



# Steady-state distributions of probability fluxes on complex networks

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## HIGHLIGHTS

- The statistical properties of the probability fluxes in complex networks are studied.
- Their stationary distributions converge to the Gaussian function regardless of the network topology.
- The average flux and the standard deviation are related through the fluctuation theorem.
- Also, the other factors that affect these two parameters are comprehensively analyzed.

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## ABSTRACT

We consider a simple model of the Markovian stochastic dynamics on complex networks to examine the statistical properties of the probability fluxes. The additional transition, called hereafter a gate, powered by the external constant force breaks a detailed balance in the network. We argue, using a theoretical approach and numerical simulations, that the stationary distributions of the probability fluxes emergent under such conditions converge to the Gaussian distribution. By virtue of the stationary fluctuation theorem, its standard deviation depends directly on the square root of the mean flux. In turn, the nonlinear relation between the mean flux and the external force, which provides the key result of the present study, allows us to calculate the two parameters that entirely characterize the Gaussian distribution of the probability fluxes both close to as well as far from the equilibrium state. Also, the other effects that modify these parameters, such as the addition of shortcuts to the tree-like network, the extension and configuration of the gate and a change in the network size studied by means of computer simulations are widely discussed in terms of the rigorous theoretical predictions.

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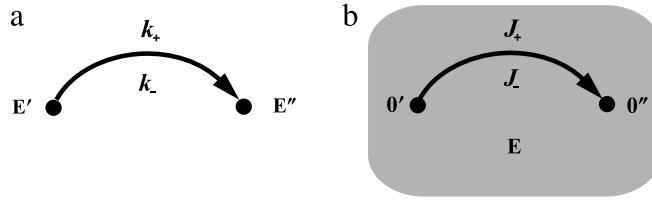
## 1. Introduction

According to the principles established by the conventional enzymology, a protein that catalyzes a chemical reaction occurs in a few stable conformational states [1]. The most simplified version of this paradigm is sketched in Fig. 1(a), where the enzyme occurs in only two distinguished states  $E'$  and  $E''$ . The transitions between them proceed with the forward and backward rate constants  $k_+$  and  $k_-$ , which depend on the molar concentrations of substrates taking part in this process. In a nonequilibrium steady state, the resultant reaction flux [2,3]

$$J = \frac{1 - e^{-a}}{k_+^{-1} + k_-^{-1} e^{-a}} \quad (1)$$

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**Fig. 1.** (a) The scheme of the enzymatic reaction that proceeds with the forward and backward rate constants  $k_+$  and  $k_-$  between two distinguished conformational states  $E'$  and  $E''$  of the protein enzyme. (b) The reaction fluxes  $J_+$  and  $J_-$  through the gate that consists of two conformational substates  $0'$  and  $0''$ . The gray plaque represents the network of conformational transitions within either the enzyme or the enzyme-substrate native state  $E$ . Arrows indicate the directions assumed to be forward.

is unbalanced, because of the dimensionless constant force  $a \equiv A/k_B T$ , defined by the ratio of the thermodynamic force (chemical affinity)  $A$  and the temperature  $T$  multiplied by the Boltzmann constant  $k_B$ . In Fig. 1(b), this oversimplified picture of the coarse-grained enzymatic kinetics is replaced by the more detailed ‘mesoscopic’ scheme, promoted in our previous papers [4,5]. The gray plaque represents an arbitrary network of stochastic transitions between numerous conformational substates, composing either the enzyme or the enzyme-substrate native state  $E$ . All these internal transitions satisfy a detailed balance condition. However, it is broken by the external transitions powered by the chemical reaction fluxes  $J_+$  and  $J_-$  through a pair of the conformational states  $0'$  and  $0''$  composing the gate. Unlike the average flux in Eq. (1), the fluxes emergent in such a mesoscopic system fluctuate in time [6–8]. Thus, they must be considered as random variables [9,10], and their statistical properties provide the scope of the present paper.

At the beginning, we define the model of the enzymatic reaction in formal terms, as a kind of a dynamical system. The states of the system, symbolized by the nodes, are assumed to be organized into the fractal scale-free network [11,12], while the stochastic transitions, determined by a set of master equations [9,13], proceed between them through the links. Our decision to choose this special type of network was justified by the recent report establishing that the network of conformational transitions within the protein native state has the fractal topology [14]. In our model, the essential component of the network is the gate destined to monitor the external transitions giving rise to the probability fluxes. In the nonequilibrium ensemble these quantities are no longer determined precisely, but undergo the stationary distributions constrained by the Andrieux–Gaspard fluctuation theorem [15,16]. The correctness of the different variants of the fluctuation theorem has been verified in the case of many experimental protocols [17–22], as well as theoretical models [23–36], for the systems that operate on the mesoscopic scales. Here, we use the method of numerical simulations and argue that in the case of the stochastic dynamics on the network equipped with a single gate, the stationary distributions of the probability fluxes converge to the Gaussian function. It turns out, that its standard deviation depends directly on the mean flux for a given value of the external force and the time period of the fluxes determination. Furthermore, the nonlinear relation between the mean flux and the external force (see Eq. (1)), which provides the key result of the present study, allows us to determine the two parameters that entirely characterize the Gaussian distribution of the probability fluxes. Thus, we show that no fitting procedure to the numerical data is needed to estimate their values. Moreover, our method works regardless of whether the system is close to or far from the equilibrium state.

We also examine the other factors that affect the Gaussian distribution of the probability fluxes, such as the addition of shortcuts to the fractal tree-like network, the change in the network size and the extension and configuration of the gate attached to the network. All these effects are thoroughly analyzed and interpreted in terms of the rigorous theoretical predictions.

## 2. Stochastic dynamics on networks with a single gate

A continuous-time evolution of the Markovian stochastic process in a discrete set of states is described by the system of differential master equations [9,10]

$$\dot{p}_l(t) = \sum_{l'} [w_{l'l} p_{l'}(t) - w_{ll'} p_l(t)], \tag{2}$$

where  $p_l(t)$  refers to the occupation probability of a state  $l$  at time  $t$ , the overdot denotes the time derivative and  $w_{l'l}$  are the transition probabilities per unit time from the state  $l$  to the adjacent states  $l'$ . In general, these transition rates do not have to complement to unity after summation over  $l'$  for a fixed  $l$ , which poses some technical problems for numerical simulations. However, on introducing a discrete time  $t = m\tau_0$ , where the number of steps  $m$  is expressed in the specified unit of time  $\tau_0$ , Eq. (2) can be rewritten as the difference master equation

$$p_l(m + 1) = p_l(m) + \sum_{l'} [u_{l'l} p_{l'}(m) - u_{ll'} p_l(m)], \tag{3}$$

with the transition probabilities

$$u_{l'l} = \tau_0 w_{l'l} \tag{4}$$

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