

Information Thermodynamics on Causal Networks

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We study nonequilibrium thermodynamics of complex information flows induced by interactions between multiple fluctuating systems. Characterizing nonequilibrium dynamics by causal networks (i.e., Bayesian networks), we obtain novel generalizations of the second law of thermodynamics and the fluctuation theorem, which include an informational quantity characterized by the topology of the causal network. Our result implies that the entropy production in a single system in the presence of multiple other systems is bounded by the information flow between these systems. We demonstrate our general result by a simple model of biochemical adaptation.

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Introduction.—Nonequilibrium equalities for small thermodynamic systems such as molecular motors have been intensively investigated in the last two decades [1,2]. The second law of thermodynamics can be derived from the Jarzynski equality [3] and the fluctuation theorems (FTs) [4–8]. The second law is expressed in terms of the ensemble average of the entropy production σ ,

$$\langle \sigma \rangle \geq 0, \quad (1)$$

where $\langle \dots \rangle$ describes the ensemble average. We note that σ reduces to the difference in the free-energy change ΔF and the work W performed on the system such that $\sigma = \beta(W - \Delta F)$, when the system is attached to a single heat bath with inverse temperature β , and the initial and final states are in thermal equilibrium.

On the other hand, in the presence of feedback control by Maxwell’s demon [9–11], the second law seems to be violated; i.e., $\langle \sigma \rangle$ can be negative. For such cases, the second law has been generalized as

$$\langle \sigma \rangle \geq \langle \Delta I \rangle, \quad (2)$$

where $\langle \Delta I \rangle$ is the mutual information that is exchanged between the system and the demon [12,13]. Such a Maxwell’s demon has been experimentally demonstrated with a colloidal particle [14]. While the relationship between information and thermodynamics has been studied in several simple setups with the demon [15–53], the general theory has been elusive for more complex cases in which multiple systems exchange information many times.

In this Letter, we derive a novel nonequilibrium equality in the presence of complex information flows between multiple stochastic systems. Our result involves a new informational term that is characterized by the topology of the causal structure of the dynamics. The informational quantity consists of the initial correlation between the target system and other systems, the information transfer from the system to others during the dynamics, and the final correlation between them. Our result can reproduce

inequality (2) for special cases. In order to describe nonequilibrium dynamics of multiple systems, we use Bayesian networks (BNs) [54] that topologically represent the causal structure of the dynamics.

Our theory is applicable to quite a broad class of non-equilibrium dynamics such as an information transfer between multiple Brownian particles and information processing in autonomous nanomachines. We illustrate our result by a chemical model of biological adaptation with time-delayed feedback. Our result implies that information processing plays a crucial role in biochemical reactions.

Bayesian networks.—First, we briefly discuss the basic concepts of BNs [see also Fig. 1(a)]. Let $\mathcal{A} = \{a_j | j = 1, 2, \dots, N_{\mathcal{A}}\}$ be the set of random variables that are associated with the nodes of a BN, where $N_{\mathcal{A}}$ is the number of the nodes. When an edge $a_{j'} \rightarrow a_j$ exists, there is a causal relationship from $a_{j'}$ to a_j , where we say that $a_{j'}$ is a parent of a_j . We denote by $\text{pa}(a_j)$ the set of parents of a_j . Here, the order of a_1, a_2, \dots is determined by the causal relationship in the BN such that a_j cannot be a parent of $a_{j'}$ if $j' < j$. This order is referred to as the topological ordering. We characterize stochastic dynamics in the BN by the conditional probability $p(a_j | a_{j-1}, \dots, a_1) = p(a_j | \text{pa}(a_j))$

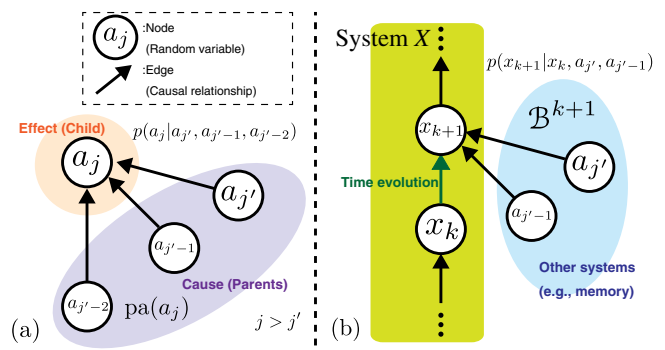


FIG. 1 (color online). (a) Schematic of a BN. (b) Stochastic dynamics of system X under the influence of other systems.

that describes the probability of a_j under the condition of a particular realization of $\text{pa}(a_j)$. We write $p(a_j|\emptyset) = p(a_j)$, where \emptyset is the empty set. Because of the chain rule in the probability theory, we obtain the joint probability distribution of the all random variables [54],

$$p(\mathcal{A}) = \prod_{j=1}^{N_{\mathcal{A}}} p(a_j|\text{pa}(a_j)). \quad (3)$$

The ensemble average of the arbitrary function $g(\mathcal{A})$ is defined as $\langle g \rangle \equiv \sum_{\mathcal{A}} p(\mathcal{A})g(\mathcal{A})$.

We next describe how we use BNs to describe stochastic dynamics [see also Fig. 1(b)]. We consider a situation in which system X interacts with other systems. The probability distribution of all the systems for the entire process is given by Eq. (3), where a_j corresponds to a state of a system at a particular time. \mathcal{A} consists of all states in the time evolution of both system X and other systems.

We also use the notation X to describe the time evolution of system X ; we write $X \equiv \{x_k | k = 1, 2, \dots, N\} (\subseteq \mathcal{A})$, where x_k is the state of system X at time k , and \subseteq is the symbol of the subset. We assume that x_k is a parent of x_{k+1} . We also assume that x_k cannot be a parent of $x_{k'}$ for $k' \neq k + 1$. We note that the time evolution of X is characterized by the chain $x_1 \rightarrow x_2 \rightarrow \dots \rightarrow x_N$.

For instance, Fig. 2(a) shows an expansion of a single-molecule gas, which can be described by the BN shown in Fig. 2(b). This BN shows the time evolution such that $p(x_1, x_2) = p(x_2|x_1)p(x_1)$, where x_1 and x_2 , respectively, describe the initial and final positions of the particle. In Fig. 2(c), we illustrate the Szilard engine [10] that is a standard model of Maxwell's demon. Figure 2(d) shows the corresponding BN, where m_1 describes a memory state that is correlated with x_1 . This BN shows the time evolution of the total system $p(x_1, x_2, m_1) = p(x_2|x_1, m_1)p(m_1|x_1)p(x_1)$.

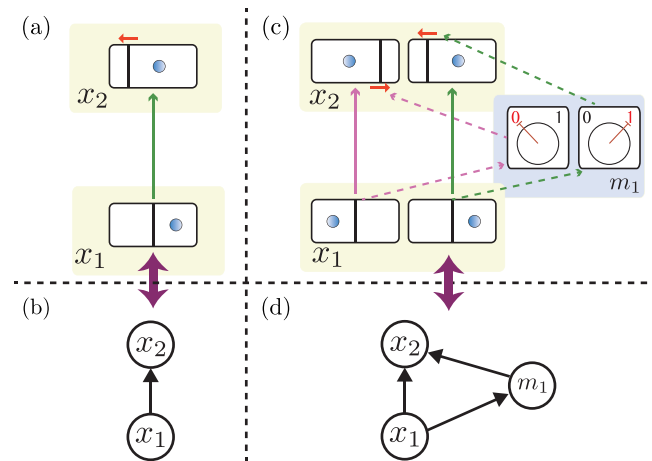


FIG. 2 (color online). (a) Time evolution of a single-molecule gas without feedback control. (b) BN corresponding to (a). (c) The Szilard engine with feedback control by a memory device. (d) BN corresponding to (c).

Entropy production and mutual information.—We introduce the entropy production in stochastic thermodynamics in terms of the BN. We assume that system X is coupled to heat baths with inverse temperatures β_α ($\alpha = 1, 2, \dots, n_{\text{bath}}$). Let Q_α be the heat absorbed by X from the α th bath. Because of the standard definition in stochastic thermodynamics [2], the entropy production in X is given by $\sigma \equiv \Delta s_{\text{bath}} + \ln p(x_1) - \ln p(x_N)$, where x_1 (x_N) is the initial (final) state of X and $\Delta s_{\text{bath}} \equiv -\sum_\alpha \beta_\alpha Q_\alpha$ is the entropy change in the baths. Let $\Delta s_{\text{bath}}^{k+1}$ be the entropy change in the baths from time k to $k + 1$ such that $\Delta s_{\text{bath}} = \sum_{k=1}^{N-1} \Delta s_{\text{bath}}^{k+1}$. In quite a broad class of nonequilibrium dynamics, including multidimensional Langevin dynamics (see the Supplemental Material [55]), $\Delta s_{\text{bath}}^{k+1}$ satisfies the detailed FT [7,8],

$$\Delta s_{\text{bath}}^{k+1} \equiv \ln \frac{p(x_{k+1}|x_k, \mathcal{B}^{k+1})}{p_B(x_k|x_{k+1}, \mathcal{B}^{k+1})}, \quad (4)$$

where \mathcal{B}^{k+1} is defined as $\mathcal{B}^{k+1} \equiv \text{pa}(x_{k+1}) \setminus \{x_k\}$ with \setminus indicating the relative complement of two sets. \mathcal{B}^{k+1} means the set of random variables which affect the time evolution of X from states x_k to x_{k+1} [see also Fig. 1(b)]. p_B describes the probability distribution of backward paths.

We next introduce mutual information that plays a crucial role in this study. Let \mathcal{A}_1 , \mathcal{A}_2 , and \mathcal{A}_3 be arbitrary sets of random variables. We define $I(\mathcal{A}_1:\mathcal{A}_2|\mathcal{A}_3) \equiv \ln p(\mathcal{A}_1, \mathcal{A}_2|\mathcal{A}_3) - \ln p(\mathcal{A}_1|\mathcal{A}_3) - \ln p(\mathcal{A}_2|\mathcal{A}_3)$, where we write $I(\mathcal{A}_1:\mathcal{A}_2|\mathcal{A}_3 = \emptyset) = I(\mathcal{A}_1:\mathcal{A}_2)$. Its ensemble average $\langle I(\mathcal{A}_1:\mathcal{A}_2|\mathcal{A}_3) \rangle$ is the mutual information between \mathcal{A}_1 and \mathcal{A}_2 under the condition of \mathcal{A}_3 .

Main result.—In order to discuss the main result, we introduce set $\mathcal{C} \equiv \{a_1, a_2, \dots, a_J\} \setminus X$, where a_J is chosen to satisfy $a_J = x_N$ [see also Fig. 3(a)]. Here, \mathcal{C} is the history of the other systems that can affect the final state x_N . We denote the elements of \mathcal{C} as $\mathcal{C} = \{c_l | l = 1, 2, \dots, N'\}$, where c_1, c_2, \dots are in the topological ordering.

We now state the main result of this Letter. In the foregoing setup, we have a new generalization of the integral fluctuation theorem (IFT),

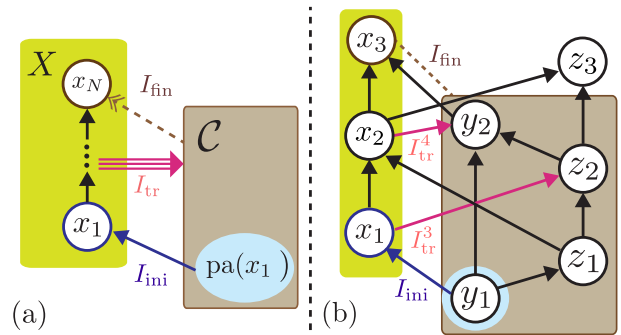


FIG. 3 (color online). (a) Schematic of \mathcal{C} and $\text{pa}(x_1)$. \mathcal{C} is the history of other systems that can affect the final state x_N . $\text{pa}(x_1)$ describes the variables correlated with the initial state x_1 . (b) An example of a BN that describes three-body interactions.

$$\langle \exp[-\sigma + \Theta] \rangle = 1. \quad (5)$$

Here, the key quantity Θ is the informational quantity characterized by the topology of the BN,

$$\Theta \equiv I_{\text{fin}} - I_{\text{ini}} - \sum_{l=1}^{N'} I_{\text{tr}}^l, \quad (6)$$

$$I_{\text{fin}} \equiv I(x_N; \mathcal{C}), \quad (7)$$

$$I_{\text{ini}} \equiv I(x_1; \text{pa}(x_1)), \quad (8)$$

$$I_{\text{tr}}^l \equiv I(c_l; \text{pa}_X(c_l) | \mathcal{C}_{l-1}), \quad (9)$$

where $\mathcal{C}_{l-1} \equiv \{c_{l'} | l' = 1, 2, \dots, l-1\}$ and $\text{pa}_X(a_j) \equiv \text{pa}(a_j) \cap X$, with \cap indicating the intersection. Here, I_{ini} characterizes the initial correlation between X and the other systems, while I_{fin} characterizes the final correlation that remains at the end of the dynamics. On the other hand, I_{tr}^l is the transfer entropy [56] that characterizes the information transfer into c_l from X during the dynamics (see the Supplemental Material [55]). For example, in the case of Fig. 3(b), we obtain $I_{\text{fin}} = I(x_3; \{y_1, z_1, z_2, y_2\})$, $I_{\text{ini}} = I(x_1; y_1)$, $I_{\text{tr}}^1 = I_{\text{tr}}^2 = 0$, $I_{\text{tr}}^3 = I(z_2; x_1 | y_1, z_1)$, and $I_{\text{tr}}^4 = I(y_2; x_2 | y_1, z_1, z_2)$. We will discuss the proof of Eq. (5) later.

By using the Jensen inequality for convex functions, i.e., $\langle \exp[g] \rangle \geq \exp[\langle g \rangle]$, we obtain

$$\langle \sigma \rangle \geq \langle I_{\text{fin}} \rangle - \langle I_{\text{ini}} \rangle - \sum_{l=1}^{N'} \langle I_{\text{tr}}^l \rangle, \quad (10)$$

which is a novel generalization of the second law of thermodynamics for subsystem X in the presence of complex information flows.

In the following, we illustrate that our main result (5) can reproduce known nonequilibrium relations for special cases in a unified way, and moreover, can lead to new generalizations of the IFT.

Example 1.—We consider the Markov chain shown in Fig. 4(a). We have $\mathcal{C} = \emptyset$ and $\text{pa}(x_1) = \emptyset$, and therefore $I_{\text{fin}} = 0$, $I_{\text{ini}} = 0$, and $\Theta = 0$. We then reproduce the conventional IFT, $\langle \exp[-\sigma] \rangle = 1$, which leads to inequality (1).

Example 2.—We next consider a system with feedback control shown in Fig. 4(b), where m_1 describes a state of the memory. State x_1 is measured by the memory, and the outcome m_1 is used for the feedback control. We have $\mathcal{C} = \{m_1\}$ and $\text{pa}(x_1) = \emptyset$, and therefore $I_{\text{fin}} = I(x_N; m_1)$, $I_{\text{ini}} = 0$, $I_{\text{tr}}^1 = I(x_1; m_1)$, and $\Theta = I(x_N; m_1) - I(x_1; m_1)$. We then reproduce a generalized IFT obtained in Ref. [13], $\langle \exp[-\sigma + \Delta I] \rangle = 1$, which leads to inequality (2). We note that in the case of the discrete repeated feedback, a previous result [24] can be derived from Eqs. (5) and (10) (see the Supplemental Material [55]).

Example 3.—We next consider the two-dimensional Langevin equation that describes an interaction between two Brownian particles,

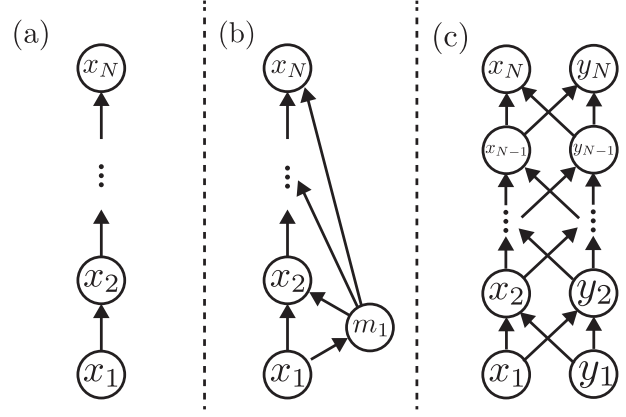


FIG. 4. (a) BN corresponding to a simple Markov chain. (b) BN corresponding to feedback control. (c) BN corresponding to two Brownian particles.

$$\gamma^x \frac{dx}{dt}(t) = f^x(x(t), y(t)) + \xi^x(t), \quad (11)$$

$$\gamma^y \frac{dy}{dt}(t) = f^y(x(t), y(t)) + \xi^y(t), \quad (12)$$

where t is time, γ^x and γ^y are friction coefficients, f^x and f^y are mechanical forces, and ξ^x and ξ^y are independent white-Gaussian noises with variances $2\gamma^x/\beta^x$ and $2\gamma^y/\beta^y$, respectively. Let Δt be an infinitesimal time interval. We discretize the dynamics as $x_k \equiv x(t = k\Delta t)$ and $y_k \equiv y(t = k\Delta t)$, and introduce the corresponding BN by Fig. 4(c), where system X corresponds to one particle with coordinate $x(t)$. We then have $\mathcal{C} = \{y_1, \dots, y_{N-1}\}$ and $\text{pa}(x_1) = \emptyset$, and therefore, $I_{\text{fin}} = I(x_N; \{y_1, \dots, y_{N-1}\})$, $I_{\text{ini}} = 0$, $I_{\text{tr}}^l = I(x_{l-1}; y_l | y_{l-1}, \dots, y_1)$, and $\Theta = I_{\text{fin}} - \sum_{l=1}^{N-1} I_{\text{tr}}^l$. We note that $\Delta s_{\text{bath}} = -\beta^x Q_x$, where Q_x is the heat absorbed by system X from the bath [57] (see the Supplemental Material for details [55]).

In this case, inequality (10) implies that the entropy production of one particle is bounded by the information flow into the other particle and the final correlation with it. As shown in the Supplemental Material [55], such a result is valid for multidimensional cases, in general, which enables us to characterize the entropy production in one particle that interacts with multiple particles in terms of information exchanges between them. We note that the entropy production in a single particle of a multidimensional Langevin system is closely related to experiments on the role of the hidden degrees of freedom [58,59].

Model of biological adaptation.—We next discuss an application of our general result to a biochemical system. The significance of information processing in biochemical networks has been presented, for example, in Refs. [60–62]. In particular, feedback control plays a key role in biological adaptations such as bacterial chemotaxis [63,64]. We show that the free-energy difference is bounded by an informational quantity in the presence of a

chemical feedback loop in a simple model of adaptation with the time-delay effect [65].

The model is characterized by a negative feedback loop between two systems: output system O and memory system M [see Fig. 5(a)]. We assume that each of O and M has a binary state described by 0 or 1. This model is described by the following master equations:

$$\frac{dp_0^X(t)}{dt} = -\omega_{0,1}^X(t)p_0^X(t) + \omega_{1,0}^X(t)p_1^X(t), \quad (13)$$

$$\frac{dp_1^X(t)}{dt} = -\omega_{1,0}^X(t)p_1^X(t) + \omega_{0,1}^X(t)p_0^X(t), \quad (14)$$

where $p_0^X(t)$ and $p_1^X(t)$ are, respectively, the probabilities of the states 0 and 1 with $X = O, M$ at time t . The transition rate $\omega_{\mu,\nu}^X$ ($\mu, \nu = 0, 1$) is assumed to be

$$\omega_{\mu,\nu}^X(t) = \frac{1}{\tau^X} \exp\{-\beta^X[\Delta_{\mu\nu}^X - F_{\mu}^X(t)]\}, \quad (15)$$

where τ^X is a time constant, β^X is the inverse temperature of a heat bath coupled to X , $F_{\mu}^X(t)$ is the effective free energy of the state μ at time t , $\Delta_{\mu\nu}^X$ is a barrier that satisfies $\Delta_{\mu\nu}^X = \Delta_{\nu\mu}^X$. This transition rate is well established in chemical reaction models [1].

Let o_k (m_k) be the state of O (M) at time $t = k\delta$ ($t = k\delta - \delta'$), where δ is the time interval with $\delta > \delta'$. The feedback loop between O and M is described by $F_{\mu}^M(t)$ [$F_{\mu}^O(t)$] that depends on o_k (m_k) [see also Fig. 5(c)]; we assume that $F_{\mu}^M(t)$ depends on o_k at time $k\delta - \delta' \leq t \leq (k+1)\delta - \delta'$, and that $F_{\mu}^O(t)$ depends on m_{k+1} and m_k at time $k\delta \leq t \leq (k+1)\delta$. The m_k dependence of $F_{\mu}^O(t)$ describes the effect of time-delayed feedback.

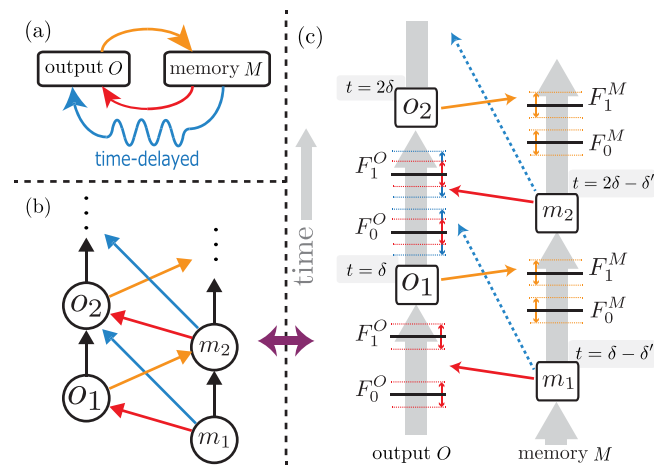


FIG. 5 (color online). (a) Feedback loop of a time-delayed chemical reaction model. (b) BN that describes our model. (c) The free-energy levels and the interactions between output O and memory M . For instance, $F_{\mu}^O(t)$ at time $\delta \leq t \leq 2\delta$ depends on m_1 and m_2 .

By applying Eqs. (7)–(10) to the BN in Fig. 5(b), we obtain two inequalities in the time evolution from $\{o_1, m_1\}$ to $\{o_2, m_2\}$,

$$\langle -\beta^M Q_M \rangle \geq \langle \ln p(o_1, m_2) \rangle - \langle \ln p(o_1, m_1) \rangle, \quad (16)$$

$$\langle -\beta^O Q_O \rangle \geq \langle \ln p(o_2, m_1, m_2) \rangle - \langle \ln p(o_1, m_1, m_2) \rangle, \quad (17)$$

where Q_X is equal to the effective free-energy difference in this system (see the Supplemental Material [55]). The right-hand sides of Eqs. (16) and (17) are the changes in the two-body and three-body Shannon entropies, respectively. This three-body Shannon entropy includes the states of different times m_1 and m_2 . This is a crucial difference between the conventional thermodynamics and our result. We numerically illustrate the validity of Eq. (17) in Fig. 6. We stress that these bounds are calculated from the probability distribution that can be experimentally measured in principle [60–62].

Derivation of the main result.—From the definition of Θ in Eqs. (6)–(9), we obtain

$$\begin{aligned} \Theta &= \ln \left(\frac{p(x_N, \mathcal{C})p(x_1)}{p(x_N)p(\mathcal{C})p(x_1|\text{pa}(x_1))} \prod_{l=1}^{N'} \frac{p(c_l|\mathcal{C}_{l-1})}{p(c_l|\text{pa}_X(c_l), \mathcal{C}_{l-1})} \right) \\ &= \ln \frac{p(x_1)p(x_N, \mathcal{C})}{p(x_N)p(x_1|\text{pa}(x_1)) \prod_{l=1}^{N'} p(c_l|\text{pa}(c_l))} \\ &= \ln \frac{p(x_1)p(x_N, \mathcal{C}) \prod_{k=2}^N p(x_k|\text{pa}(x_k))}{p(x_N)p(X, \mathcal{C})}. \end{aligned} \quad (18)$$

We then use mathematical properties of BNs [54], $p(c_l|\text{pa}_X(c_l), \mathcal{C}_{l-1}) = p(c_l|\text{pa}(c_l))$ and $p(X, \mathcal{C}) = \prod_{k=1}^N \prod_{l=1}^{N'} p(x_k|\text{pa}(x_k))p(c_l|\text{pa}(c_l))$ (see the Supplemental Material [55]). From Eqs. (3), (4), and (18), we arrive at the main result (5),

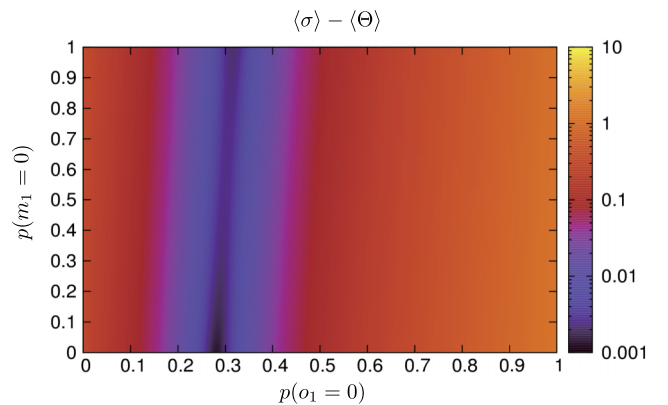


FIG. 6 (color online). Numerical illustration of the non-negativity of $\langle \sigma \rangle - \langle \Theta \rangle = \langle -\beta^O Q_O \rangle + \langle \ln p(o_1, m_1, m_2) \rangle - \langle \ln p(o_2, m_1, m_2) \rangle$. We set the initial states to $p(o_1, m_1) = p(o_1)p(m_1)$. The amount of $\langle \sigma \rangle - \langle \Theta \rangle$ is close to 0 when the initial states are close to the stationary state of this system. The parameter set is noted in the Supplemental Material [55].

$$\begin{aligned} \langle \exp[-\sigma + \Theta] \rangle &= \sum_{\mathcal{A}} p(\mathcal{D}|\mathcal{C}, X) \prod_{k=2}^N p_B(x_{k-1}|x_k, \mathcal{B}^k) p(x_N, \mathcal{C}) \\ &= 1, \end{aligned} \quad (19)$$

where $\mathcal{D} \equiv \mathcal{A} \setminus (\mathcal{C} \cup X)$. Here, we used $\mathcal{B}^k \subseteq \mathcal{C}$ ($k = 2, \dots, N$) and the normalization of the probability.

Conclusion.—In general causal networks, we have derived a novel generalization of the IFT [Eq. (5)]. We have obtained a generalized second law of thermodynamics (10), which sets a fundamental bound on the entropy production of a single system in the presence of multiple other systems, where the exchanged information between these systems plays a crucial role.

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