Beat of a current

Pedro E. Harunari,^{1,2,*} Alberto Garilli,² and Matteo Polettini²

¹Instituto de Física da Universidade de São Paulo, 05314-970 São Paulo, Brazil ²Department of Physics and Materials Science, University of Luxembourg, Campus Limpertsberg, 162a avenue de la Faïencerie, L-1511 Luxembourg, Grand Duchy of Luxembourg

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The fluctuation relation, a milestone of modern thermodynamics, is only established when a set of fundamental currents can be measured. Here we prove that it also holds for systems with hidden transitions if observations are carried "at their own beat," that is, by stopping the experiment after a fixed number of visible transitions, rather than the elapse of an external clock time. This suggests that thermodynamic symmetries are more resistant to the loss of information when described in the space of transitions.

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Consider the "symbolism of atomic measurements," as Schwinger called quantum mechanics [1]: transitions in the energy spectrum of atoms were then only visible through spectral lines, i.e., the emission of photons. Or else, consider a chemical reactor fed by the in- and outtake of some controlled species: while flows can be monitored, the abundance of the reactants is only accessible by scanning with devices that involve internal degrees of freedom—e.g., magnetic, vibrational, and electronic (NMR, UV/Vis, and infrared [2–5] spectroscopy). Yet again, as in Fig. 1, consider myosins carrying cargoes on actin filaments: their motion can be monitored via imaging techniques, but not their ATP-ADP metabolic cycle [6–8].

The physics of open systems is a discourse about transitions and transformations. However, our modern understanding based on continuous-time Markov chains is tightly bound to notions of the system's internal state. Take the fluctuation relation, the most encompassing result about nonequilibrium systems, stating that for currents c cumulated up to some stopping time τ the log-ratio of their positive to negative probabilities is linear:

$$\ln \frac{p_{\tau}(\boldsymbol{c})}{p_{\tau}(-\boldsymbol{c})} = \boldsymbol{f} \cdot \boldsymbol{c}.$$
(1)

The above relation holds at times $\tau = t$ beat by an external clock (upon a proper choice of preferred initial distribution [9], or asymptotically) only if the observer has access to all currents and forces in the system's state space, up to boundary contributions. Instead, it does not generally hold if some of the currents are not visible.

Our main result is that a local current $c = n_{\uparrow} - n_{\downarrow}$, that is, the number of times a certain transition denoted \uparrow occurs minus that of the opposite transition \downarrow , obeys the fluctuation relation when counted "at its own beat," namely the number of times $\tau \equiv n = n_{\uparrow} + n_{\downarrow}$ that either \uparrow or \downarrow are performed, regardless of what happens within the system in the meanwhile. The second main contribution is the introduction of the formalism of Markov chains in the space of transitions, rather than states, which we prove to correctly describe the statistics of observables at the total number of visible transitions. We illustrate this in Fig. 1. While the Letter is self-contained, we refer at various points to the Supplemental Material (SM) [10].

Setup. We work with autonomous continuous-time Markov chains x(t) from t = 0 to some stopping time $\tau \in [0, +\infty)$

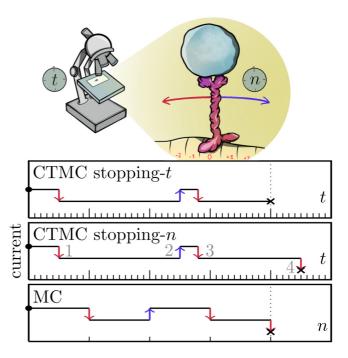


FIG. 1. When monitoring a current, trajectories are usually collected at the beat of an external clock (continuous-time Markov chain stopping t). A new paradigm, allowing for the fluctuation relation recovery, involves ending the observation at the internal notion of time given by number of transitions n (continuous-time Markov chain stopping n). Furthermore, the notion of time can be completely washed away by a Markov chain in transition space (Markov chain).

^{*}pedro.harunari@uni.lu

with rates r(x|y) of jumping from y to x. All probabilities here and in the following can in principle be derived from a well-known path probability density $p({x(t), t \in [0, \tau]})$ that in simulations will be produced by the Doob-Gillespie algorithm [11]. The state space can be depicted as a graph with states as nodes and transitions as directed links—for example,

Notice that not all transitions need to be reversible. Removal of links $1 \leftrightarrow 2$ and $3 \leftrightarrow 4$ makes the graph into a tree, which supports no stationary current [12]. We will instead focus on one link only, belonging to some cycle. Without loss of generality we take $\uparrow = 1 \leftarrow 2$ and $\downarrow = 2 \leftarrow 1$ as our visible transitions, on the assumption that there are no other mechanisms connecting 1 and 2 directly. We further assume *hidden irreducibility*, i.e., the existence of a nonzero probability path between any pair of states not containing visible transitions.

For a physical picture, these transitions could be associated with measurable emission and absorption of photons of energy ε with a thermal bath at inverse temperature β . Local detailed balance then grants that

$$\frac{r(1|2)}{r(2|1)} = \exp\beta\varepsilon.$$
(3)

We assume nondegeneracy, that is, $1 \leftrightarrow 2$ is the only transition exchanging photons of that energy, and that the temperature can be regulated.

We define *R* as the rate matrix with entries $R_{x,y} := r(x|y) - \delta_{x,y}r(y)$, with $r(y) = \sum_{x} r(x|y)$ the exit rate out of state *y*, and δ Kronecker's. Consider the induced chain of states visited by the process $\mathbf{x} = \{x_m \leftarrow x_{m-1} \leftarrow \dots \leftarrow x_0\}$, and let the taboo function $\theta(\mathbf{x})$ be zero whenever any two consecutive states are either (1,2) or (2,1); otherwise it is 1. We define the taboo matrix *T* with entries $T_{x,y} := \theta(x, y) = 1 - \delta_{x,1}\delta_{y,2} - \delta_{y,1}\delta_{x,2}$ and the survival rate matrix $S := R \circ T$, where \circ is componentwise Hadamard multiplication. In other words, the survival rate matrix is identical to *R* but for $S_{1,2} = 0 = S_{2,1}$.

Trans-transition probabilities. Letting $p_t(\mathbf{n}|x)$ be the probability that, starting from x, one observes total numbers $\mathbf{n} = (n_{\uparrow}, n_{\downarrow})$ of transitions \uparrow, \downarrow up to time t, the survival probability of not performing any visible transition is found to be (see SM [10]) [13,14]

$$p_t(\mathbf{0}|x) = \sum_{y} [\exp tS]_{y,x}.$$
 (4)

Taking minus the time derivative we find

$$-\frac{d}{dt}p_t(\mathbf{0}|x) = r(1|2)[e^{tS}]_{2,x} + r(2|1)[e^{tS}]_{1,x}, \qquad (5)$$

where we used the fact that columns of *R* add up to zero. On the right-hand side the two contributions can be proven (cf. Appendix A of [14]) to be respectively the rates at which \uparrow or \downarrow are performed for the first time in the time interval [t, t + dt), defining a renewal Markov process in the space of

transitions (or, if the transitions are thought to be prolonged for the whole duration of the interval, a semi-Markov process as in Ref. [15]). Integrating the first contribution over time we find

$$p(\uparrow | \uparrow) := -r(1|2) [S^{-1}]_{2,1}, \tag{6}$$

where we used the fact that the eigenvalue of *S* with largest real part is negative (see SM [10]) [16], implying $\lim_{t\to\infty} e^{tS} = 0$. Equation (6) is indeed the probability that the next transition is \uparrow , given that the previous was \uparrow , by (i) the strong Markov property that grants that the process in state space stays Markov for any notion of stopping time (in this case, that of the next transition), and (ii) by the fact that no two microscopic transitions contribute to the same observable. We dub this and other similar expressions (see SM [10]) $p(\ell | \ell')$, where ℓ (for "link") denotes a generic transition $\in \{\uparrow, \downarrow\}$, the *trans-transition* probabilities. A useful formula for their interpretation is (see SM [10])

$$-[S^{-1}]_{x,x_0} = \frac{1}{r(x)} \sum_{\mathbf{x} : x_0 \rightsquigarrow x} \theta(\mathbf{x}) \, p(\mathbf{x}|x_0), \tag{7}$$

where the sum runs over all trajectories, of any length, that go from x_0 to x. $p(\mathbf{x}|x_0)$ is the probability of the induced Markov chain that can be obtained from transition rates, and $\theta(\mathbf{x})$ filters the trajectories that include visible transitions. Notice that, by hidden irreducibility, trans-transition probabilities are positive.

Markov chain in transition space. We can arrange transtransition probabilities in a trans-transition matrix

$$P := \begin{pmatrix} p(\uparrow \mid \uparrow) & p(\uparrow \mid \downarrow) \\ p(\downarrow \mid \uparrow) & p(\downarrow \mid \downarrow) \end{pmatrix}.$$
(8)

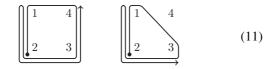
By normalization of Eq. (5) with respect to t, columns of P add up to unity. Therefore P is a discrete-time transition matrix in the following space of transitions:

Thus, the sequence of visible transitions is a Markov chain in transition space, which by hidden irreducibility is fully connected. Notice that here the Markov property is preserved by lifting the observable process into a different space. Other decimation procedures anchored on states typically break Markovianity, which is only recovered in the limit of timescale separation [17,18].

Now consider the probability $p_n(\ell)$ that the *n*th transition is ℓ . Collect them in a vector \vec{p}_n and let $s(\ell)$ and $t(\ell)$ denote the source and target states of the transition. Then, given the initial state probability $q_0(x)$ of being in x at clock time t = 0, once obtained the probability of the first transition as

$$p_1(\ell) = -r(t(\ell)|s(\ell)) \sum_{x} [S^{-1}]_{s(\ell),x} q_0(x), \qquad (10)$$

which is also normalized (see SM [10]), we can further evolve the process in transition space by $\vec{p}_n = P^{n-1}\vec{p}_1$. Notice that the Markov chain's "beat" is that of the occurrences of visible transitions, rather than the clock time *t* or the total number of jumps in state space usually considered. *Paths and time reversal.* We can depict induced chains x as walks in the above graph in Eq. (2), e.g.,



Searching for the visible transitions in x we can map paths in state space into paths in transition space $x \mapsto \ell = \{\ell_n \leftarrow \ell_{n-1} \leftarrow \ldots \leftarrow \ell_1\}$. Notice that the two example paths above correspond to the same path $\uparrow \uparrow \downarrow$ in transition space, on the left-hand side:

$$\begin{array}{c} \uparrow \quad \downarrow \\ \uparrow \quad \downarrow \\ \end{array} \tag{12}$$

On the right-hand side is the time-reversed path in transition space, which upon the hidden irreducibility hypothesis always exists, despite the fact that not all state-space paths afford a time-reversed process, e.g., the second in Eq. (11). Notice that we do not only invert the order of the transitions, but also flip their direction. Time reversal is involutive, and therefore bijective.

The probability of transition path ℓ is

$$p(\boldsymbol{\ell}) = p_1(\ell_1) \prod_{k=1}^{n-1} p(\ell_{k+1} | \ell_k).$$
(13)

We now compare it to that of its time-reversed, both sampled from the same initial distribution, by taking their ratio. The time-reversed of $p(\ell|\bar{\ell})$ is itself; therefore all such terms cancel out and we are left with

$$\frac{p(\boldsymbol{\ell})}{p(\overline{\boldsymbol{\ell}})} = \frac{p_1(\ell_1)}{p_1(\overline{\ell}_n)} \left[\frac{p(\uparrow|\uparrow)}{p(\downarrow|\downarrow)} \right]^{n_{\uparrow\uparrow}(\boldsymbol{\ell}) - n_{\downarrow\downarrow}(\boldsymbol{\ell})}, \tag{14}$$

where $n_{\ell\ell'}(\ell)$ is the number of times trans-transition $\ell \to \ell'$ occurs along the path.

Currents and the fluctuation relation. Letting $j(\ell) := \delta_{\ell,\uparrow} - \delta_{\ell,\downarrow}$ be the instantaneous current, signaling when a transition occurs, we focus on the cumulated current (or charge)

$$c(\boldsymbol{\ell}) := \sum_{k=1}^{n} j(\ell_k) = n_{\uparrow}(\boldsymbol{\ell}) - n_{\downarrow}(\boldsymbol{\ell}), \qquad (15)$$

where n_{ℓ} is the number of times transition ℓ has been performed along the process. Notice that it can only take values $\{-n, -n+2, \ldots, n-2, n\}$, and that it is antisymmetric by time reversal, $c(\bar{\ell}) = -c(\ell)$. Importantly, we can also express it in terms of the trans-transition numbers $n_{\ell\ell'}$ as

$$c(\boldsymbol{\ell}) = n_{\uparrow\uparrow}(\boldsymbol{\ell}) - n_{\downarrow\downarrow}(\boldsymbol{\ell}) + \frac{j(\ell_1) + j(\ell_n)}{2}.$$
 (16)

The first term is due to the fact that occurrences of $\uparrow \downarrow$ and $\downarrow \uparrow$ always reset the current to its initial value, and therefore only self-loops contribute to it. The second boundary term is less intuitive, and is explained in Fig. 2.

The central result of this Letter is found (see SM [10]) by plugging this latter expression into Eq. (14) and summing over all intermediate transitions $\ell_2, \ldots, \ell_{n-1}$. After standard manipulations we find the fluctuation relation for the joint

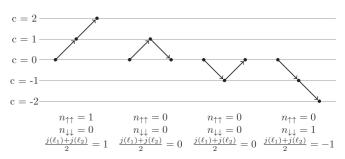


FIG. 2. The diagram shows how boundary terms contribute to the current by displaying trajectories of length n = 2, uniquely formed by boundary terms. Longer trajectories will only change the values of $n_{\uparrow\uparrow}$ and $n_{\downarrow\downarrow}$ and Eq. (16) will hold.

probability of the charge and of the first and last transitions

$$p_n(c, \ell_1, \ell_n) = p_n(-c, \overline{\ell_n}, \overline{\ell_1}) \exp[f^{\varnothing}c + u(\overline{\ell_n}) - u(\ell_1)], \quad (17)$$

where, given an arbitrary constant v , the effective force f^{\varnothing}

[19] and the effective potential u are given by

$$f^{\varnothing} := \ln \frac{p(\uparrow | \uparrow)}{p(\downarrow | \downarrow)}, \quad u(\ell) := \frac{j(\ell)f^{\varnothing}}{2} - \ln p_1(\ell) + v.$$
(18)

Parametrizing the visible rates by the principle of local detailed balance $r(2|1)/r(1|2) = \exp \beta \varepsilon$ with β a tunable inverse temperature (in units of Boltzmann's constant) and of a fixed energy increment ε , the effective affinity can be shown to be given by $f^{\emptyset} = (\beta - \beta^{\emptyset})\varepsilon$ where β^{\emptyset} is the stalling value that makes the visible current vanish on average [20,21]. Thus, operationally, provided ε is known from microphysical considerations, all one has to do to obtain f^{\emptyset} is to tune the temperature to the stalling state and measure the difference.

The potential u can be made to vanish by selecting as preferred initial distribution (marked *)

$$p_1^*(\ell) \propto p(\ell|\ell) \tag{19}$$

with v chosen to fix the normalization. In view of Eq. (10), a state-space precursor of this distribution is $q_0^*(1) \propto p(\downarrow | \downarrow)$, $q_0^*(2) \propto p(\uparrow | \uparrow)$, else zero. When the potential vanishes one can further marginalize for the current in Eq. (17) by summing over ℓ_1 and ℓ_n to obtain our central result, the fluctuation relation at finite number of total visible transitions

$$\frac{p_n(c)}{p_n(-c)} = \exp f^{\varnothing} c.$$
(20)

Figure 3 illustrates the validity of the fluctuation relation for the state-space continuous-time Markov chain at stopping n, prepared from \vec{q}_0^* , and the transition-space Markov chain, prepared from \vec{p}_1^* . It also displays the failure of the fluctuation relation for the continuous-time Markov chain at clock time, prepared from the so-called stalling distribution, which is the best candidate for the preferred initial distribution given that it satisfies the integral fluctuation relation $\langle \exp f^{\varnothing} c \rangle = 1$ [19]. The fluctuation relation also holds asymptotically, beyond the finite values of charge explored in these numerical simulations, as revealed by a symmetry in the stationary scaled cumulant generating function (see SM [10]) [9,22].

Discussion and conclusions. Three different stochastic processes are at play in this work. We started with a

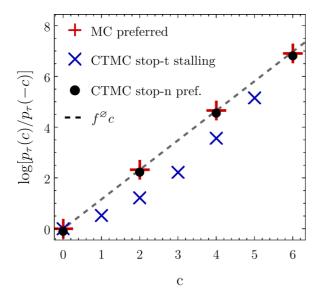


FIG. 3. Log-ratio $\ln p_{\tau}(+c)/p_{\tau}(-c)$, $c \ge 0$, for different stopping times and processes in a four-state system: state-space continuous-time Markov chain at stopping *t* sampled from the stalling distribution (CTMC stop *t* stalling) and at stopping *n* sampled from the preferred distribution (CTMC stop *n* pref.), and the transition-space Markov chain also sampled from the preferred distribution (MC preferred). Only the latter two satisfy the fluctuation relation. More details of the simulation can be found in the Supplemental Material [10].

continuous-time Markov chain sampled from some distribution \vec{q}_0 and evolving by generator *R* up until final clock time *t*. The second is in all identical, but, as already suggested in Refs. [23,24], and explored for run-and-tumble particles with fixed number of jumps [25–27], it runs until *n* transitions are observed. Finally, we introduced a discrete-time Markov chain in transition space with (trans-)transition matrix *P* sampled from \vec{p}_1 . Other internal notions of time have been considered in Refs. [28,29]

The latter two produce the same current statistics, as evidenced by red crosses and black dots in Fig. 3, thus confirming our second main point, viz., the appropriateness of the concept of Markov chains in the space of transitions for the study of transitions at their own beat. An additional statistical advantage of working at fixed number of transitions is that no events of charge c > n can possibly occur, thus making the distribution of compact support—while at clock time events of rare activity produce noise in the tails that are hard to characterize in simulations.

The results presented here hold only if every visible transition, \uparrow or \downarrow , arises from a unique and well-defined transition in state space. Otherwise, if two transitions produce the same signal, the so-called renewal property is lost, and correspondingly the time series of transitions is not Marko-

vian [i.e., there will be a difference in probability between $p(\uparrow | \downarrow, \downarrow)$ and $p(\uparrow | \downarrow, \uparrow)$, etc.]. A different question is whether the fluctuation relation holds for several independent transitions. Work in progress by the authors suggests that monitoring the number of occurrences of the visible transitions is not enough, and that one needs to additionally consider cross-information.

Many facts that are true for processes in state space may not be true in transition space, and vice versa. One example is the notion of time reversal, where the requirement of also flipping the transition's direction resembles the time reversal of the momentum variable in underdamped Langevin dynamics. Thus, as anticipated in Ref. [30], this formalism may serve as a candidate for "second-order" Markov processes as the basis for transition-based coarse-graining [14,15,30–33].

Our central result, Eq. (20), is obtained from the combination of the formalism in Refs. [14,30] and the introduced notion of stopping *n*, further assessing the fluctuating nature of single currents. The present fluctuation relation holds even when the fundamental set is not fully accessible, composing a relevant observation for understanding the thermodynamic consistency of currents flowing in the vast class of partially observed systems. Another connection between these works is the entropic interpretation: Usually, exponents of fluctuation relations are measures of dissipation. Indeed, the effective affinity times the visible current $f^{\varnothing}c$ bounds the entropy production of a stochastic process from below, as shown in [14,30].

From the present fluctuation relation and the definition of Markov processes in transition space, thermodynamic considerations beyond dissipation inference might arise: for example, an associate thermodynamic uncertainty relation [34–36], the usage of Martingale theory [37] to explore the beat of a current as a random stopping time, connections to fluctuating heat and work that are now accessible at small scales [38,39], the measurement of effective affinities from current statistics [40], and the usage of discrete-time processes to efficiently assess some details of continuous-time Markov chains (see SM [10]).

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