Exact computation of current cumulants in small Markovian systems

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Abstract. We describe an algorithm computing the exact value of the mean current, its variance, and higher order cumulants for stochastic driven systems. The method uses a Rayleigh-Schrödinger perturbation expansion of the generating function of the current, and can be extended to compute covariances of multiple currents. As an example of application of the method, we give numerical evidence for a simple relation [Eq. (5)] between the second and the fourth cumulants of the current in a symmetric exclusion process.

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GOAL

In phenomena like charge transport in nano-electromechanical systems [1, 2, 3, 4, 5, 6] or in life processes like molecular motors or like ion-transport through a single membrane channel, one easily reaches energy scales as low as a few k_BT [7, 8]. Therefore, the physics and the chemistry of these small systems must talk about fluctuations, not only because they are very much present but also because some processes actually make use of these fluctuations. Moreover, the experimental output is often in terms of current cumulants, which should inform us about important features of the system dynamics.

A central quantity is the fluctuating current j, which gives the time-averaged number of particles or quanta that pass trough a given surface, and its large deviation function $I(j)$, describing the shape of its probability distribution $p(j) \simeq \exp(-T\,I(j))$ for very long time intervals T. One is interested in its full shape, as its tail can contain signatures of interesting physics. However, the asymptotic estimate of these tails is problematic as they involve fluctuations that become rare for $T \to \infty$. We describe a numerical scheme to compute exactly (up to numerical round-off's) the cumulants of these current fluctuations in general small Markovian systems. We emphasize that our algorithm is exact and can be systematically implemented to produce cumulants of in principle arbitrary order. Practical limitations such as memory storage make it however most efficient for the statistical mechanics of systems that are not too large. Finally, our method is based on general theoretical considerations and its interpretation involves a relation between current and traffic (dynamical activity) fluctuations.

Mathematically, our approach uses a type of Rayleigh-Schrödinger perturbation expansion for the largest eigenvalue of a matrix that is obtained as a perturbation of the original Markov generator; a full account can be found in [9]. It can be seen as a

modification and adaption to classical nonequilibrium models, of a technique developed within the framework of full counting statistics for quantum transport [10], see also [4, 5, 11, 12, 13, 14, 15]. Our approach is somewhat complementary to a recent efficient algorithm for the (approximate) estimate of the large deviation function [16, 17].

EXAMPLE MODEL

To illustrate our focus we consider the well studied one-dimensional boundary driven simple symmetric exclusion process (SSEP), for which several rigorous results are available [18, 19]. A state is represented by an array (η_i) of N units, which can either be empty ($\eta_i = 0$) or occupied by one particle ($\eta_i = 1$). A transition takes place when a particle moves to a neighboring empty site (with rate 1) or if it enters/exits from one of the end sites, which are in contact with reservoirs at different chemical potentials (α at $i = 1$ and α' at $i = N$). For example, a transition from a state η to a state ξ due to the entrance of a particle from the left reservoir ($\eta_1 = 0 \to \eta_1 = 1$ and the rest of the array is unchanged) takes place with rate $k(\eta,\xi) = \exp(\alpha/2)$. Observe that we impose the physical condition of local detailed balance, meaning that the rates should obey

$$k(\eta,\xi) = a(\eta,\xi)\,\exp\Big[\frac{\text{entropy flux}}{2}\Big] \tag{1}$$

with some symmetric prefactor $a(\eta,\xi) = a(\xi,\eta)$. Here, we have taken $a = 1$ and the irreversible entropy flux from the left particle reservoir is α per entering particle. We expect that systematically a net particle current flows through the system, from the side with higher chemical potential. As we follow the path or trajectory $\eta(t)$ over some time-interval $t \in [0,T]$ we can read the number of particles that enter from the left (left time-integrated particle current) and the number of particles that exit to the right. These are of course fluctuating currents, as the path $(\eta(t))$ is random with a distribution obtained from the Markov dynamics. For our purposes, the information on the dynamics is summarized in the generator L, an $M \times M$ matrix with elements $L(\eta,\xi) = k(\eta,\xi)$ for $\eta \neq \xi$ and $L(\eta,\eta) = -\sum_\xi k(\eta,\xi)$. Exactly because of the nonequilibrium condition $\alpha \neq \alpha'$, the matrix L need not even be diagonalizable. For the final algorithm, that involves a departure from the more standard Rayleigh-Schrödinger set-up, as we might not have an orthogonal basis of eigenvectors.

PATH-SPACE IDENTITY

To understand the theoretical point of departure of the method, it is useful to separate the time-antisymmetric part from the time-symmetric part in the path-space distribution of the Markov process. Under the condition of local detailed balance (1), the time-antisymmetric part is directly related to the variable entropy flux and the time-symmetric part measures the dynamical activity, called *traffic* [20, 21] in the system. Because of the normalization of the path-space distribution these two sectors have related fluctuations, as we will make explicit below in (4). Specifically, we consider ensembles of bonds $B = \{\eta \to \xi\}$ that all equally contribute to the same time-integrated mesoscopic current

$J_B = \int_0^T dJ_B(t)$. In our example, we can take B_1 containing all transitions getting one particle into the system and coming from the left reservoir, and B_2 consisting of all transitions in which a particle leaves the system to the right reservoir. We denote by $-B$ the ensemble of reversed transitions, giving rise to an instantaneous current $dJ_{-B} = -1$. We are then interested in the various moments and correlations between the J_B's. These can be obtained from the cumulant-generating function

$$g(\sigma) = \frac{1}{T} \log\langle \exp \sum_B \sigma_B J_B \rangle \tag{2}$$

in the steady state of the system. For example the second (partial) derivatives with respect to $\sigma_{B_1}, \sigma_{B_2}$ give a covariance between two currents. The point is now that the exponent in (2) can be read as an excess entropy flux $\sum_B \sigma_B J_B$, whose fluctuations are the same as that of a dynamical activity in a Markov model with extra driving. To make that last point, we imagine an extra driving by modifying the rates to

$$L_\sigma(\eta, \xi) = k(\eta, \xi)\, e^{\sigma(\eta,\xi)}$$

for some antisymmetric function σ, which, allowing some abuse of notation, is $\sigma(\eta, \xi) = \pm\sigma_B$ if $(\eta, \xi) \in \pm B$. One should check the local detailed balance condition (1) to see that some extra entropy flux is imposed. Both the original Markov process (with generator L) and the modified one (with generator L_σ) have a path-space distribution with action, respectively A and A_σ, and for which

$$\begin{aligned} \exp\left[T\, g(\sigma)\right] &= \langle e^{-A+\sum_B \sigma_B J_B} \rangle_{\rm eq} \\ &= \langle e^{-A_\sigma}\, e^{-A+A_\sigma+\sum_B \sigma_B J_B} \rangle_{\rm eq} \end{aligned} \tag{3}$$

with respect to some fixed equilibrium reference dynamics. If we therefore arrange that the time-antisymmetric parts of A and A_σ differ exactly by the excess entropy flux, we keep the excess in dynamical activity (time-symmetric parts):

$$-A + A_\sigma + \sum_B \sigma_B J_B = \int_0^T V(\eta(t), \sigma)\, dt$$

for a particular function V on the state space, that also depends on the σ. That function $V(\eta)$ essentially measures the difference in escape rates from η for the original process with respect to the one modified by the σ's. The conclusion is a general path-space identity

$$g(\sigma) = \frac{1}{T} \log\langle \exp \int_0^T V(\eta(t), \sigma)\, dt \rangle_\sigma \tag{4}$$

where the last expectation is for the modified steady state. The formula (4) is more ready for asymptotic evaluation as $T \uparrow +\infty$ since V is a multiplication operator. The algorithm must then give a systematic expansion in the σ_B of the largest eigenvalue (in the sense of its real part) of the matrix $\mathscr{L} = L_\sigma + V(\cdot, \sigma) = L + \mathscr{R} = L + \sum_B \sum_{n\geq 1} (\sigma_B)^n \mathscr{L}_B^{(n)}$, where $\mathscr{R}$ is the matrix with non-zero elements $[e^{\pm\sigma_B} - 1]k(\eta, \xi)$ only in ensembles $\pm B$'s, where the rates of L_σ are different from the rates of L. The details of this

expansion are in [9]. We just briefly mention that this expansion does not have the advantage of dealing with symmetric matrices, as in the original Rayleigh-Schrödinger method for quantum mechanical operators. The solution of the problem goes via the use of *resolvents*. Interestingly, the final results include the group inverse G of the generator L as a main actor [22, 23]. This matrix contains all the informations needed to compute the dynamical quantities of interest, like the stationary distribution $\langle\rho|$ and the cumulants. For example, the variance of a current takes the form $C_{BB} = \langle\rho|\mathscr{L}_B^{(2)}|1\rangle - \langle\rho|\mathscr{L}_B^{(1)} G \mathscr{L}_B^{(1)}|1\rangle$ (by $|1\rangle$ we mean a vector of 1's).

ILLUSTRATION

We end with a discussion of some results for the open SSEP introduced above. For the SSEP on a ring, cumulants $Q^{(n)}$ of the current have been computed theoretically [24]. Formulas for the mean current and its variance are also available for the boundary-driven SSEP, while formulas for cumulants of order $n \geq 3$ are known up to order $1/N$ [18, 19]. Being one-dimensional and finite, there is only one relevant current in the system, which we identify with the entrance of a particle from the left reservoir. Our data, for system sizes up to $N = 14$, at equilibrium with half-filling ($\alpha = \alpha' = 0$)[1] perfectly agree with the theoretical value: $C^{(2)} = Q^{(2)} = (2N)^{-1}$. In the same conditions, for the fourth cumulant we observe

$$C^{(4)} = (C^{(2)})^2 = \frac{1}{(2N)^2} \tag{5}$$

for $N \leq 14$, while to order $1/N$ one has $Q^{(4)} = 0$ [18, 19]. The relation (5) is slightly different from the one found for the SSEP at equilibrium on a ring, where the asymptotic values of the second and fourth cumulants of the current are related by $Q^{(4)} = \frac{1}{2}(Q^{(2)})^2$ [24]. It turns out that the addition of a term $= (Q^{(2)})^2$ to $Q^{(4)}$ yields a good approximation of $C^{(4)}$ for finite N also out of equilibrium, see the Fig. 1(a). Finally, we have tested that the relation (5) is not valid for $\alpha = \alpha' \neq 0$ (no half-filling) or for $\alpha = -\alpha' \neq 0$ (a case of half-filling out of equilibrium), see Fig. 1(b).

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[1] The chemical potentials α and α' correspond to reservoirs with particle density $\rho_a = \exp(\alpha/2)/[\exp(\alpha/2) + \exp(-\alpha/2))$ and $\rho_b = \exp(\alpha'/2)/[\exp(\alpha'/2) + \exp(-\alpha'/2))$ in [18, 19].

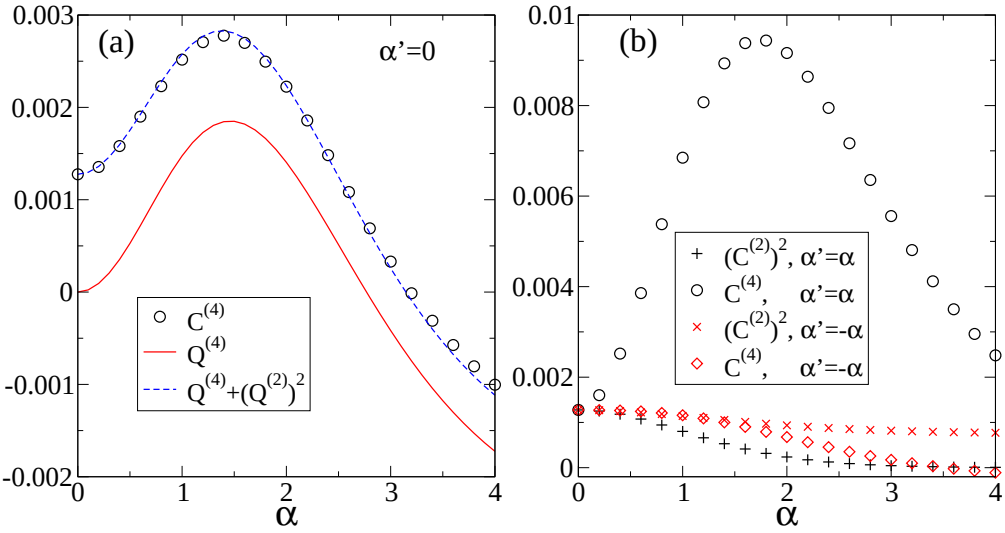

FIGURE 1. (a) Fourth cumulant ($C^{(4)}$) of the open SSEP as a function of α, and the theoretical value ($Q^{(4)}$) by Derrida and coworkers, for $N = 14$ and $\alpha' = 0$. The theoretical $Q^{(4)} + (Q^{(2)})^2$ is also shown. (b) $(C^{(2)})^2$ and $C^{(4)}$ vs α for $N = 14$, with $\alpha' = \alpha$ and $\alpha' = -\alpha$ (see legend).

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