

Simple bounds on fluctuations and uncertainty relations for first-passage times of counting observables

Juan P. Garrahan

*School of Physics and Astronomy and Centre for the Mathematics and Theoretical Physics of Quantum Non-equilibrium Systems,
University of Nottingham, Nottingham NG7 2RD, United Kingdom*

(Received 10 January 2017; published 23 March 2017)

Recent large deviation results have provided general lower bounds for the fluctuations of time-integrated currents in the steady state of stochastic systems. A corollary are so-called thermodynamic uncertainty relations connecting precision of estimation to average dissipation. Here we consider this problem but for counting observables, i.e., trajectory observables which, in contrast to currents, are non-negative and nondecreasing in time (and possibly symmetric under time reversal). In the steady state, their fluctuations to all orders are bound from below by a Conway-Maxwell-Poisson distribution dependent only on the averages of the observable and of the dynamical activity. We show how to obtain the corresponding bounds for first-passage times (times when a certain value of the counting variable is first reached) and their uncertainty relations. Just like entropy production does for currents, dynamical activity controls the bounds on fluctuations of counting observables.

DOI: [10.1103/PhysRevE.95.032134](https://doi.org/10.1103/PhysRevE.95.032134)

I. INTRODUCTION

In this paper we try to connect three recent developments in the theory of stochastic systems. The first are general bounds on the fluctuations of time-integrated currents [1–4]. Obtained by means Level 2.5 [5–7] dynamical large deviation methods [8–12], these results stipulate general lower bounds for fluctuations at any order of all empirical currents in the stationary state of a stochastic process [1–4]. A corollary are thermodynamic uncertainty relations [13–15] connecting the estimation error of time-integrated currents to overall dissipation.

The second development are fluctuation relations for first-passage times (FPTs) [16–18], similar to those of more standard observables such as work or entropy production. From these an uncertainty relation connecting dissipation to the time needed to determine the direction of time can be derived [16]. These results indicate a relation between the fluctuations of observables in dynamics over a fixed time, with fluctuations in stopping times.

The third development is trajectory ensemble equivalence [19–22] between ensembles of long trajectories subject to different constraints. For example, for long times, the ensemble of trajectories conditioned on a fixed value of a time-integrated quantity is equivalent to that conditioned only on its average [19,20] (cf. microcanonical or canonical equivalence of equilibrium ensembles [23]). Similarly, the ensemble of trajectories of fixed total time and fluctuating number of jumps is equivalent to that of fixed number of jumps but fluctuating time [21,22] (cf. fixed volume and fixed pressure static ensembles [23]).

The works in Refs. [1–4] and [13–18] focus on trajectory observables asymmetric under time reversal, such as empirical currents, which can be positive or negative and can increase and decrease with time. Here we consider instead trajectory observables which are always non-negative and strictly non-decreasing with time. We call these counting observables. An example is the total number of configuration changes in a trajectory, or dynamical activity [11,24,25], sometimes also called “traffic” or “frenesi” [5,26,27]. Here we show that

from the bounds to the rate functions of counting observables, via trajectory ensemble equivalence, we can derive the corresponding bounds for arbitrary fluctuations of FPTs.

After introducing the basics of dynamical large deviations, in Sec. III we show that the rate functions of counting observables are bounded from above by a Conway-Maxwell-Poisson distribution (a generalization of the Poisson distribution that allows for non-Poissonian number fluctuations [28]). The corresponding bound for the cumulant generating function was first found in Ref. [2] (called “exponential bound”); here we rederive it straightforwardly via Level 2.5 large deviations; cf. [1]. In Sec. IV we consider the large deviations of FPTs and establish the correspondence between the FTP and observable generating functions. This allows us, in Sec. V, to derive a general bound on FPT rate functions from the large deviations of the observable distributions. From these bounds FPT uncertainty relations follow. An important observation is that the bounds on fluctuations of a counting observable and its FPTs are controlled by the average dynamical activity, in analogy to the role played by the entropy production in the case of currents [1,13]. We hope these results will add to the growing body of work applying large deviation ideas and methods to the study of dynamics in driven systems [29–41], glasses [25,42–47], protein folding and signaling networks [48–51], open quantum systems [52–64], and many other problems in nonequilibrium [65–72].

II. STOCHASTIC DYNAMICS AND LARGE DEVIATIONS OF COUNTING OBSERVABLES

We consider systems evolving as continuous time Markov chains [73], with master equation

$$\partial_t P_t(x) = \sum_{x,y \neq x} W_{yx} P_t(y) - \sum_x R_x P_t(x), \quad (1)$$

where $P_t(x)$ is the probability being in configuration x at time t , W_{xy} the transition rate from x to y , and $R_x = \sum_{y \neq x} W_{xy}$ the escape rate from x . In operator form the master equation reads

$$\partial_t |P_t\rangle = \mathcal{L} |P_t\rangle, \quad (2)$$

with probability vector $|P_t\rangle = \sum_x P_t(x)|x\rangle$, where $\{|x\rangle\}$ is an orthonormal configuration basis. The master operator is

$$\mathcal{L} = \mathcal{W} - \mathcal{R} = \sum_{x,y \neq x} W_{xy}|y\rangle\langle x| - \sum_x R_x|x\rangle\langle x|, \quad (3)$$

where \mathcal{W} and \mathcal{R} indicate the off-diagonal and diagonal parts of \mathcal{L} , respectively. This dynamics is realized by stochastic trajectories, such as $\omega = (x_0 \rightarrow x_{t_1} \rightarrow \dots \rightarrow x_{t_K})$. This trajectory has K jumps, with the jump between configurations $x_{t_{i-1}}$ and x_{t_i} occurring at time t_i , with $0 \leq t_1 \leq \dots \leq t_K \leq t$, and no jump between t_K and t . We denote by $\pi_t(\omega)$ the probability of ω within the ensemble of trajectories of total time t .

Properties of the dynamics are encoded in trajectory observables, i.e., functions of the whole trajectory, $A(\omega)$, which are time additive, that is, on average they increase linearly with the time extent of trajectories. For this reason these observables are sometimes also called ‘‘time extensive’’ (even though for a given trajectory ω the value of $A(\omega)$ may not necessarily always grow linearly in time). Examples include time-integrated currents or dynamical activities. Time extensivity of their averages implies that at long times their probabilities and moment generating functions have large deviation forms [8–12],

$$P_t(A) = \sum_{\omega} \delta[A - A(\omega)]\pi_t(\omega) \approx e^{-t\varphi(A/t)}, \quad (4)$$

$$Z_t(s) = \sum_{\omega} e^{-sA(\omega)}\pi_t(\omega) \approx e^{t\theta(s)}, \quad (5)$$

where the rate function $\varphi(a)$ and the scaled cumulant generating function $\theta(s)$ are related by a Legendre transform [8–12],

$$\varphi(a) = -\min_s [\theta(s) + s a]. \quad (6)$$

In what follows we focus on trajectory observables defined in terms of the jumps in a trajectory,

$$A(\omega) = \sum_{xy} \alpha_{xy} Q_{xy}(\omega), \quad (7)$$

where $Q_{xy}(\omega)$ is the number of jumps from x to y in trajectory ω . We will assume all $\alpha_{xy} \geq 0$. This means that $A(\omega)$ is non-negative and nondecreasing with time. We call $A(\omega)$ a counting observable as it counts the number of certain kinds of jumps in the trajectory. Furthermore, when $\alpha_{xy} = \alpha_{yx}$ these observables are symmetric under time reversal, in contrast to time-integrated currents which are antisymmetric (and therefore neither necessarily positive nor nondecreasing with time). An important example of a counting observable is the total number of jumps or dynamical activity [5,11,24],

$$K(\omega) = \sum_{xy} Q_{xy}(\omega). \quad (8)$$

For observables such as Eq. (7) the moment generating function Eq. (5) can be written as

$$Z_t(s) = \langle -|e^{t\mathcal{L}_s}|x_0\rangle, \quad (9)$$

where \mathcal{L}_s is the tilted operator [8–12],

$$\mathcal{L}_s = \mathcal{W}_s - \mathcal{R} = \sum_{x,y \neq x} e^{-\alpha_{xy}s} W_{xy}|y\rangle\langle x| - \mathcal{R}, \quad (10)$$

and $\langle -| = \sum_x \langle x|$. The function $\theta(s)$ is then given by the largest eigenvalue of \mathcal{L}_s .

III. LEVEL 2.5 AND FLUCTUATION BOUNDS

The computation of large deviation functions as the ones in Eqs. (4) and (5) for arbitrary observables and dynamics is difficult in general. There is however one case where the rate function can be written down explicitly [5–7].

Consider a trajectory ω of total time extent t . Imagine that in this trajectory the system visits configuration x a number of times: there is a jump into x at time $t_{x,1}^{(in)}$ and out of it at time $t_{x,1}^{(out)}$, another jump into x at $t_{x,2}^{(in)}$ and out of it at $t_{x,2}^{(out)}$, and so on. Adding up all these time intervals gives the overall amount of time $M_x(\omega)$ that ω spends in x , or residence time, $M_x(\omega) = (t_{x,1}^{(out)} - t_{x,1}^{(in)}) + (t_{x,2}^{(out)} - t_{x,2}^{(in)}) + \dots$. Repeating this analysis for all configurations x , and dividing by t , we can define a probability vector $\vec{m}(\omega)$ with components $m_x(\omega) = t^{-1}M_x(\omega)$, with $\sum_x m_x(\omega) = 1$. The vector $\vec{m}(\omega)$ is called the empirical measure of trajectory ω , as it provides the estimate that can be inferred from the states visited during this trajectory to the true average distribution over configurations of the dynamics.

As mentioned in Sec. II, time extensive observables obey a LD principle for long times, Eqs. (4)–(6). This goes by the name of ‘‘level 1’’ of LDs [12]. Given that the entries of the empirical measure are also time extensive observables it follows that the whole $\vec{m}(\omega)$ vector also obeys a LD principle at long times [8–12], $P_t(\vec{m}) = \sum_{\omega} \pi_t(\omega) \prod_x \delta[m_x - m_x(\omega)] \approx e^{-tI(\vec{m})}$, where $I(\vec{m})$ is the corresponding LD rate function. This is known as ‘‘level 2’’ of LDs [8–12].

A trajectory also has transitions between configurations. We denote by $Q_{xy}(\omega)$ the total number of jumps between configurations x and y in trajectory ω , and we collect them as the elements of the matrix $\mathbf{Q}(\omega)$ which contains the number of jumps between any two configurations in the trajectory. If we divide by the total trajectory time t we obtain the flux, $\mathbf{q}(\omega) = t^{-1}\mathbf{Q}(\omega)$, which corresponds to the empirical rates for all the possible transitions as estimated from the trajectory. As for the case of the empirical measure, given that the entries of $\mathbf{Q}(\omega)$ are time additive, the whole of $\mathbf{q}(\omega)$ obeys a LD principle at long times [8–12], $P_t(\mathbf{q}) = \sum_{\omega} \pi_t(\omega) \prod_{xy} \delta[q_{xy} - q_{xy}(\omega)] \approx e^{-tI(\mathbf{q})}$, with $I(\mathbf{q})$ the corresponding rate function.

Just like for LD at level 1, in general it is difficult to find explicit forms for the rate functions of either the empirical measure or the flux. However, the rate function $I(\mathbf{q}, \vec{m})$ for the joint probability of the empirical measure *and* the flux, where

$$P_t(\mathbf{q}, \vec{m}) = \sum_{\omega} \pi_t(\omega) \prod_x \delta[m_x - m_x(\omega)] \times \prod_{xy} \delta[q_{xy} - q_{xy}(\omega)] \approx e^{-tI(\mathbf{q}, \vec{m})}, \quad (11)$$

has an explicit form in the stationary state dynamics of Eq. (2). This remarkable result is known as ‘‘level 2.5’’ of large deviations [5–7]. The joint rate function reads

$$I(\mathbf{q}, \vec{m}) = \sum_{xy} q_{xy} \left[\ln \left(\frac{q_{xy}}{m_x W_{xy}} \right) - 1 \right] + \sum_x m_x R_x, \quad (12)$$

where \vec{m} and \mathbf{q} must obey the probability conserving conditions,

$$\sum_x m_x = 1, \quad \sum_y q_{xy} = \sum_y q_{yx}. \quad (13)$$

This rate function is minimized (its minimum value being zero) when \vec{m} and \mathbf{q} take the stationary average values

$$m_x = \rho_x, \quad q_{xy} = \rho_x W_{xy}, \quad (14)$$

where ρ_x is the stationary distribution, $\mathcal{L}[\rho] = 0$. The rate function for a trajectory observable such as Eq. (7) can then be obtained by *contraction* [8–12],

$$\varphi(a) = \min_{\mathbf{q}, \vec{m}: a = \text{Tr}(\boldsymbol{\alpha} \cdot \mathbf{q})} I(\mathbf{q}, \vec{m}), \quad (15)$$

where $\text{Tr}(\boldsymbol{\alpha} \cdot \mathbf{q}) = \sum_{xy} \alpha_{xy} q_{xy}$ and $a = A/t$.

An upper bound for $\varphi(a)$ can be obtained following the procedure of Ref. [1]. From Eq. (15), any pair of empirical measure \vec{m} and flux \mathbf{q} that satisfies Eq. (13) and has $a = \sum_{xy} \alpha_{xy} q_{xy}$ will give an upper bound to $\varphi(a)$. A convenient and simple choice is

$$m_x^* = \rho_x, \quad q_{xy}^* = \frac{a}{\langle a \rangle} \rho_x W_{xy}, \quad (16)$$

where $\langle a \rangle = \sum_{xy} \alpha_{xy} \rho_x W_{xy}$. We then get, with $I_*(a) = I(\mathbf{q}^*, \vec{m}^*)$,

$$\varphi(a) \leq I_*(a) = \frac{\langle k \rangle}{\langle a \rangle} \left[\ln \left(\frac{a}{\langle a \rangle} \right) - (a - \langle a \rangle) \right], \quad (17)$$

where $\langle k \rangle = \sum_{xy} \rho_x W_{xy} = \sum_x \rho_x R_x$ is the average dynamical activity (per unit time). The rate function on the right side of Eq. (17) is that of a Conway-Maxwell-Poisson (CMP) distribution [28], a generalization of the Poisson distribution for a counting variable with non-Poissonian number fluctuations.

From the Legendre transform Eq. (6), the upper bound Eq. (17) also implies a lower bound for the scaled cumulant generating function $\theta(s)$,

$$\theta(s) \geq \theta_*(s) = \langle k \rangle \left[\exp \left(-s \frac{\langle a \rangle}{\langle k \rangle} \right) - 1 \right]. \quad (18)$$

The expression on the right is the scaled cumulant generating function of a CMP distribution. This last result was first derived in Ref. [2] in a slightly different manner.

Figure 1 illustrates the bounds Eqs. (17) and (18) for the elementary example of a two-level system. The exact rate function $\varphi(a)$ and the upper bound $I_*(a)$ have the same minimum at $\langle a \rangle$, but the fluctuations of a are larger than those given by $I_*(a)$ for all a . The exact cumulant generating function $\theta(s)$ and its lower bound $\theta_*(s)$ have the same slope at $s = 0$, but $\theta_*(s)$ has derivatives which are smaller in magnitude to all orders that those of $\theta(s)$, again indicating that the CMP approximation provides lower bounds for the size of fluctuations of a .

As occurs with the analogous bounds on time-integrated currents [1–4], an immediate consequence of the bounds on the rate function or cumulant generating function are the thermodynamic uncertainty relations [13–15]. From Eq. (17) or Eq. (18) we get a lower bound for the variance of the observable in terms of its average and the average activity

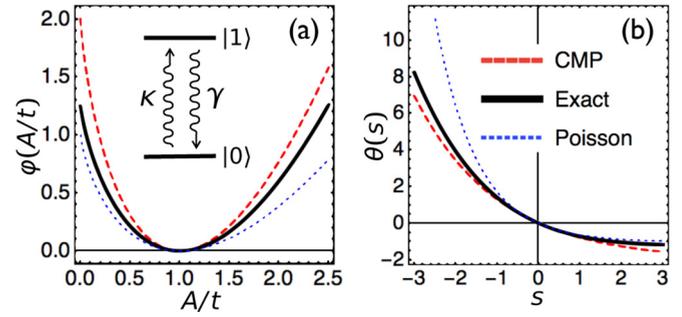


FIG. 1. Bounds on observable fluctuations for a two-level system. Transition rates are $W_{10} = \gamma$ and $W_{01} = \kappa$. We consider as observable A the total number of $1 \rightarrow 0$ jumps. In the stationary state $\langle a \rangle = \langle A \rangle/t = \gamma\kappa/(\gamma + \kappa)$. The average activity per unit time is $\langle k \rangle = 2\langle a \rangle$. Panel (a) shows the rate function $\varphi(A/t)$ [full (black)] for $\gamma = 5$ and $\kappa = 1.25$. The rate function is bounded from above everywhere by a CMP rate function, Eq. (17) [dashed (red)]. We also show for comparison a Poisson rate function with mean $\langle a \rangle$ [dotted (blue)]. Panel (b) shows the corresponding scaled cumulant generating function $\theta(s) = \frac{1}{2}[\sqrt{(\gamma - \kappa)^2 + 4\gamma\kappa e^{-s}} - (\gamma + \kappa)]$ [full (black)]. It is monotonic in s since $A \geq 0$, and is bounded from below, Eq. (18), by $\theta_*(s) = \frac{2\gamma\kappa}{\gamma + \kappa}(e^{-s/2} - 1)$ [dashed (red)]. For the case $\kappa = \gamma$ the bounds become exact in this simple model.

(cf. [2])

$$\text{var}(a) = \frac{\theta''(0)}{t} \geq \frac{\theta_*''(0)}{t} = \frac{\langle a \rangle^2}{\langle k \rangle t}. \quad (19)$$

This in turn provides an upper bound for precision of estimation of the observable A in terms of the signal-to-noise ratio (i.e., inverse of the error),

$$\text{SNR}(A) = \frac{\langle A \rangle}{\sqrt{\text{var}(A)}} \leq \sqrt{\langle K \rangle}, \quad (20)$$

where $\langle K \rangle = t \langle k \rangle$. Just like in the case of integrated currents [13–15], where there is an unavoidable tradeoff between precision and dissipation, the uncertainty in the estimation of a counting observable is bounded generically by the overall average activity in the process.

IV. LARGE DEVIATIONS OF FIRST-PASSAGE TIME DISTRIBUTIONS

We consider now the statistics of first-passage times (FPT) (also called stopping times), the times at which a certain trajectory observable first reaches a threshold value. This implies a change of focus from ensembles of trajectories of total fixed time to ensembles of trajectories of fluctuating overall time [21,74,75]. Recently, distributions of FPT associated with entropy production have been shown to obey fluctuation relations [16–18] reminiscent of those of currentlike observables. This suggests a duality between observable and FPT statistics, which in turn is connected to the equivalence between fixed time and fluctuating time trajectory ensembles; see e.g. [21,22].

We focus on stopping times for counting observables as defined in Eq. (7). For simplicity we assume that the coefficients α_{xy} are either zero or 1, so that $A(\omega)$ counts a subset of all possible jumps in a trajectory and takes integer values.

(These assumptions can be relaxed at the expense of slightly more involved expressions without changing the essence of the results.)

Let us consider the structure of trajectories associated with FPT events for a fixed value A of the observable $A(\omega)$. Such a trajectory will have A jumps for which $\alpha_{xy} = 1$, occurring at times $0 \leq t_1 \leq \dots \leq t_{A-1} \leq t_A = \tau$ with τ being the FPT through $A(\omega) = A$. In between these jumps the evolution will be one where only jumps with $\alpha_{xy} = 0$ occur. The weight of this trajectory is related to the amplitude of a matrix product state [76],

$$\langle y | \tilde{\mathcal{W}} e^{(t_A - t_{A-1})\mathcal{L}_\infty} \dots \tilde{\mathcal{W}} e^{(t_2 - t_1)\mathcal{L}_\infty} \tilde{\mathcal{W}} e^{t_1 \mathcal{L}_\infty} | x \rangle. \quad (21)$$

This expression is the weight of all trajectories starting in x and ending in y , after A jumps that contribute to the observable, occurring at the specified times t_i ($i = 1, \dots, A$), and with an arbitrary number of the other jumps. Here \mathcal{L}_∞ is the tilted operator Eq. (10) at $s \rightarrow \infty$, so that all transitions associated to $A(\omega)$ are suppressed. The factors $e^{\Delta t \mathcal{L}_\infty}$ encode dynamics which do not contribute to increasing the observable and which occur between the times t_i . The operator

$$\tilde{\mathcal{W}} = \mathcal{L} - \mathcal{L}_\infty \quad (22)$$

includes all the transitions that increase $A(\omega)$ by one unit, and Eq. (21) has A insertions of $\tilde{\mathcal{W}}$. Integrating Eq. (21) over intermediate times and summing over the final configuration formally yields the FPT distribution,

$$F_x(\tau | A) = \int_{0 \leq t_1 \dots \leq \tau} \langle - | \tilde{\mathcal{W}} e^{(\tau - t_{A-1})\mathcal{L}_\infty} \dots \tilde{\mathcal{W}} e^{t_1 \mathcal{L}_\infty} | x \rangle.$$

This expression simplifies via a Laplace transform,

$$\hat{F}_x(\mu | A) = \int_0^\infty dt e^{-\mu t} F_x(\tau | A) = \langle - | \mathcal{F}_\mu^A | x \rangle, \quad (23)$$

where the transfer operator reads

$$\mathcal{F}_\mu = \tilde{\mathcal{W}} (\mu - \mathcal{L}_\infty)^{-1}. \quad (24)$$

When A is large, $A \gg 1$, the Laplace transformed FTP distribution has a large deviation form,

$$\hat{F}_x(\mu | A) \approx e^{A g(\mu)}, \quad (25)$$

where $e^{g(\mu)}$ is the largest eigenvalue of \mathcal{F}_μ . Note the similarities between Eqs. (23)–(25) and Eqs. (5)–(10).

The eigenvalues of \mathcal{F}_μ and \mathcal{L}_s are directly related. From Eqs. (10), (22), and (24) we can write

$$e^{-s} \mathcal{F}_\mu = (\mathcal{L}_s - \mu)(\mu - \mathcal{L}_\infty)^{-1} + 1. \quad (26)$$

Consider now a row vector $\langle l |$ which is a left eigenvector both of \mathcal{F}_μ and \mathcal{L}_s , with eigenvalue $e^{g(\mu)}$ and $\theta(s)$, respectively. Multiplying Eq. (26) by $\langle l |$ and rearranging we get

$$(e^{-s+g(\mu)} - 1)l = [\theta(s) - \mu]l(\mu - \mathcal{L}_\infty)^{-1}. \quad (27)$$

We see that for $\langle l |$ to be a simultaneous eigenvector of \mathcal{F}_μ and \mathcal{L}_s we need to have $g(\mu) = s$ and $\theta(s) = \mu$. That is, g is the functional inverse of θ and vice versa,

$$\theta(s) = g^{-1}(s), \quad g(\mu) = \theta^{-1}(\mu). \quad (28)$$

For the case where the counting observable is the dynamical activity, Eq. (8), the analysis above is that of “ x -ensemble”

of Ref. [21], i.e., the ensemble of trajectories of fixed total number of jumps but fluctuating time.

For the general problem of the FPTs for arbitrary counting observables, Eqs. (23)–(24) coincide with the FPT distributions first obtained in Ref. [17] in a different way. The derivation in Ref. [17] proceeds in the standard manner used for example in the proof of FPT distributions for diffusion processes [73]. It relates the probability of having accumulated A up to time t , to the probability of reaching A at time $\tau \leq t$ for the first time followed by no increment in A from τ to t ,

$$P_t(A | x) = \sum_y \int_0^t d\tau P_{t-\tau}(0 | y) F_{xy}(\tau | A), \quad (29)$$

where $P_t(A | x)$ is Eq. (4) with the initial condition made explicit, and $F_{xy}(\tau | A)$ refers to the FPT distribution for time τ and final configuration y . If we transform from A to s , cf. Eqs. (4), (5), and (9), we can rewrite Eq. (29) as matrix elements of

$$e^{t \mathcal{L}_s} = \int_0^t d\tau e^{(t-\tau)\mathcal{L}_\infty} \hat{\mathcal{F}}_s(\tau), \quad (30)$$

where $\langle y | \hat{\mathcal{F}}_s(\tau) | x \rangle = \sum_A e^{-sA} F_{xy}(\tau | A)$. After a Laplace transform and rearranging we get

$$\hat{\mathcal{F}}_{s\mu} = (\mu - \mathcal{L}_\infty)(\mu - \mathcal{L}_s)^{-1}. \quad (31)$$

This last expression is the same as that in Ref. [17] after a discrete Laplace transform from A to s . We can invert the $A \rightarrow s$ transformation as follows. The left-hand side (LHS) of Eq. (31) is

$$\hat{\mathcal{F}}_{s\mu} = \sum_{A=0}^\infty e^{-sA} \hat{\mathcal{F}}_\mu(A), \quad (32)$$

while the RHS can be rewritten as

$$\begin{aligned} & (\mu - \mathcal{L}_\infty)(\mu - \mathcal{L}_s)^{-1} \\ &= [1 - e^{-s} \tilde{\mathcal{W}} (\mu - \mathcal{L}_\infty)^{-1}]^{-1} \\ &= \sum_{A=0}^\infty e^{-sA} [\tilde{\mathcal{W}} (\mu - \mathcal{L}_\infty)^{-1}]^A. \end{aligned} \quad (33)$$

Equating Eqs. (32) and (33) term by term we get that

$$\hat{\mathcal{F}}_\mu(A) = \mathcal{F}_\mu^A, \quad (34)$$

with \mathcal{F}_μ given by Eq. (24), showing that our derivation is equivalent to that of Ref. [17]. The advantage of expressing the FPT distribution in terms of its generating function Eq. (24) as we have done here is that it allows for a direct extraction of its large deviation function, see Eqs. (25) and (28), giving access to the full statistics of FPTs in the limit of large A .

V. BOUNDS ON FPT DISTRIBUTIONS

Equations (23)–(28) establish a connection between the statistics of a counting observable, at fixed overall time, and the statistics of the FPT for a fixed value of said observable. This connection is due to the equivalence [21,22] between the ensemble of trajectories of fixed time, but where the observable is allowed to fluctuate (in a manner controlled by the field s conjugate to the observable), with the ensemble of fixed

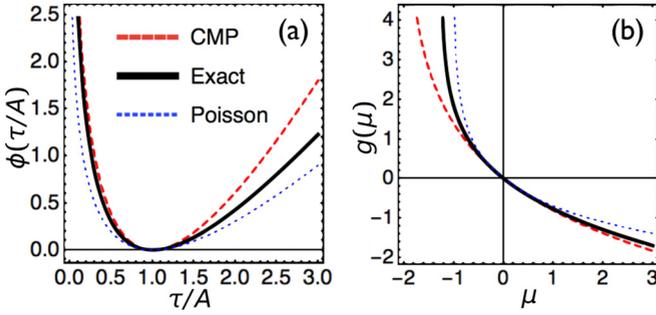


FIG. 2. Bounds on first-passage time fluctuations for the two-level system of Fig. 1. The FPT τ is defined as the time when a total A of up or down jumps $1 \rightarrow 0$ is reached. In the stationary state $\langle \tau \rangle = A/\langle a \rangle = A(\gamma + \kappa)/(\gamma\kappa)$. Panel (a) shows the rate function $\phi(\tau/A)$ [full (black)] for $\gamma = 5$ and $\kappa = 1.25$, and assuming the initial state is zero. The rate function is bounded from above everywhere by $\phi_*(\tau/A)$, Eq. (37) [dashed (red)]. We also show for comparison the FPT rate function of a Poisson process with the same mean [dotted (blue)]. Panel (b) shows the FPT scaled cumulant generating function $g(\mu) = \ln(\gamma\kappa) - \ln[(\gamma + \mu)(\kappa + \mu)]$ [full (black)]. It is bounded from below, Eq. (35), by $g_*(\mu)$ [dashed (red)].

observable but where the time extension of trajectories is allowed to fluctuate (in a manner controlled by the field μ conjugate to time). This equivalence holds in the limit of large observable or time, where the relation between the controlling fields is given by Eq. (28). We can now use the results of Sec. III on bounds on observable fluctuations to infer the corresponding bounds on FPT fluctuations.

The bound Eq. (18) on the cumulant generating function of A provides a lower bound to the FPT scaled cumulant generating function $g(\mu)$ through Eq. (28). Inverting θ_* in Eq. (18) we get

$$g(\mu) \geq g_*(\mu) = -\frac{\langle k \rangle}{\langle a \rangle} \ln \left(\frac{\mu}{\langle k \rangle} + 1 \right). \quad (35)$$

For large A the FPT distribution also has a large deviation form,

$$F(\tau|A) \approx e^{-A\phi(\tau/A)}, \quad (36)$$

where $\phi(\tau/A)$ is obtained from $g(\mu)$ by a Legendre transform similar to Eq. (6). From Eq. (35) we then obtain an upper bound for the FPT rate function,

$$\begin{aligned} \phi(\tau/A) &\leq \phi_*(\tau/A) \\ &= -\frac{\langle k \rangle}{\langle a \rangle} \left[\ln \left(\frac{\tau \langle a \rangle}{A} \right) - \left(\frac{\tau \langle a \rangle}{A} - 1 \right) \right]. \end{aligned} \quad (37)$$

Figure 2 illustrates the upper bound of the FPT rate function, Eq. (37), and the lower bound of the FPT cumulant generating function, Eq. (35), for the same two-level model of Fig. 1.

The bound function $\phi_*(\tau/A)$ has its minimum at the exact value of the average FPT,

$$\langle \tau \rangle_A = \frac{A}{\langle a \rangle}, \quad (38)$$

where $\langle \cdot \rangle_A$ indicates average in the FPT ensemble of fixed A . That the average FPT is given by the inverse of the observable per unit time follows immediately from Eq. (28). The second

derivative of $\phi_*(\tau/A)$ at its minimum provides a lower bound for the variance of the FPT. From Eq. (37), or alternatively Eq. (35), we get

$$\frac{\text{var}(\tau)}{A} = g''(0) \geq g_*''(0) = \frac{1}{\langle a \rangle \langle k \rangle}. \quad (39)$$

This in turn gives a bound on the precision with which one can estimate the FPT,

$$\text{SNR}(\tau) = \frac{\langle \tau \rangle_A}{\sqrt{\text{var}(\tau)}} \leq \sqrt{\langle K_A \rangle}, \quad (40)$$

where $\langle K_A \rangle = \langle \tau \rangle_A \langle k \rangle$. As for case of the uncertainty for the observable, Eq. (20), the precision of estimation of the FPT is limited by the total average activity, in this case for trajectories of length $t = \langle \tau \rangle_A$.

VI. CONCLUSIONS

We have discussed general bounds on fluctuations of counting observables, hopefully complementing the more detailed recent results on current fluctuations [1–4]. While empirical currents are the natural trajectory observables to consider in driven problems [1–5, 29, 30, 33, 35, 36, 40], counting observables such as the dynamical activity are central quantities for systems with complex equilibrium dynamics, such as glass formers [24, 25, 42, 43, 46]. (And even for driven systems it is revealing to study the dynamical phase behavior in terms of both empirical currents and activities; see e.g. [33, 36, 40, 45].)

The bounds are a straightforward consequence of the Level 2.5 large deviation [5–7] description, Eq. (12), which provides an explicit (and useful) minimization principle for rate functions. But as remarked in [4], these bounds may be more or less descriptive depending on whether they are tight or loose, which in turn depends on how good the variational ansatz is. As observed in [2], the ansatz Eq. (16) is akin to a mean-field approximation that homogenizes the connections between states. For any counting observable which is a subset of the overall activity the rate function is bound by a CMP distribution with sub-Poissonian number fluctuations; see Eqs. (17) and (18). For the elementary example of Fig. 1 the bound is tight, but more complex problems of interest often display large (that is, super-Poissonian) number fluctuations [24, 42, 43, 46, 48, 53].

For a simple illustration of this consider Fig. 3 which shows the rate functions for an observable and its FPT in a three-level system. The observable is the number of jumps between states zero and 1—see Fig. 3(a) for the level scheme—and under the conditions of the figure the dynamics is intermittent and correlated in time. The CMP curves give the bounds to the rate functions, as described in the previous sections. In contrast to Figs. 1 and 2 the bounds are not tight. Figures 1 and 2 also showed the corresponding Poisson rate functions, and due to the particular nature of the two-level system, they appear to lower bound the true rate functions. But this is not the case in general, as Fig. 3 shows. It would be interesting to find alternative yet simple variational ansatzes that can capture such strong fluctuation behavior. Nevertheless, there are still important consequences that follow even from these simple bounds. An immediate one is that the dynamical activity cannot be sub-Poissonian, which in turn implies an

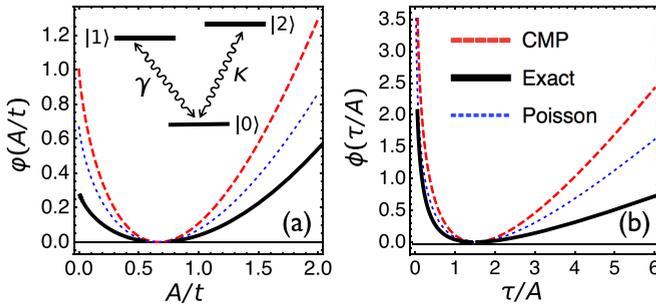


FIG. 3. Bounds on rate functions for a three-level system. Transition rates are $W_{10} = W_{01} = \gamma$ and $W_{02} = W_{20} = \kappa$. We consider as observable A the total number of $1 \rightarrow 0$ jumps. Panel (a) shows the rate function $\phi(A/t)$ [full (black)] for $\gamma = 1$ and $\kappa = 0.5$. The rate function is bounded from above everywhere by a CMP rate function, Eq. (17) [dashed (red)]. We also show for comparison a Poisson rate function with mean $\langle a \rangle$ [dotted (blue)]. Panel (b) shows the FPT rate function $\phi(\tau/A)$ [full (black)]. The rate function is bounded from above everywhere by $\phi_*(\tau/A)$, Eq. (37) [dashed (red)]. The CMP bounds are not tight, due to the intermittent nature of the dynamics (i.e., events are correlated in time, or “bunched”) making the event statistics super-Poissonian.

exponential in time complexity for the efficient sampling of trajectories conditioned on it; cf. [36].

We have also shown how to obtain related general bounds on the distributions of first-passage times. Again this complements for counting observables, and generalizes, recent

results on FPTs for currentlike quantities [16–18]. We did this by exploiting the correspondence between the large deviation functions of observables and those of FPTs, Eqs. (25)–(28). Note that this correspondence works for observables which are nondecreasing in time. For these, the zero increment probability $P_t(0|y)$, Eq. (29), is directly related to the tilted operator \mathcal{L}_∞ , leading to the ensemble correspondence, Eqs. (25)–(28). For currents, however, a zero observable does not imply the absence of jumps that contribute to the observable (only that their contribution adds up to zero), and the correspondence breaks down (or at least we have not been able to relate the corresponding cumulant generating functions in that case). Just like in the case of activities, the FPTs are bounded by the distribution of times of a CMP process, Eqs. (35) and (37), as illustrated in Fig. 2.

As occurs for currents [13–15], the bounds to rate functions give rise to thermodynamic uncertainty relations constraining the precision of estimation of both observables and FPTs, Eqs. (20) and (40). For empirical currents, which are time-asymmetric, precision is limited by the average entropy produced [13–15]. In turn, for counting observables and their FPTs, the corresponding limit is set by the average dynamical activity, suggesting that this quantity might play as important a role in the dynamics as the overall dissipation.

ACKNOWLEDGMENT

This work was supported by EPSRC Grant No. EP/M014266/1.

- [1] T. R. Gingrich, J. M. Horowitz, N. Perunov, and J. L. England, *Phys. Rev. Lett.* **116**, 120601 (2016).
- [2] P. Pietzonka, A. C. Barato, and U. Seifert, *Phys. Rev. E* **93**, 052145 (2016).
- [3] P. Pietzonka, A. C. Barato, and U. Seifert, *J. Phys. A* **49**, 34LT01 (2016).
- [4] T. R. Gingrich, G. M. Rotskoff, and J. M. Horowitz, [arXiv:1609.07131](https://arxiv.org/abs/1609.07131).
- [5] C. Maes and K. Netocny, *Europhys. Lett.* **82**, 30003 (2008).
- [6] L. Bertini, A. Faggionato, and D. Gabrielli, [arXiv:1212.6908](https://arxiv.org/abs/1212.6908).
- [7] L. Bertini, A. Faggionato, and D. Gabrielli, *Stoc. Proc. Appl.* **125**, 2786 (2015).
- [8] A. Dembo and O. Zeitouni, *Large Deviation Techniques and Applications*, 2nd ed. (Springer, New York, 1998).
- [9] D. Ruelle, *Thermodynamic Formalism* (Cambridge University Press, Cambridge, UK, 2004).
- [10] P. Gaspard, *Chaos, Scattering and Statistical Mechanics* (Cambridge University Press, Cambridge, UK, 2005).
- [11] V. Lecomte, C. Appert-Rolland, and F. van Wijland, *J. Stat. Phys.* **127**, 51 (2007).
- [12] H. Touchette, *Phys. Rep.* **478**, 1 (2009).
- [13] A. C. Barato and U. Seifert, *Phys. Rev. Lett.* **114**, 158101 (2015).
- [14] A. C. Barato and U. Seifert, *J. Phys. Chem. B* **119**, 6555 (2015).
- [15] M. Poletti, A. Lazarescu, and M. Esposito, *Phys. Rev. E* **94**, 052104 (2016).
- [16] E. Roldán, I. Neri, M. Dörpinghaus, H. Meyr, and F. Jülicher, *Phys. Rev. Lett.* **115**, 250602 (2015).
- [17] K. Saito and A. Dhar, *EPL* **114**, 50004 (2016).
- [18] I. Neri, E. Roldan, and F. Jülicher, *Phys. Rev. X* **7**, 011019 (2017).
- [19] R. Chetrite and H. Touchette, *Phys. Rev. Lett.* **111**, 120601 (2013).
- [20] R. Chetrite and H. Touchette, *Ann. Henri Poincaré* **16**, 2005 (2015).
- [21] A. A. Budini, R. M. Turner, and J. P. Garrahan, *J. Stat. Mech.* (2014) P03012.
- [22] J. Kiukas, M. Guta, I. Lesanovsky, and J. P. Garrahan, *Phys. Rev. E* **92**, 012132 (2015).
- [23] L. Peliti, *Statistical Mechanics in a Nutshell* (Princeton University Press, Princeton, NJ, 2011).
- [24] J. P. Garrahan, R. L. Jack, V. Lecomte, E. Pitard, K. van Duijvendijk, and F. van Wijland, *Phys. Rev. Lett.* **98**, 195702 (2007).
- [25] J. P. Garrahan, R. L. Jack, V. Lecomte, E. Pitard, K. van Duijvendijk, and F. van Wijland, *J. Phys. A* **42**, 075007 (2009).
- [26] C. Maes, K. Netocny, and B. Wynants, *Physica A* **387**, 2675 (2008).
- [27] U. Basu, M. Krüger, A. Lazarescu, and C. Maes, *Phys. Chem. Chem. Phys.* **17**, 6653 (2015).
- [28] G. Shmueli, T. P. Minka, J. B. Kadane, S. Borle, and P. Boatwright, *J. R. Stat. Soc. C-App.* **54**, 127 (2005).
- [29] J. L. Lebowitz and H. Spohn, *J. Stat. Phys.* **95**, 333 (1999).
- [30] R. M. L. Evans, *Phys. Rev. Lett.* **92**, 150601 (2004).

- [31] C. Giardinà, J. Kurchan, and L. Peliti, *Phys. Rev. Lett.* **96**, 120603 (2006).
- [32] B. Derrida, *J. Stat. Mech.* (2007) P07023.
- [33] C. Appert-Rolland, B. Derrida, V. Lecomte, and F. van Wijland, *Phys. Rev. E* **78**, 021122 (2008).
- [34] T. Bodineau and C. Toninelli, *Commun. Math. Phys.* **311**, 357 (2012).
- [35] C. P. Espigares, P. L. Garrido, and P. I. Hurtado, *Phys. Rev. E* **87**, 032115 (2013).
- [36] R. L. Jack, I. R. Thompson, and P. Sollich, *Phys. Rev. Lett.* **114**, 060601 (2015).
- [37] M. Ueda and S.-i. Sasa, *Phys. Rev. Lett.* **115**, 080605 (2015).
- [38] R. L. Jack and R. Evans, *J. Stat. Mech.* (2016) 093305.
- [39] P. Tsoibgni Nyawo and H. Touchette, *Phys. Rev. E* **94**, 032101 (2016).
- [40] D. Karevski and G. M. Schutz, *Phys. Rev. Lett.* **118**, 030601 (2017).
- [41] Y. Baek, Y. Kafri, and V. Lecomte, *Phys. Rev. Lett.* **118**, 030604 (2017).
- [42] M. Merolle, J. P. Garrahan, and D. Chandler, *Proc. Natl. Acad. Sci. USA* **102**, 10837 (2005).
- [43] L. O. Hedges, R. L. Jack, J. P. Garrahan, and D. Chandler, *Science* **323**, 1309 (2009).
- [44] J. Kurchan, [arXiv:0901.1271](https://arxiv.org/abs/0901.1271).
- [45] T. Speck and J. P. Garrahan, *Eur. Phys. J. B* **79**, 1 (2011).
- [46] T. Speck, A. Malins, and C. P. Royall, *Phys. Rev. Lett.* **109**, 195703 (2012).
- [47] C. Flindt and J. P. Garrahan, *Phys. Rev. Lett.* **110**, 050601 (2013).
- [48] J. K. Weber, R. L. Jack, and V. S. Pande, *J. Am. Chem. Soc.* **135**, 5501 (2013).
- [49] A. S. J. S. Mey, P. L. Geissler, and J. P. Garrahan, *Phys. Rev. E* **89**, 032109 (2014).
- [50] S. Vaikuntanathan, T. R. Gingrich, and P. L. Geissler, *Phys. Rev. E* **89**, 062108 (2014).
- [51] J. K. Weber, D. Shukla, and V. S. Pande, *Proc. Natl. Acad. Sci. USA* **112**, 10377 (2015).
- [52] M. Esposito, U. Harbola, and S. Mukamel, *Rev. Mod. Phys.* **81**, 1665 (2009).
- [53] J. P. Garrahan and I. Lesanovsky, *Phys. Rev. Lett.* **104**, 160601 (2010).
- [54] J. M. Hickey, S. Genway, I. Lesanovsky, and J. P. Garrahan, *Phys. Rev. A* **86**, 063824 (2012).
- [55] C. Ates, B. Olmos, J. P. Garrahan, and I. Lesanovsky, *Phys. Rev. A* **85**, 043620 (2012).
- [56] I. Lesanovsky, M. van Horssen, M. Guță, and J. P. Garrahan, *Phys. Rev. Lett.* **110**, 150401 (2013).
- [57] M. Znidaric, *Phys. Rev. Lett.* **112**, 040602 (2014).
- [58] M. Znidaric, *Phys. Rev. E* **89**, 042140 (2014).
- [59] D. Bernard and B. Doyon, *Ann. Henri Poincaré* **16**, 113 (2015).
- [60] S. Pigeon, L. Fusco, A. Xuereb, G. De Chiara, and M. Paternostro, *Phys. Rev. A* **92**, 013844 (2015).
- [61] M. van Horssen and M. Guță, *J. Math. Phys.* **56**, 022109 (2015).
- [62] S. Gherardini, S. Gupta, F. S. Cataliotti, A. Smerzi, F. Caruso, and S. Ruffo, *New J. Phys.* **18**, 013048 (2016).
- [63] S. Deffner, *New J. Phys.* **18**, 011001 (2016).
- [64] C. Monthus, [arXiv:1701.05090](https://arxiv.org/abs/1701.05090).
- [65] M. Baiesi, C. Maes, and B. Wynants, *Phys. Rev. Lett.* **103**, 010602 (2009).
- [66] A. A. Budini, *Phys. Rev. E* **84**, 011141 (2011).
- [67] C. De Bacco, A. Guggiola, R. Kühn, and P. Paga, *J. Phys. A: Math. Theor.* **49**, 184003 (2016).
- [68] J. Szavits-Nossan and M. R. Evans, *J. Stat. Mech.* (2015) P12008.
- [69] G. Verley, *Phys. Rev. E* **93**, 012111 (2016).
- [70] M. V. S. Bonança and C. Jarzynski, *Phys. Rev. E* **93**, 022101 (2016).
- [71] T. Nemoto, F. Bouchet, R. L. Jack, and V. Lecomte, *Phys. Rev. E* **93**, 062123 (2016).
- [72] T. Speck, *Phys. Rev. E* **94**, 022131 (2016).
- [73] C. Gardiner, *Handbook of Stochastic Methods* (Springer, Berlin, 2004).
- [74] P. G. Bolhuis, *J. Chem. Phys.* **129**, 114108 (2008).
- [75] R. J. Harris and H. Touchette, *J. Phys. A: Math. Theor.* **50**, 10LT01 (2017).
- [76] J. P. Garrahan, *J. Stat. Mech.* (2016) 073208.