P^*)^{j-i}$ if $i \leqslant j$, where P^* is the adjoint of P for the scalar product $\langle . | . \rangle_j$ over Ω_j. Note that P is the usual transition matrix appearing in the master equation associated to the discrete-step Markov chain $\omega_0, \dots, \omega_{N-1}$, as we may write the propagation of transient probability measures as

$$p(\omega_{j+1}) = \sum_{\omega_j} p(\omega_j) P(\omega_j, \omega_{j+1}). \tag{26}$$

In this equation, intepreted in matrix notation, the probability measures $p(\omega_{j+1})$ and $p(\omega_{j+1})$ appear as row vectors.

Nevertheless, as we assume periodicity, i.e. stationarity of this Markov chain of local paths $\omega_0, \dots, \omega_{N-1}$, the master equation (26) is of little use here, except to notice that $p(\omega_j)$ must be the dominant left-eigenvector of P, of eigenvalue 1. The viewpoint explicited above, and used in (25), sees P as describing the propagation of the conditional mean of an observable instead of the transient probability measures: this is the 'Heisenberg viewpoint' dual to the master equation.

From the knowledge of P we can compute the mean product of any two time-summed observables $g = g_0 + \dots + g_{N-1}$ and $f = f_0 + \dots + f_{N-1}$ over an arbitrary number N of intervals, as given by (25), which now becomes

$$\langle g | f \rangle = \sum_i \langle g_i | f_i \rangle_i + \sum_{i,j:i>j} \langle g_i | P^{i-j} f_i \rangle_j + \sum_{i,j:i<j} \langle g_j | (P^*)^{j-i} f_i \rangle_j \tag{27}$$

or, equivalently:

$$\langle g | f \rangle = \sum_i \langle g_i | f_i \rangle_i + \sum_{i,j:i>j} \langle (P^*)^{i-j} g_j | f_i \rangle_i + \sum_{i,j:i<j} \langle P^{j-i} g_j | f_i \rangle_i. \tag{28}$$

To proceed, we exploit Markovianity and periodicity further, as they imply the possibility to define a concept of 'state space' to the Markov chain. This state space is such that to a path ω_i we can associate a source state $s(\omega_i)$ and a target state $t(\omega_i)$, with the properties that $s(\omega_{i+1}) = t(\omega_i)$ and that ω_i, ω_{i+1} are independent given the state $t(\omega_i)$. With the knowledge of the probability measure on the paths, one can always build in principle (albeit in a non-unique way) a notion of state complying with these properties, as being a sufficient statistics of the past for the future and conversely [36, 37]. In most applications, the reverse situation occurs, where a natural notion of state is given, from which a notion of path is built as a (discrete or continuous) list of successive states. Once a state space X is fixed, together with the source map s and target map t, one may endow a probability measure on X as $p(x) = \sum_{t(\omega_i)=x} p(\omega_i) = \sum_{s(\omega_{i+1})=x} p(\omega_{i+1})$. From this we define a Hilbert space of square-summable real observables $\mathcal{L}^2(X)$ on the state space X, with scalar product denoted $\langle \cdot | \cdot \rangle$.

We now have natural linear mappings between the path observables and the state observables. In particular given an observable $f_i(\omega_i)$, we denote Sf_i the mean of f_i knowing the source state. In other words,

$$(Sf_i)(x) = \sum_{\omega_i:s(\omega_i)=x} \frac{p(\omega_i)}{p(x)} f_i(\omega_i).$$

In other terms, we can write the operator S as a matrix whose entry $S(x, \omega_i)$ is $p(\omega_i)/p(x)$ if $x = s(\omega_i)$ and 0 otherwise.

The adjoint operator S^* is even simpler to express. It lifts a state observable to a path observable: if $h(x)$ is a state observable, then $(S^*h)(\omega_i) = h(s(\omega_i))$. If we think of S^* as a matrix (with rows indexed by paths and columns indexed by states), its entry $S^*(\omega_i, x)$ is 1 if $s(\omega_i) = x$ and 0 otherwise: we see here that S^* is the 'source incidence matrix', a binary matrix relating each path with its source. This is observed by writing down the identity defining S^*, namely $\langle S^*h|f_i \rangle = \langle h|Sf \rangle_X$ for all state observables h and all path observables f_i.

Similar considerations apply for T, the target conditional mean operator, and T^*, the 'target incidence matrix'. A trivial observation is that $S1 = T1 = 1$: the constant unit path-observable is mapped to the constant unit state-observable. Another observation is that $SS^* = TT^* = Id_X$, the identity on $\mathcal{L}^2(X)$. Moreover, we have $P = T^*S$ and $P^* = S^*T$.

4.3. Graph-theoretic interpretation and gradient-like observables

First we draw attention to a graph-theoretic interpretation of $T^* - S^*$: in matrix terms, each row corresponds to a path ω_i, with a -1 in the column corresponding to state $s(\omega_i)$, a $+1$ in the column corresponding to state $t(\omega_i)$, and zero entries otherwise. In other words it is the usual *incidence matrix* of the graph whose nodes are states and edges are paths of length Δt.

Defining a state observable $h : X \to \mathbb{R}$, we can derive a corresponding 'gradient-like' observable along (local) paths, denoted Δh, as the increment of h along the path:

$$\Delta h(\omega_i) = h(t(\omega_i)) - h(s(\omega_i)). \tag{29}$$

One can write compactly $\Delta h = (T^* - S^*)h$. Therefore the space of gradient-like observables is the image space of the incidence matrix $T^* - S^*$. It can also be characterized as the observable that sum to zero over each cycle of the graph ('no curl'). Gradient-like observables have zero mean value, $\langle \Delta h \rangle = 0$, which directly follows from (29) and stationarity (which states that source and target of a random path are identically distributed). In the Hilbert space formalism, we can also write:

$$\langle \Delta h \rangle = \langle 1|\Delta h \rangle_i = \langle 1|(T^* - S^*)h \rangle_i = \langle (T - S)1|h \rangle_X = 0.$$

If gradient-like observables are legitimate, it implies that their mean can be computed with any averaging observable M_i of the space of legitimate observables:

$$0 = \langle \Delta h \rangle = \langle M_i|\Delta h \rangle_i = \langle M_i|(T^* - S^*)h \rangle_i = \langle (T - S)M_i|h \rangle_X.$$

In particular, if every gradient-like observable is legitimate then we conclude that $SM_i = TM_i$ for every averaging observable of the legitimate space. In particular, we then have

$$Sm_i = Tm_i \tag{30}$$

for the legitimate averaging observable m: the mean value of m along a path knowing that its source is x equals the mean value of m along a path knowing that its target is x, for every state x. This condition is helpful in the proof of the periodic uncertainty relation as we see next.

Examples of gradient-like observables along a path include work of a conservative force (if the states of the Markov chain represent the states of a physical system and the state observable h is the potential energy) and displacement (if states of the Markov chain are each associated to a unique spatial position of the system, which is the state observable).

4.4. The periodic uncertainty relation: statement of the main result

We are finally in the position to state the periodic uncertainty relation.

We assume that over a single period of a periodic Markovian system the gradient-like observables are legitimate (or even more generally, the averaging observable m_i satisfies (30)). Then the precision that can be achieved over N periods, divided by N, is less than the precision that can be achieved in a single period, equation (24).

This is our most general statement of the periodic uncertainty relation. After the proof, we specialize it to antisymmetric observables, and to time-summed observables supported by the transitions of continuous time Markov chain.

4.5. The periodic uncertainty relation: proof

We prove the periodic uncertainty relation using the mapping between trajectories and state space. Under the assumptions introduced in the previous subsections suppose that for a certain space of legitimate observables on Ω_i, we find a zero-mean averaging observable M_i, i.e. checking $\langle M_i|f_i \rangle_i = \langle f_i \rangle$ for every

legitimate observable f_i. We now introduce the crucial assumption that M_i is such that $SM_i = TM_i$. Then it is easily checked with the identities derived at the end of section 4.2 that $PP^*M_i = PM_i$ and $P^*PM_i = P^*M_i$.

Let us get back to the computation of $\langle g|f \rangle$, for $g = g_0 + \cdots + g_{N-1}$ and $f = f_0 + \cdots + f_{N-1}$. Recall from (28) that the total contribution of f_i in this sum is

$$\langle P^i g_0 + P^{i-1} g_1 + \cdots + P g_{i-1} + g_i + (P^*) g_{i+1} + \cdots + (P^*)^{N-i-2} g_{N-2} + (P^*)^{N-i-1} g_{N-1} | f_i \rangle_i. \qquad (31)$$

Assume that we take $g_0 = M_i$ and $g_1 = \ldots = g_{N-1} = (Id - P)M_i$. Then the contribution of f_i to $\langle g|f \rangle$ reduces to $\langle M_i|f_i \rangle_i$ (using among others the fact that $P^*(Id - P)M_i = 0$). Thus g is a zero-mean averaging observable over Ω, as $\langle g|f \rangle = \sum_i \langle M_i|f_i \rangle_i = \langle f \rangle$ for every legitimate f. Therefore the precision over the N periods is bounded by $\langle g|g \rangle$, which develops as

$$\mathfrak{p}_{\max} \leqslant \langle M_i|M_i \rangle_i + (N-1)\langle (Id-P)M_i|(Id-P)M_i \rangle_i$$
$$= N \langle M_i|M_i \rangle_i - (N-1)\langle PM_i|PM_i \rangle_i \qquad (32)$$
$$\leqslant N \langle M_i|M_i \rangle_i \qquad (33)$$

using $\langle PM_i|PM_i \rangle_i = \langle M_i|P^*PM_i \rangle_i = \langle M_i|P^*M_i \rangle_i = \langle PM_i|M_i \rangle_i = \langle M_i|PM_i \rangle_i$. Therefore, $\langle M_i|M_i \rangle_i$ is not only a bound on the precision over one period but also a bound over the precision over N periods, if scaled with a factor N. In particular, if the legitimate averaging observable m_i satisfies

$$Sm_i = Tm_i, \qquad (34)$$

then the observable M_i given by (4) also satisfies $SM_i = TM_i$. Moreover $\langle M_i|M_i \rangle_i = \mathfrak{p}_{\max}(\Omega_i)$. Equation (34) states the equivalence of conditioning the average of m over the initial or the final state. In particular this is true when all gradient-like observables are legitimate, as stated in section 4.3. This concludes the proof of the periodic uncertainty relation, as stated above.

4.6. The periodic uncertainty relation for time-antisymmetric observables

In this section assume that the legitimate observables over one period Ω_i are the time-antisymmetric observables, $f_i(\omega_i) = -f_i(\overline{\omega}_i)$, for some definition time-reversal, i.e. any involutive symmetry of Ω_i. We also assume that the path on a period (which up to now has been defined as an element of some arbitrary abstract space Ω_i, from which we can derive a source state and a target state) is a discrete or continuous sequence of states of a Markov process, and the time-reversal simply consists in taking this sequence in reverse order. This is the case when the Markov process models an overdamped system, fully described at all times by 'even' quantities, not changing sign under time reversal.

In this framework, it is clear that gradient-like observables are legitimate, as they are time-antisymmetric. Indeed, time-reversal of a path swaps source and targets, thus changes the sign of Δh in (29). Note that this does not hold in general for underdamped process, where the time-reversal of a path running from x to y is not a path from y to x, but a path between a different pair of states (typically obtained from y and x by 'flipping momenta').

Alternatively we can prove directly that (30) holds for the legitimate averaging observable m_i defined by (14) in the following way. It is enough to show that $S(1 - m_i) = T(1 - m_i)$, since $S1 = T1$. But $1 - m_i = \frac{\overline{p}}{p + \overline{p}}$, thus $S(1 - m_i)$ evaluated at state x reads

$$S(1 - m_i) = \frac{1}{p(x)} \sum_{\omega_i : s(\omega_i) = x} \frac{p(\omega_i)\overline{p}(\omega_i)}{p(\omega_i) + \overline{p}(\omega_i)}. \qquad (35)$$

As this expression is symmetric for time-reversal, this is also $T(1 - m_i)$ evaluated at state x. It is essential for the proof above that state x has an even parity under time reversal. Namely, quantities like momenta are excluded as in overdamped systems.

Therefore we can apply the periodic uncertainty relation (24).

In particular, applying (18) to a single period, we find that the precision of N periods is bounded by

$$\frac{\mathfrak{p}_{\max}(\Omega)}{N} \leqslant \frac{e^{\langle \sigma_i \rangle} - 1}{2}, \qquad (36)$$

where $\langle \sigma_i \rangle$ is now the Kullback–Leibler divergence over a single interval. This is valid for arbitrary protocols (being understood that $\langle \sigma_i \rangle$ is not necessarily the entropy production). This includes in particular the result in [23] as a limit case $N \to \infty$, which was proved originally by large deviation techniques, for overdamped systems under time-symmetric protocols.

This includes the discrete-time stationary Markov chain case, where $\Delta t = 1$. The continuous-time stationary Markov chain case is obtained as the limit $\Delta t \to 0$. This is further discussed in section 5 below.

4.7. The activity bound as a periodic uncertainty relation

Finally, we used the above results to prove the activity bound [35]: the precision of an observable that is the weighted sum of the transitions undergone by a finite-state continuous time Markov chain during an arbitrary time interval is bounded by the mean number of transitions over that same interval.

In the first step, we find the maximum precision over a short time interval Δt. Over such an interval, we consider that zero or one transition takes place, as multiple transitions are extremely unlikely in such a short time. The legitimate observables are those that take zero value over constant paths (where zero transitions occur).

Let us first consider a general setting (absolutely no assumption on Ω). When the legitimate observables are defined as those that take zero value on a given subset Ω_z, we find that the legitimate averaging observable m is the function that takes zero value on Ω_z and unit value on $\Omega \backslash \Omega_z$. Therefore the maximum normalized precision is $\langle m|m \rangle = 1 - p(\Omega_z)$ and the maximum precision is $p(\Omega_z)^{-1} - 1$.

Coming back to the case of stationary finite state Markov chains over a short time interval Δt, we take Ω_z as the constant paths, and m_i assigns a unit weight to all transitions. The normalized precision $1 - p(\Omega_z)$ is the probability of a transition, which is also the mean number of transitions over Δt. This is proportional to Δt, and also equal in the first order to the the maximum precision (as second moment and variance differ by an order of Δt^2).

Now, gradient-like observable are clearly legitimate, as they take zero value on constant paths (alternatively, we can also check that (34) is satisfied, as the left-hand side now computes the probability flow leaving a state, and the right-hand side computes the probability flow entering a state). Therefore the periodic uncertainty principle applies, and the precision available over any time interval is no larger than the expected number of transitions: this is the activity bound.

5. Time anti-symmetric observables of stationary Markov processes

In the case of stationary (jump or diffusive) processes over a total time interval $[0, t_\mathrm{f}]$, the period is infinitesimal, $\Delta t = t_\mathrm{f}/N \rightarrow 0$, and so is $\langle \sigma_i \rangle$. Then (36) reduces to

$$\frac{\mathfrak{p}_{\max}}{t_\mathrm{f}} \leqslant \frac{\langle \sigma_i \rangle}{2\Delta t} \underset{\rightarrow}{=} \frac{\langle \dot{\sigma} \rangle}{2}, \tag{37}$$

with $\langle \dot{\sigma} \rangle$ the mean entropy production rate. Hence, we recover the entropy bound for arbitrary time intervals, previously proved with information-theoretic means [24].

Beyond recovering these results with a unified method, we can derive far sharper bounds. In particular, as already mentioned in section 4.7, for a stationary continuous-time Markov process precision and normalized precision over an infinitesimal time interval Δt coincide. So, in view of (15), the precision over a time interval $t_\mathrm{f} = N\Delta t$ is bounded by

$$\frac{\mathfrak{p}_{\max}}{t_\mathrm{f}} \leqslant \frac{1}{\Delta t} \sum_e \frac{(p_e - p_{\bar{e}})^2}{p_e + p_{\bar{e}}} \tag{38}$$

where p_e is the probability of a transition along a path e relating a source state $s(e)$ to a target state $t(e)$ over an infinitesimal time interval Δt. The flow is defined as $j_e := p_e/\Delta t$. In a finite state jump process, e is a transition between two different states, and j_e factors as $p_{s(e)} w_e$ for stationary state probability $p_{s(e)}$ and jumping rate w_e. We know that (38) can be relaxed to $\mathfrak{p}_{\max}/t_\mathrm{f} \leqslant (d/\Delta t) \tanh(\langle \sigma \rangle / 2d)$ with $d = \frac{1}{2}\sum_e |p_e - p_{\bar{e}}|$. We obtain in particular the simple and novel bound,

$$\frac{\mathfrak{p}_{\max}}{t_\mathrm{f}} \leqslant \frac{d}{\Delta t} = \frac{1}{2}\sum_e |j_e - j_{\bar{e}}| \tag{39}$$
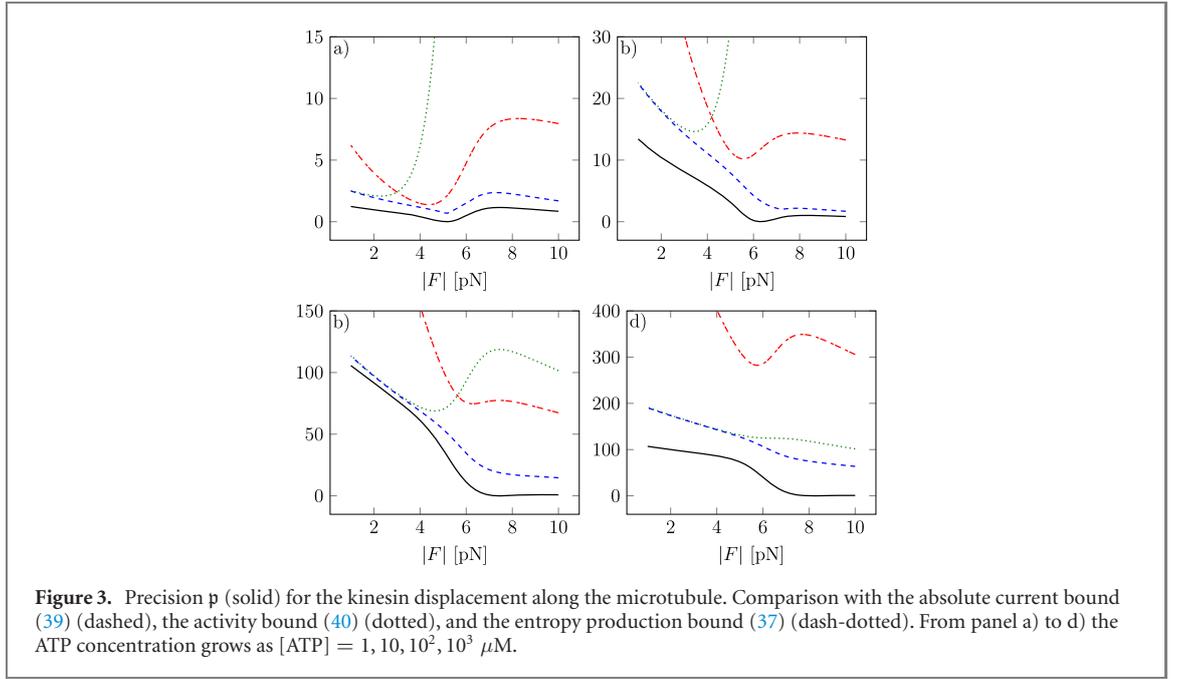
which we call the *absolute current bound*, valid for all stationary (jump or diffusion) Markov processes.

In the case of finite state jump processes, it is evidently tighter than the activity bound,

$$\frac{\mathfrak{p}_{\max}}{t_\mathrm{f}} \leqslant \frac{1}{2}\sum_e (j_e + j_{\bar{e}}). \tag{40}$$

As we have seen in section 4.7 this last bound applies to all time-summed observables taking non-zero values only on the transitions (thus zero values on the constant paths), without any request of time-antisymmetry [35], as a direct consequence of the periodic uncertainty relation.

Note that the mean entropy production rate in (37) when written in terms of the forward flow j_e and the backward one $j_{\bar{e}}$ reads $\langle \dot{\sigma} \rangle = \frac{1}{2}\sum_e (j_e - j_{\bar{e}}) \ln \frac{j_e}{j_{\bar{e}}}$. Therefore, (37), (39) and (40) require the same amount of

Figure 3. Precision $\mathfrak{p}$ (solid) for the kinesin displacement along the microtubule. Comparison with the absolute current bound (39) (dashed), the activity bound (40) (dotted), and the entropy production bound (37) (dash-dotted). From panel a) to d) the ATP concentration grows as $[\text{ATP}] = 1, 10, 10^2, 10^3$ μM.

information of the microscopic dynamics to be computed, namely, knowledge of j_e and $j_{\bar{e}}$ on each edge.

6. Example

We illustrate the different bounds for stationary Markovian dynamics on a benchmark example [35] which provides a minimal model for the molecular motor kinesin moving under load along a microtubule. Kinesin is either in a low energy state (1) with both heads on the microtubule or in a high energy state (2) with only one head attached. Transitions from state 1 to state 2 happen with or without ATP consumption, and cause both forward and backward motion along the microtubule (with half step size $\ell \simeq 4$ nm). Each of these four transitions $e = 1, \ldots, 4$ out of each state $x = 1, 2$ (making eight possible transitions) has an associated rate w_{xe}, given by [33, 34]:

$$w_{11} = \omega e^{-\epsilon + \theta_a^+ f}, \qquad\qquad w_{22} = \omega e^{-\theta_b^- f},$$

$$w_{12} = \omega' e^{-\epsilon - \theta_a^- f}, \qquad\qquad w_{22} = \omega' e^{\theta_b^+ f},$$

$$w_{13} = \alpha e^{-\epsilon + \theta_a^+ f} k_0 [\text{ATP}], \quad w_{23} = \alpha e^{-\theta_b^- f},$$

$$w_{14} = \alpha' e^{-\epsilon - \theta_a^- f} k_0 [\text{ATP}], \quad w_{24} = \alpha' e^{\theta_b^+ f}.$$

The control parameters are the ATP concentration, $[\text{ATP}]$, and the external loading force $F < 0$, with $f = F\ell/(k_{\text{B}}T)$ being its associated dimensionless work along the length ℓ. Typical ranges for *in vitro* experiments are $1\,\mu\text{M} \lesssim [\text{ATP}] \lesssim 10^3\,\mu\text{M}$ and $1\,\text{pN} \lesssim |F| \lesssim 10\,\text{pN}$. Other parameters encode kinetic details. The constants $\omega, \omega', \alpha, \alpha'$ are the bare rates for the two (forward and backward) pathways corresponding to ATP hydrolysis and thermal activation, and $\theta_{a,b}^{\pm}$ are loading factors accounting for different repartition of the force F among the transitions. All these parameters are chosen as in [33, 35], i.e. extracted from fits of experimental velocity data.

Note that in this case displacement is not a gradient-like observable, because each state of the Markov process is not associated with a single position of the kinesin.

In figure 3 we plot $\mathfrak{p}$ for the displacement (analytically obtained in appendix C) and the various bounds. We see that our simpler novel bound (39) outperforms the activity bound and entropy production bounds without requiring further information.

7. Conclusions

The general approach here introduced solely exploits the properties of the Hilbert space of observables and the presence of a (broken) involutive symmetry. Therefore, it is not restricted to trajectories of random systems endowed with some notion of time-reversal symmetry. Rather, Ω can be, e.g., the configuration space of a classical or quantum system and the involution may be parity, charge conjugation, spin reversal, etc.

For example, imagine a classical Ising system of n spins s_i, in an external magnetic field h, equilibrated at inverse temperature β. The Gibbs probability measure is thus

$$p(\{s_i\}) \propto e^{-\beta[H_0(\{s_i\}) - h\mathcal{M}]}, \tag{41}$$

where $H_0(\{s_i\}) = H_0(\{-s_i\})$ is the interaction Hamiltonian and $\mathcal{M} = \sum_{i=1}^{n} s_i$ is the system magnetization. If we consider spin reversal $\overline{s}_i = -s_i$, entailing the legitimate observables $f(\{s_i\}) = -f(\{-s_i\})$, then (18) is an upper bound on the precision of, e.g. the magnetization, taking the form (see with [39])

$$\frac{\langle \mathcal{M} \rangle^2}{\mathrm{Var}\,\mathcal{M}} \leqslant \frac{e^{\beta h \langle \mathcal{M} \rangle} - 1}{2}. \tag{42}$$

Beyond the classical case, it is also evident that the same Hilbert uncertainty principle apply to the quantum case. The spin system is then characterized by a density matrix ρ rather than a probability measure, and the mean and second moment of an observable f (now a Hermitian matrix) are computed as the trace of ρf and $\rho f f^*$ respectively. Now for any subspace of legitimate observables, one may again find an appropriate maximum precision. Further examples may arise from broken symmetries of order larger than 2 (for example spatial rotational or translational symmetries) or in case of *spontaneously* broken symmetries emerging in the thermodynamic limit. We leave these exciting opportunities of generalization for future investigations.

Acknowledgments

Appendix A. Bound for arbitrary time-varying protocols

Here, we tackle the case a random system subject to arbitrary time-varying protocols. In this case some meaningful observables, such as work and heat, are not time-antisymmetric in the naive sense of time-reversal as reading the list of states in reverse order, because work and heat depend on the parameters of the time-varying protocol.

For this reason, we consider the auxiliary configuration space $\Omega = \Omega_{\mathrm{forw}} \times \Omega_{\mathrm{back}}$, which is the space of all pairs of paths (ω, ω'), endowed with the direct product measure $p(\omega, \omega') = p_{\mathrm{forw}}(\omega) p_{\mathrm{back}}(\omega')$. Here $p_{\mathrm{forw}}(\omega)$ evaluates the probability of ω in the forward protocol, and $p_{\mathrm{back}}(\omega')$ is the probability computed in the time-reversed protocol.

On Ω we consider the involution $(\omega, \omega') \mapsto (\overline{\omega}', \overline{\omega})$. In other words the involution reverses *and swaps* the paths. We consider the legitimate observables on Ω as those that take the form $F(\omega, \omega') = f(\omega) + f'(\omega')$ and are antisymmetric for the involution, which is equivalent to the identity $f(\omega) = -f'(\overline{\omega})$. One checks that protocol-dependent thermodynamic variables, such as heat are indeed anti-symmetric for this involution, where in this case f (resp., f') denotes the heat exchanged along the path as computed from the forward (resp., backward) protocol.

We can now apply the bound (18) of the main text, only with the linear form $\langle f \rangle$ occurring in (2) now being the sum $\langle f \rangle = \langle f \rangle_{\mathrm{forw}} + \langle f' \rangle_{\mathrm{backw}}$ of means according to the forward and backward protocol (similarly for the variance). Moreover, $\langle \sigma \rangle$ turns out to be

$$\langle \sigma \rangle = \left\langle \ln \frac{p_{\mathrm{forw}}}{p_{\mathrm{back}}} \right\rangle_{\mathrm{forw}} + \left\langle \ln \frac{p_{\mathrm{back}}}{p_{\mathrm{forw}}} \right\rangle_{\mathrm{back}}.$$

In this way we retrieve the recent result of [30], which is there derived with a large deviation argument. We refer to that paper for a discussion on the meaning and importance of this bound.

Appendix B. Computing the variance of a time-summed observable in a stationary finite-state continuous-time Markov chain

We indicate here how to evaluate numerically the variance and covariances of observables for a stationary ergodic finite-state Markov chain over asymptotically large time intervals. This is useful to evaluate the variance of the displacement observable in the kinesin model, as we show in the next section. A continuous-time Markov chain is often represented by a master equation, or Kolmogorov forward equation, computing the evolution of a transient probability towards stationarity:

$$\dot{p}(y) = \sum_x p(x)L(x,y), \quad \text{or} \quad \dot{p} = pL \tag{B.1}$$

in matrix notation, where p is a row vector and L is the Laplacian matrix encoding the rates: $L(x,y) = w_{x\to y}$, the rate at which the Markov chain, in state y, transitions to another state x. The diagonal entry is picked so that every row sums to zero: $L(x,x) = -\sum_{y\neq x} w_{x\to y}$, to ensure preservation of total probability. To make an explicit link with the periodic case exposed above, we take Ω_i as the space of paths of some arbitrary duration Δt. It is then useful to write the discrete-time master equation which propagates the state over an interval Δt:

$$p_{t+\Delta t} = p_t e^{\Delta t L}.$$

As we already observed in last section, the master equation is of little use for a stationary Markov chain, and we prefer the observable viewpoint. Given a state observable h, assigning value $h(x)$ on each state x, then $e^{\Delta t L}h$ is a state observable assigning to each x the mean value of h at time $t + \Delta t$ knowing that the state at time t is x. The mean value at time t given the state at time $t + \Delta t$ is encoded in the state observable $e^{\Delta t L^*}h$. Here L^* denotes the adjoint of L under the natural scalar product on states, which is defined elementwise with $(L^*)(x,y) = \frac{p(y)}{p(x)}L(y,x)$. In the same way that the path-to-path operator P factorizes as $P = T^*S$, the state-to-state operator factorizes as $e^{\Delta t L} = ST^*$. Therefore for $k > 0$, we can write $P^k = T^*e^{(k-1)\Delta t L}S$.

We now consider $\langle g|f\rangle$ in the case where all f_i are zero-mean and identical to one another, and all g_j are zero-mean and identical to one another. In this case, (31) provides the scaling of the covariance $\langle g|f\rangle$ with N:

$$\lim_{N\to\infty} \frac{\langle g|f\rangle}{N} = \langle (\sum_{k>0} P^k + \sum_{k>0} (P^*)^k + Id)g_i|f_i\rangle_i$$

We can rewrite $\sum_{k>0} P^k g_i = T^*(Id - e^{\Delta t L})^{-1}Sg_i$ which in the limit of short time intervals gives $\sum_{k>0} P^k g_i = -T^*(\Delta t L)^{-1}Sg_i$. Note that the inversion of the non-invertible matrix L is not problematic for an ergodic Markov chain, because L is then invertible on the subspace of zero-mean state observables, such as Sg_i. In the limit of short times, it is convenient to consider a time horizon t_f, with $N = t_f/\Delta t$, and then take $t_f \to \infty$, as we are interested in asymptotically large times.

$$\lim_{t_f\to\infty} \frac{\langle g|f\rangle}{t_f} = \Delta t^{-1}\langle (-T^*(\Delta t L)^{-1}S - S^*(\Delta t L^*)^{-1}T + Id)g_i|f_i\rangle_i$$

This expression can be processed further by expressing $\langle T^*(\Delta t L)^{-1}Sg_i|f_i\rangle_i$ as the state-space scalar product $\Delta t^{-1}\langle L^{-1}Sg_i|Tf_i\rangle_X$, and similarly for $\langle S^*(\Delta t L^*)^{-1}Tg_i|f_i\rangle_i$. Overall, the covariance for asymptotically large times is

$$\lim_{t_f\to\infty} \frac{\langle g|f\rangle}{t_f} = -\Delta t^{-2}\langle L^{-1}Sg_i|Tf_i\rangle_X - \Delta t^{-2}\langle L^{-1}Tg_i|Sf_i\rangle_X + \Delta t^{-1}\langle g_i|f_i\rangle_i. \tag{B.2}$$

which is the main result of this section.

If we want to evaluate the covariance of non-zero-mean observables, then we may first center the observable by removing the mean.

Appendix C. The kinesin model: analytic calculation of the variance

We are interested in computing the variance of the displacement for arbitrarily large times. For that purpose we use (B.3) for $f_i = g_i$ encoding the centered displacement on each path over an infinitesimal time Δt. The displacement is ± 1 on each proper transition, and zero on each constant path (Δt is short enough to ignore multiple transitions). The mean displacement $\langle f_i\rangle$ is proportional to Δt, therefore the centered displacement on each transition can still be taken to $\pm\ell$ up to a negligible transition, and is set to $-\langle f_i\rangle$ on

both constant paths. The mean displacement over Δt conditioned on the initial state $x = 1, 2$ is

$$Sf_i = \begin{pmatrix} \Delta t\, c_1 - \langle f_i \rangle \\ -\Delta t\, c_2 - \langle f_i \rangle \end{pmatrix}, \tag{C.1}$$

where $\langle f_i \rangle = \Delta t [c_1 p(1) - c_2 p(2)]$, $c_x = \ell \sum_{e=1}^{4} (-1)^{e-1} k_{xe}$. The stationary probabilities read $p(1) = a_2/(a_1 + a_2)$ and $p(2) = 1 - p(1) = a_1/(a_1 + a_2)$. The mean displacement over Δt conditioned on the final state $x = 1, 2$ is

$$Tf_i = \begin{pmatrix} -\Delta t c_2 p(2)/p(1) - \langle f_i \rangle \\ \Delta t c_1 p(1)/p(2) - \langle f_i \rangle \end{pmatrix} \tag{C.2}$$

while the Laplacian is

$$L = \begin{pmatrix} -a_1 & a_1 \\ a_2 & -a_2 \end{pmatrix}, \tag{C.3}$$

where $a_x = \sum_{e=1}^{4} w_{xe}$. Therefore the two state-space products are

$$-2\Delta t^{-2} \langle L^{-1} Sf_i | Tf_i \rangle_X = -\frac{[a_1(c_1 - \langle f_i \rangle) + a_2(c_2 + \langle f_i \rangle)][p(1)(c_1 + \langle f_i \rangle) + p(2)(c_2 - \langle f_i \rangle)]}{a_1^2 + a_2^2} \tag{C.4}$$

while the path-space scalar product is

$$\Delta t^{-1} \langle f_i | f_i \rangle_i = \ell^2 (p(1)a_1 + p(2)a_2) = \ell^2 \frac{a_1 a_2}{a_1 + a_2}. \tag{C.5}$$

Summing together (C.4) and (C.5) we obtain the variance of the displacement.

We checked these results by relying on the large deviation approach [38]. The scaled cumulant generating function of any observable f is found by 'tilting' the stochastic matrix L by $v_{xe}(q) = e^{qf_{xe}}$ into

$$L_f(q) = \begin{pmatrix} -\sum_j k_{1e} & \sum_e k_{1e} v_{1e}(q) \\ \sum_j k_{2e} v_{2e}(q) & -\sum_j k_{2e} \end{pmatrix}, \tag{C.6}$$

and looking for its leading eigenvalue $g(q)$, i.e. the one satisfying $g(0) = 0$. In (C.6), f_{xe} defines the observable f. For example, the dynamical activity is obtained for $f_{xe} = 1 \forall x, e$, while the motor displacement for $f_{1e} = -f_{2e}$, and $f_{1e} = \Delta(-\Delta)$ with e odd (even). The (scaled) mean and variance of f are calculated as $\langle f \rangle = \partial_q g|_{q=0}$ and $\mathrm{Var} f / t_f = \partial_q^2 g|_{q=0}$, respectively.

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