Entropy production and fluctuation theorems on complex networks

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Entropy production (EP) is known as a fundamental quantity for measuring the irreversibility of processes in thermal equilibrium and states far from equilibrium. In stochastic thermodynamics, the EP becomes more visible in terms of the probability density functions of the trajectories of a particle in the state space. Inspired by a previous result that complex networks can serve as state spaces, we consider a data packet transport problem on complex networks. Entropy is produced owing to the complexity of pathways as the packet travels back and forth between two nodes. The EPs are exactly enumerated along the shortest paths between every pair of nodes, and the functional form of the EP distribution is determined by extreme value analysis. The asymptote of the accumulated EP distribution is found to follow the Gumbel distribution.

I. INTRODUCTION

The concept of entropy production (EP) has received increasing attention recently as nonequilibrium phenomena have become a central issue in statistical physics [1–4]. The EP is the amount of uncompensated heat divided by the temperature in irreversible processes. This quantity corresponds to the work dissipated during irreversible process. The fluctuation theorem (FT) of EP in the nonequilibrium steady state was established in Refs. [5–7]. Crooks [8], Jarzynski [9], and others developed the FT for the dissipated work associated with other physical quantities such as the free energy. After the FT was first proposed for thermal systems, further studies were performed to obtain more general FTs and deeper understanding [10, 11]. As a result, EP could be viewed microscopically in terms of the trajectories of a single particle [12, 13]. The EP was defined as the logarithm of the ratio of the probabilities that a dynamic process proceeds in the forward and backward directions between two states in a nonequilibrium system [10, 13]. The EP distribution is formed as the integral of those EPs over all possible states and trajectories. FTs such as the integral FT and detailed FT were derived [1].

Even though the EP is well defined formally as described above, it is rarely shown explicitly, because the trajectories of a particle in the state space are virtual, and the number of trajectories increases exponentially as the number of steps is increased. Here we note that complex networks can serve as state spaces. For instance, each node in a protein folding network represents a protein conformation, and two nodes are connected by a link when a protein conformation is changed to another in consecutive steps [14]. Thus, we consider a data packet transport problem on complex networks to obtain the EP distribution explicitly. Suppose that a data packet is sent from one node to another on a complex network such as the Internet. At each time step, the packet is transmitted to a neighbor according to the router protocol at each node toward the final destination. Unless traffic is congested, packets generally travel along the shortest path between a starting node and a final destination. Recent studies using molecular dynamics simulations revealed that in protein folding dynamics, there exist a few major pathways involving multiple folds from denatured states to the natural state [14, 15], in disagreement with Levinthal's perspective [16]. Thus, the folding dynamics may proceed as biased random walks along the shortest pathway on the conformation network. Thus, it makes sense to consider only the case in which the packet is transmitted along the shortest pathways to the final destination.

Owing to extensive research in network science during the past two decades, an efficient algorithm for identifying every possible shortest path between any pair of nodes was developed, which has the computational complexity $O(N^2 \log N)$, where N is the network size [17–19]. Thus, the exact EP distribution can be obtained as long as the transport is confined to the shortest pathways. On the other hand, the flow along the shortest pathways on complex networks was used to quantify a person's influence in society [18] and the load on a router on the Internet [20].

We first integrate the EP induced by topological diversity of every shortest pathway as each pair of nodes sends and receives a data packet on a given network [20]. This dataset is complete in the sense that the data are obtained from every possible shortest pathway. Thus, the EP distribution consists of $N(N-1)$ EPs.

Next, we perform extreme value (EV) analysis [21] to determine the functional form of the asymptotic behavior of the EP distribution, called an asymptote. This method was originally developed to predict the probability of rare events such as floods of a certain level, for in-

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stance. To perform this EV analysis, we use the theorem that states that the functional form of the asymptote of a distribution is related to the distribution of the maxima of samples selected randomly from the original $N(N-1)$ elements [21]. Using this property, we find that the Gumbel distribution is the best fit to the asymptote of the n-th power of the accumulated EP distribution. Moreover, the Gumbel distribution seems to be common to other similar distributions obtained from different complex networks. On the basis of this result, we assert that the EP distribution behaves asymptotically.

Networks are a platform for interdisciplinary studies. The nodes and links of a network represent routers and optical cables on the Internet, web documents and hyperlinks on the World Wide Web, and individuals and social interactions in social networks [22]. It was found that most complex networks in the real world are heterogeneous in the number of connections at each node, called the degree. Their degree distributions follow a power-law or heavy-tailed distribution. Because the exponent λ of the degree distribution $P_d(k) \sim k^{-\lambda}$ is in the range $2 < \lambda \leq 3$, they are called scale-free networks. On the other hand, a random network introduced by Erdős and Rényi (ER) has a degree distribution following the Poisson distribution. We have considered the data packet transport problem on diverse types of model networks and find that the Gumbel distribution seems to fit all scale-free networks well.

This paper is organized as follows. In Sec. II, we introduce an EP induced by the topological complexity of the shortest pathways on networks. In Sec. III, we show that the total EP obtained from every shortest pathway satisfies the integral FT and the detailed FT (Sec. IIIA and Sec. IIIB, respectively). In Sec. IV, we obtain the EP distribution for several model networks numerically. In Sec. V, we determine the functional type of the asymptote of the accumulated EP distribution using the EV approach. We confirm that the asymptote follows the Gumbel distribution. A summary is presented in Sec. VI.

II. EP ON NETWORKS

We consider data packet transport from a source node i to a target node j along a shortest pathway α. The packet returns along the same pathway α from node j to node i. Thus, the time-forward trajectory and its corresponding time-reverse trajectory are the same. However, the probabilities to take that trajectory in each direction can be different. For this type of transport, the EP is defined as follows:

$$\Delta S^{\alpha}_{i\to j} = \ln\Big[\frac{P^{\rm F}_{i\to j,\alpha}}{P^{\rm B}_{j\to i,\alpha}}\Big] = \ln\Big[\frac{\rho_s(i)\rho(j|i)\Pi^{\alpha}_{i\to j}}{\rho_t(j)\rho(i|j)\tilde{\Pi}^{\alpha}_{i\to j}}\Big], \quad (1)$$

where $P^{\rm F}_{i\to j,\alpha}$ [$P^{\rm B}_{j\to i,\alpha}$] denotes the probability that transport occurs along the pathway α in the forward (backward) direction; $\rho_s(i)$ [$\rho_t(j)$] denotes the probability that node i (j) is selected as a source (target); and $\rho(j|i)$ [$\rho(i|j)$] is the conditional probability that node j (i) is chosen as a target, provided that node i (j) is chosen as a source. In this problem, $\rho_s(i) = \rho_t(j) = 1/N$, because the node is selected randomly from among N nodes. The conditional probability is $\rho(j|i) = \rho(i|j) = 1/(N-1)$ because the node j is randomly selected from $N-1$ nodes excluding node i. $\Pi^{\alpha}_{i\to j}$ ($\tilde{\Pi}^{\alpha}_{i\to j}$) is the transition probability from node i to node j along the shortest pathway α in the forward (backward) direction. In this paper, $\tilde{\Pi}^{\alpha}_{i\to j}$ is found to be the same as $\Pi^{\alpha}_{j\to i}$. Thus, we denote the transition probability in the backward direction as $\Pi^{\alpha}_{j\to i}$. We will show that $\Pi^{\alpha}_{i\to j}$ can differ from $\Pi^{\alpha}_{j\to i}$ owing to the topological diversity of the shortest pathways on complex networks. Thus, the EP can be nonzero.

We consider a simple example to explain how to calculate the transition probabilities in the forward and backward directions. Fig. 1 is a subgraph of a network showing the shortest pathways between two nodes, s and t. There exist three shortest pathways, which are denoted as α, β, and γ, with three hopping distances. Let us first consider packet transport along the pathway α in the forward direction from a to g. A packet starts to travel from a toward node g. At node a, the packet needs to choose either node b or node c, which we assume are chosen with equal probability, as the site of the next step. Thus, hopping from a to b occurs with probability 1/2, as does hopping from a to c. Next, it chooses node d with probability 1/2, because the pathway is divided into two possibilities. Thus, the packet arrives at node d with probability 1/4. Then it travels to the target t without any branching, i.e., with probability one. Accordingly, the transition probability along the pathway α is given as $\Pi^{\alpha}_{a\to g} = a \xrightarrow{1/2} b \xrightarrow{1/2} d \xrightarrow{1} g = 1/4$. On the other hand, when it returns from node g to a along the same pathway α, $\Pi^{\alpha}_{g\to a} = g \xrightarrow{1/3} d \xrightarrow{1} b \xrightarrow{1} a = 1/3$. Thus, the two transition probabilities are not the same: $\Pi^{\alpha}_{a\to g} \neq \Pi^{\alpha}_{g\to a}$. Further, $\rho_s(a) = \rho_t(g) = 1/N$, and $\rho(j|i) = \rho(i|j) = 1/(N-1)$. Thus, $\Delta S^{\alpha}_{a\to g} = \ln(3/4)$. Accordingly, a nonzero EP is obtained in packet transport along the pathway α. The EPs along the pathways β and γ can be similarly calculated and are listed in Table I. We can easily find that $\sum_{\alpha}\Pi^{\alpha}_{a\to g} = 1$ for any pair (a, g), whereas $\Pi^{\alpha}_{a\to g}$ cannot be the same, as $\Pi^{\alpha}_{g\to a}$ for each shortest pathway, α, β, and γ, for the sample network shown in Fig. 1.

Pathway	Forward pathway	$\Pi_{a\to g}$	Backward pathway	$\Pi_{g\to a}$	Entropy production
α	$a \xrightarrow{1/2} b \xrightarrow{1/2} d \xrightarrow{1} g$	$\frac{1}{4}$	$g \xrightarrow{1/3} d \xrightarrow{1} b \xrightarrow{1} a$	$\frac{1}{3}$	$\ln\frac{3}{4}$
β	$a \xrightarrow{1/2} b \xrightarrow{1/2} e \xrightarrow{1} g$	$\frac{1}{4}$	$g \xrightarrow{1/3} e \xrightarrow{1} b \xrightarrow{1} a$	$\frac{1}{3}$	$\ln\frac{3}{4}$
γ	$a \xrightarrow{1/2} c \xrightarrow{1} f \xrightarrow{1} g$	$\frac{1}{2}$	$g \xrightarrow{1/3} f \xrightarrow{1} c \xrightarrow{1} a$	$\frac{1}{3}$	$\ln\frac{3}{2}$

TABLE I. Probability that a packet takes each pathway in the forward and backward directions and entropy production

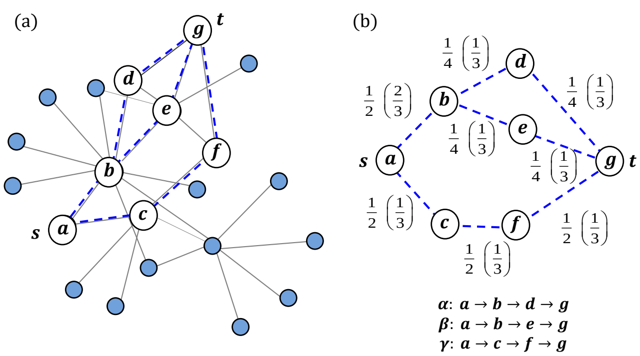

FIG. 1. (a) Sample network to illustrate the EPs along each shortest path from a to g and shortest return path from g to a. For pathway α, a data packet starts along the pathway $a \to b \to d \to g$ and returns in the backward direction. (b) At node a, there are two ways to move toward node g with equal probability. The packet takes the link $a \to b$ with probability 1/2. Next, it takes the link $b \to d$ with probability 1/2. The link $d \to g$ is taken with probability 1. Accordingly, the transition probability along the pathway α, denoted as $\Pi^{\alpha}_{a\to g}$, is found to be 1/4. In the backward direction, the transition probability $\Pi^{\alpha}_{g\to a}$ is found to be 1/3. Table I shows the transition probabilities along each shortest pathway in the forward and backward directions.

III. FLUCTUATION THEOREMS

A. The integral FT

The total EP of the system for transport of a data packet between every pair of nodes (i, j) along all the shortest pathways is written as

$$\langle \Delta S^{\alpha}_{i\to j} \rangle = \sum_i \sum_{j\neq i} \sum_{\alpha} \Delta S^{\alpha}_{i\to j} P^{\rm F}_{i\to j,\alpha}. \tag{2}$$

We find that this total entropy satisfies the so-called integral FT in the following way.

$$\begin{aligned}\langle e^{\Delta S^{\alpha}_{i\to j}} \rangle &= \sum_i \sum_{j\neq i} \sum_{\alpha} P^{\rm F}_{i\to j,\alpha} e^{-\Delta S^{\alpha}_{i\to j}} \\ &= \sum_i \sum_{j\neq i} \sum_{\alpha} \rho_s(i)\rho(j|i)\Pi^{\alpha}_{i\to j} \frac{\rho_t(j)\rho(i|j)\Pi^{\alpha}_{j\to i}}{\rho_s(i)\rho(j|i)\Pi^{\alpha}_{i\to j}} \\ &= \sum_j \sum_{i\neq j} \sum_{\alpha} \rho_s(j)\rho(i|j)\Pi^{\alpha}_{j\to i} = 1. \end{aligned} \tag{3}$$

It is demonstrated that the integer FT holds by the normalization of each factor.

B. The detailed FT

Here we obtain the EP distribution over all possible shortest pathways between every pair of nodes. The EP distribution $P_{\rm F}(\Delta S_{\rm tot})$ for a forward process from node i to node j is given by

$$\begin{aligned} &P_{\rm F}(\Delta S_{\rm tot}) \\ &= \sum_i \sum_{j\neq i} \sum_{\alpha} \delta(\Delta S_{\rm tot} - \Delta S^{\alpha}_{i\to j})\rho_s(i)\rho(j|i)\Pi^{\alpha}_{i\to j} \\ &= \sum_j \sum_{i\neq j} \sum_{\alpha} \delta(\Delta S_{\rm tot} - \Delta S^{\alpha}_{i\to j})\rho_t(j)\rho(i|j)\Pi^{\alpha}_{j\to i} e^{\Delta S^{\alpha}_{i\to j}} \\ &= \sum_j \sum_{i\neq j} \sum_{\alpha} \delta(\Delta S_{\rm tot} + \Delta S^{\alpha}_{j\to i})\rho_t(j)\rho(i|j)\Pi^{\alpha}_{j\to i} e^{\Delta S_{\rm tot}} \\ &= P_{\rm B}(-\Delta S_{\rm tot}) e^{\Delta S_{\rm tot}}, \end{aligned} \tag{4}$$

where we used $\Delta S^{\alpha}_{i\to j} = -\Delta S^{\alpha}_{j\to i}$, and $P_{\rm B}$ denotes the EP distribution in the backward process. The relation $P_{\rm F}(\Delta S) = P_{\rm B}(-\Delta S_{\rm tot})e^{\Delta S_{\rm tot}}$ is known as the detailed FT and is an instance of the Gallavotti–Cohen symmetry of the probability density function [7]. We confirm the detailed FT numerically in Fig. 2. We drop the subindex "tot" hereafter.

IV. NUMERICAL RESULTS

We perform numerical simulations to obtain EPs based on transport along every shortest pathway between all possible pairs of nodes on several networks: the

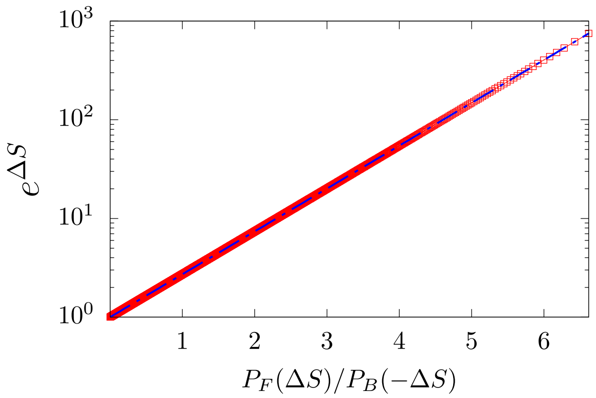

FIG. 2. Plot of the detailed FT. The ratio of the EP distributions in the forward and backward directions is equal to $e^{\Delta S}$. Numerical data are obtained from BA model networks on which a data packet is sent and returned between every pair of nodes along the shortest pathways. Data points lie exactly on the straight line with slope one.

Barabási–Albert (BA) model [23], ER model [24], and Chung–Lu (CL) model [25] with the degree exponents $\gamma = 2.2$ and $\gamma = 2.5$. The EP distributions $P(\Delta S)$ representing both $P_{\mathrm{F}}(\Delta S)$ and $P_{\mathrm{B}}(\Delta S)$ on these networks are shown in Fig. 3. All these networks were constructed with the same mean degree $\langle k\rangle = 8$ and system size $N = 2^{11} \times 10$. We obtain these EP distributions on the giant component of each network. The EP distributions have different shapes. The width of the EP distribution on the BA model is generally wide, whereas that on the ER model is generally narrow. This result arises from the extent of the topological diversity of each type of network.

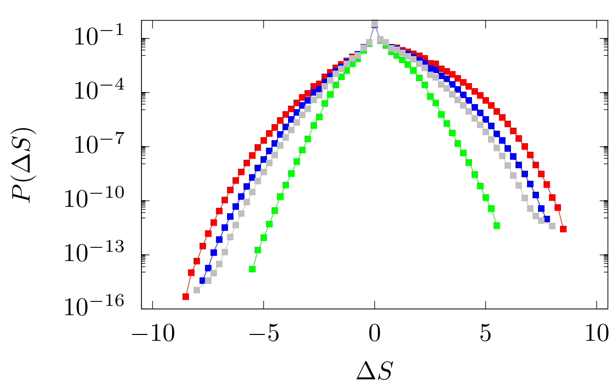

FIG. 3. EP distributions on the four model networks: BA model, scale-free CL model with degree exponent $\gamma = 2.2$, scale-free CL model with degree exponent $\gamma = 2.5$, and ER model, from top to bottom. Data are obtained from the giant component of each model network of system size $N = 2^{11} \times 10$ and mean degree $\langle k\rangle = 8$. They are averaged over 300 configurations. All EP distributions exhibit peaks at $\Delta S = 0$, which are attributed to transport along untangled pathways.

In statistical mechanics, the entropy is an extensive quantity with respect to the system size N. However, in this problem, the length d_{st} of each pathway plays a role similar to that of N in Euclidean space. Thus, we rescale the EP ΔS by the path length and define $\Delta S/d_{st}$. The EP distributions obtained for different network sizes N collapse onto a single curve, as shown in Fig. 4.

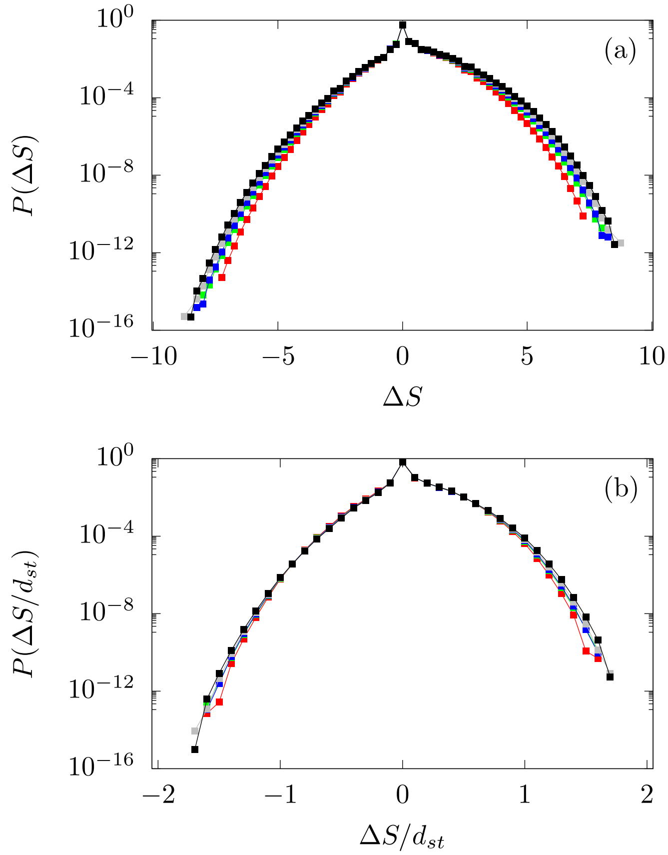

FIG. 4. (a) EP distribution on BA networks of different system sizes, $N = 4096, 8192, 10240, 14336$, and 20480. As N is increased, the EP curves tend to converge to the asymptotic one. (b) Distribution of EPs divided by the Hamming distance d_{st} between a source (s) and a target (t) for each pathway, that is, $\Delta S/d_{st}$. The system sizes are the same as those in (a). The data for the different system sizes collapse onto a single curve.

V. ASYMPTOTE OF THE EP DISTRIBUTION

To determine the functional form of the asymptote of the EP distribution, we follow the Fisher and Tippett method for EV analysis [26]. We consider the dataset composed of $N_e \equiv N(N-1)$ EPs obtained from all the shortest pathways between every pair of nodes of a given network such as the BA model, for instance. Next, we select ℓ elements randomly from among N_e elements and construct a set. Repeating this construction m times, we set up m sets of size ℓ. Let us consider a distribution

$H(\{y_i\})$ of the largest elements of each set $i = 1, \ldots, m$, which is denoted as y_i. Then the largest value among $\{y_i\}$ $(i = 1, \cdots, m)$ is the largest value of those ℓm elements selected randomly from N_e, where the elements are not necessarily distinct. To quantify this, we consider the accumulated distribution of $P(\Delta S)$, i.e., $F(x) = \text{Prob}\{\Delta S \le x\}$, that is, $F(x) = \int_{-\infty}^{x} d\Delta S P(\Delta S)$. The probability that the largest value y_i of a set i of size ℓ is less than x is given as $F^\ell(x)$. Next, the probability that the largest value among those ℓm elements is less than x is given as $F^{\ell m}(x)$. If there is an asymptote for large ℓ, $F^\ell(x)$ and $F^{\ell m}(x)$ would have the same functional form. On the other hand, we recall the extreme value theory. Let us define an asymptote $G(z)$ as

$$G(z) \equiv \text{Prob}\left\{\frac{M_\ell - \beta_\ell}{\alpha_\ell} \le z\right\}, \tag{5}$$

where M_ℓ is a random variable representing the maximum value from a set of size ℓ. α_ℓ and β_ℓ are appropriate sequences of ℓ to make the maximum value M_ℓ bounded for general ℓ. Then it is known that $G(z)$ satisfies the following stability postulate [21]:

$$G^n(z) = G(a_n z + b_n). \tag{6}$$

Using this postulate, we find the relation between $F^\ell(x)$ and $F^{\ell m}(x)$: Because the stability postulate is the ideal case as $\ell \to \infty$ limit, we try to find a finite ℓ such that the following relation holds.

$$\{F^\ell(x)\}^m = F^\ell(a_m x + b_m). \tag{7}$$

We find empirically that for $\ell = 1000$, $a_m = 1$ as shown in Fig. 5(a), in which the guide curves (dashed curves) shift in parallel for different ms. Next, we find $b_m \approx -0.42 \ln m$ as shown in the inset of Fig 5(b). Thus, we write $b_m \approx c \ln m$ for large m with $c = -0.42$. These imply that $\alpha_\ell = 1$ and $\beta_\ell \sim \ln \ell$ in Eq. (**??**). Because of Eq. (**??**), $F^\ell(x) = G(x - \beta_\ell)$.

We determine the logarithm of $G(x)$ as

$$-\ln G(x) = e^{-\frac{1}{c}(x-u)}, \tag{8}$$

where u is measured to be $u \approx 1.49$. The distribution $G(x)$ is known as the Gumbel distribution in the EV theory.

The functional form of $G(x)$ enables us to derive the EP distribution using the relation,

$$P(\Delta S) = \frac{dF^\ell(x)}{dx} \frac{1}{\ell F^{\ell-1}(x)}\Big|_{x=\Delta S}, \tag{9}$$

leading to

$$P(x) = \frac{e^{-\frac{1}{c}(x-u)}}{ce^{e^{-\frac{1}{c}(x-u)}}} \xrightarrow{x=\Delta S \to \infty} \frac{1}{c} e^{-\frac{1}{c}\Delta S}. \tag{10}$$

We emphasize that this functional form was obtained using $F^\ell(x)$ in the large-ℓ limit.

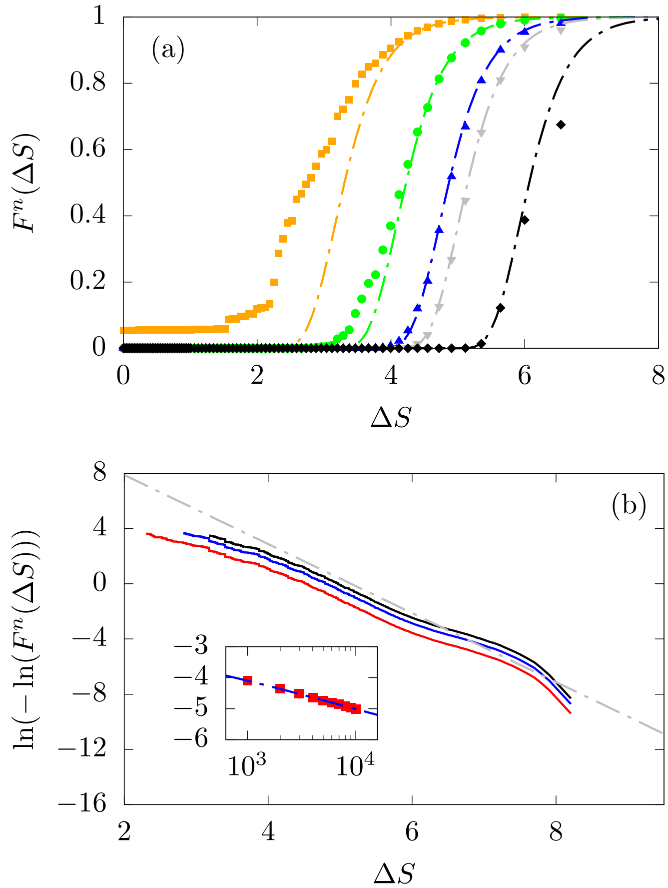

FIG. 5. (a) Test of the Gumbel distribution for the ℓ-th power of the accumulated EP distribution, $F^\ell(\Delta S)$, for BA model networks of size $N/10 = 2^{11}$. Dot-dashed curves represent $F^\ell(a_m \Delta S + b_m)$ with $\ell = 1000$, $a_m = 1$, and $b_m \approx \ln m$. The m values are taken to make $n(=\ell m) = 10^2, 10^3, 5 \times 10^3, 10^4$, and 10^5 from left to right. Data points (symbols) are obtained by exact enumeration. One can see that for $n = 10^3 - 10^5$, dashed curves seem to be fit to the data points. (b) Plot of $\ln(-\ln(F^{\ell m}(\Delta S)))$ versus ΔS to test $a_m \Delta S + b_m$ for $\ell = 10^3$ and $m = 3$, 6, and 9. Parallel alignment of data points for different ms to the straight dash-dotted line implies $a_m = 1$. Inset: Plot of b_m versus $10^3 \cdot m$ on semilogarithmic scale.

We remark that this EP distribution function is different from the recently derived work distribution function, $P(W) \propto \exp(-W)/\sqrt{W}$, in their functional forms [27, 28].

VI. SUMMARY

In this paper, we considered the EP distribution arising from the complexity of the shortest pathways from one node to another on complex networks. We showed that this EP distribution satisfies well-known FTs, i.e., the integral FT and detailed FT. To obtain the result, we considered a data packet transport problem in which a packet travels back and forth between every pair of nodes along the shortest pathways. At a branching node along the way, a packet chooses one branch randomly. The effect of this random choice is similar to that of the stochastic noise in the Langevin equation. Owing to the complexity of the shortest pathways, the probabilities of taking a shortest pathway in the forward and backward directions are different, resulting in a nonzero EP. We calculated this difference explicitly and determined the functional form in the large-EP limit. This work is helpful for understanding the origin of the EP arising in the Langevin dynamics with stochastic processes.

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