Information Thermodynamics on Causal Networks

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(Dated: October 10, 2013)

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 informatic 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.

Introduction. Nonequlibrium 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:

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

where $\langle \ldots \rangle$ 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

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

where $\langle \Delta I \rangle$ is the mutual information that is exchanged between the system and the demon [12, 13]. Such 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 [15–54], 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 informatic term that is characterized by the topology of the causal structure of the dynamics. The informatic 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
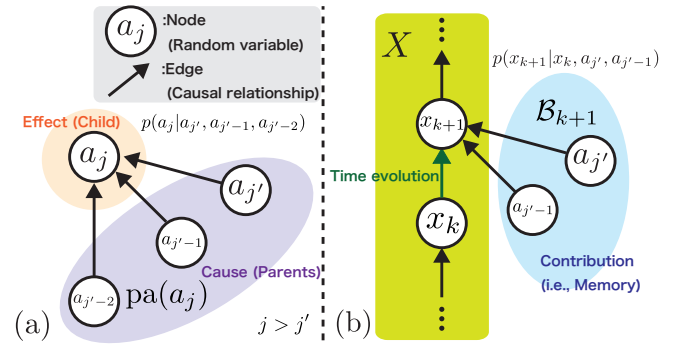

FIG. 1: (color online). (a) Schematic of general BN. (b) Stochastic dynamics of system X under the influence of other systems.

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) [55] that topologically represents the causal structure of the dynamics.

Our theory is applicable to quite a broad class of nonequilibrium 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 (BNs). First, we briefly discuss the basic concepts of BNs (see also Fig. 1 (a)). Let $\mathcal{A} = \{a_j | j = 1, 2, \ldots, N_{\mathcal{A}}\}$ 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 $\mathrm{pa}(a_j)$ the set of parents of a_j. Here, the order of $a_1, a_2, \cdots$ is determined by the causal relationship in BN such that
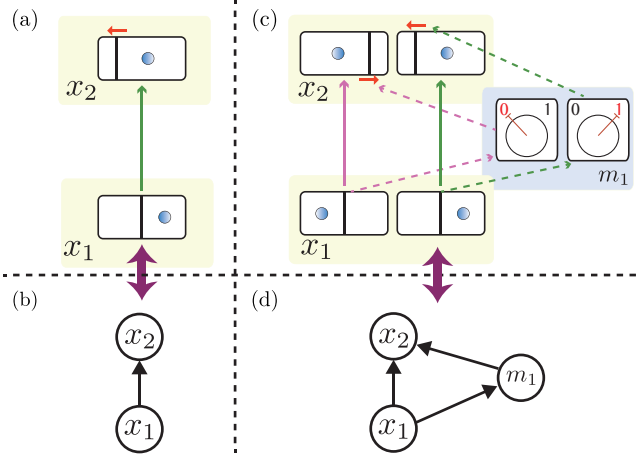
FIG. 2: (color online). (a) Time evolution of a single-molecule gas without feedback control. (b) BN corresponding to (a). (c) The Szilard engine with feedback control by a memory device. (d) BN corresponding to (c).

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 BN by conditional probability $p(a_j|a_{j-1}, \ldots, a_1) = p(a_j|\mathrm{pa}(a_j))$ that describes the probability of a_j under the condition of a particular realization of $\mathrm{pa}(a_j)$. We write $p(a_j|\emptyset) = p(a_j)$, where $\emptyset$ is the empty set. Due to the chain rule in the probability theory, we obtain the joint probability distribution of the all random variables [55]:

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

The ensemble average of 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 that system X interacts with other systems. The probability distribution of the all 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 use notation X to also describe the time evolution of system X; we write $X \equiv \{x_k|k = 1, 2, \ldots, N\}$ ($\subseteq \mathcal{A}$), 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 chain $x_1 \to x_2 \to \cdots \to x_N$.

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 $p(x_1, x_2, m_1) = p(x_2|x_1, m_1)p(m_1|x_1)p(x_1)$.

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 ($\alpha = 1, 2, \ldots, n_\alpha$). Let Q_α be the heat absorbed by X from the α-th bath. Due to the standard definition in stochastic thermodynamics [2], the entropy production in X is given by $\sigma \equiv \Delta s_{\mathrm{bath}} + \ln p(x_1) - \ln p(x_N)$, where x_1 (x_N) is the initial (final) state of X and $\Delta s_{\mathrm{bath}} \equiv -\sum_\alpha \beta_\alpha Q_\alpha$ is the entropy change in the baths. Let $\Delta s_{\mathrm{bath}}^{k+1}$ be the entropy change in the baths from time k to $k + 1$ such that $\Delta s_{\mathrm{bath}} = \sum_{k=1}^{N-1} \Delta s_{\mathrm{bath}}^{k+1}$. In quite a broad class of nonequilibrium dynamics including multidimensional Langevin dynamics (see Supplemental Material), $\Delta s_{\mathrm{bath}}^{k+1}$ satisfies the detailed FT [7, 8]:

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

where $\mathcal{B}^{k+1}$ is defined as $\mathcal{B}^{k+1} \equiv \mathrm{pa}(x_{k+1}) \setminus \{x_k\}$ 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 state 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 $I(\mathcal{A}_1 : \mathcal{A}_2|\mathcal{A}_3 = \emptyset) = I(\mathcal{A}_1 : \mathcal{A}_2)$. This 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 $\mathcal{C}$ such that $\mathcal{C} \equiv \{a_1, a_2, \cdots, a_J\} \setminus X$, where a_J is chosen to satisfy $a_J = x_N$ (see also Fig. 3 (a)). Here, $\mathcal{C}$ is a history of the other systems that can affect the final state x_N. We denote the elements of $\mathcal{C}$ as $\mathcal{C} = \{c_l|l = 1, 2, \ldots, N'\}$, where $c_1, c_2, \cdots$ 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 FT (IFT):

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

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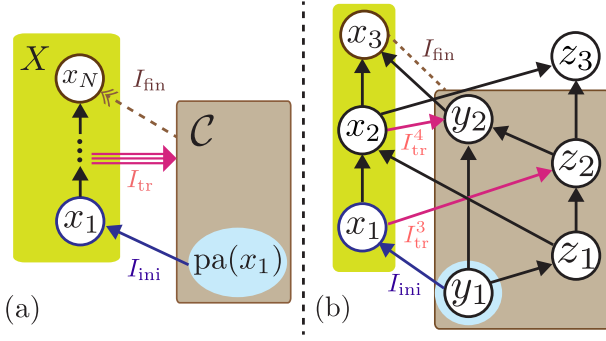
FIG. 3: (color online). (a) Schematic of $\mathcal{C}$ and $\mathrm{pa}(x_1)$. $\mathcal{C}$ is a history of other systems that can affect the final state x_N. $\mathrm{pa}(x_1)$ is the variables correlated with the initial state x_1. (b) An example of BN that describes three-body interactions.
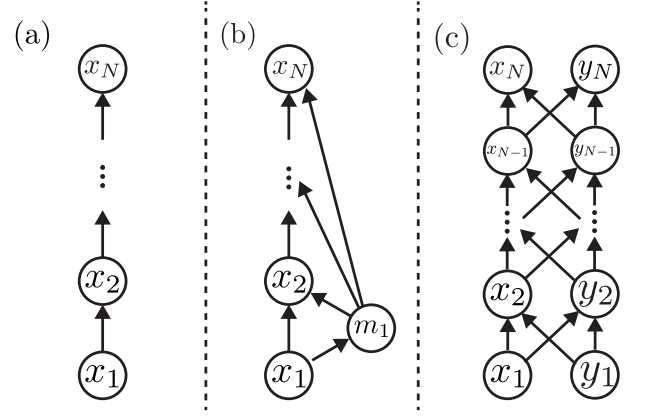

FIG. 4: (a) BN corresponding to a simple Markov chain. (b) BN corresponding to feedback control. (c) BN corresponding to two Brownian particles.

acterized by the topology of the BN:

$$\Theta \equiv I_{\mathrm{fin}} - I_{\mathrm{ini}} - \sum_{l=1}^{N'} I_{\mathrm{tr}}^l, \tag{6}$$

$$I_{\mathrm{fin}} \equiv I(x_N : \mathcal{C}), \tag{7}$$

$$I_{\mathrm{ini}} \equiv I(x_1 : \mathrm{pa}(x_1)), \tag{8}$$

$$I_{\mathrm{tr}}^l \equiv I(c_l : \mathrm{pa}_X(c_l) | \mathcal{C}_{l-1}), \tag{9}$$

where $\mathcal{C}_{l-1} \equiv \{c_{l'} | l' = 1, 2, \ldots, l-1\}$ and $\mathrm{pa}_X(a_j) \equiv \mathrm{pa}(a_j) \cap X$ 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 Supplemental Material). For example, in the case of Fig. 3 (b), we obtain $I_{\mathrm{fin}} = I(x_3 : \{y_1, z_1, z_2, y_2\})$, $I_{\mathrm{ini}} = I(x_1 : y_1)$, $I_{\mathrm{tr}}^1 = I_{\mathrm{tr}}^2 = 0$, $I_{\mathrm{tr}}^3 = I(z_2 : x_1 | y_1, z_1)$ and $I_{\mathrm{tr}}^4 = I(y_2 : x_2 | y_1, z_1, z_2)$. 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

$$\langle \sigma \rangle \geq \langle I_{\mathrm{fin}} \rangle - \langle I_{\mathrm{ini}} \rangle - \sum_{l=1}^{N'} \langle I_{\mathrm{tr}}^l \rangle, \tag{10}$$

which is a novel generalization of the second law of thermodynamics for the 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 (a). We consider the Markov chain shown in Fig. 4 (a). We have $\mathcal{C} = \emptyset$ and $\mathrm{pa}(x_1) = \emptyset$, and therefore $I_{\mathrm{fin}} = 0$, $I_{\mathrm{ini}} = 0$, and $\Theta = 0$. We then reproduce the conventional IFT: $\langle \exp[-\sigma] \rangle = 1$, which leads to inequality (1).

Example (b). 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 $\mathrm{pa}(x_1) = \emptyset$, and therefore $I_{\mathrm{fin}} = I(x_N : m_1)$, $I_{\mathrm{ini}} = 0$, $I_{\mathrm{tr}}^1 = I(x_1 : m_1)$, 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 Supplemental Material).

Example (c). We next consider the two-dimensional Langevin equation that describes an interaction between two Brownian particles:

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

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

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 a small 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 $\mathcal{C} = \{y_1, \ldots, y_{N-1}\}$ and $\mathrm{pa}(x_1) = \emptyset$, and therefore $I_{\mathrm{fin}} = I(x_N : \{y_1, \ldots, y_{N-1}\})$, $I_{\mathrm{ini}} = 0$, $I_{\mathrm{tr}}^l = I(x_{l-1} : y_l | y_{l-1}, \ldots, y_1)$, and $\Theta = I_{\mathrm{fin}} - \sum_{l=1}^{N-1} I_{\mathrm{tr}}^l$. We note that $\Delta s_{\mathrm{bath}} = -\beta^x Q_x$, where Q_x is the heat absorbed by system X from the bath [57] (see Supplemental Material for details).

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 Supplemental Material, such a result is valid for multidimensional cases in general, which
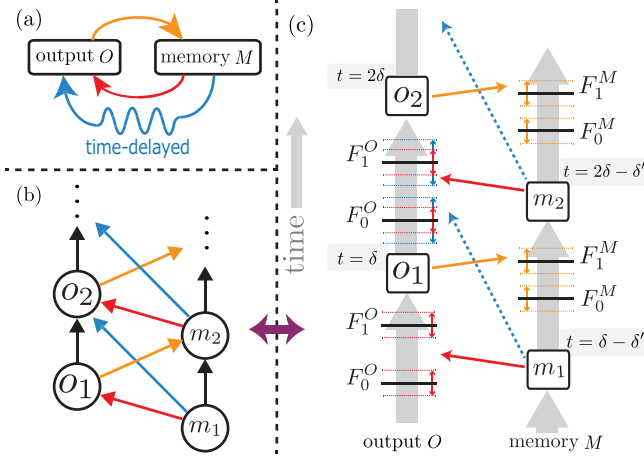
FIG. 5: (color online). (a) Feedback loop of a time-delayed chemical reaction model. (b) BN that describes our model. (c) The free energy levels and the interactions between output O and memory M. For instance, $F_\mu^O(t)$ at time $\delta \leq t \leq 2\delta$ depends on m_1 and m_2.

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 value 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 Supplemental Material.

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 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 informatic 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 driven by the following master equation:

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

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

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

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

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
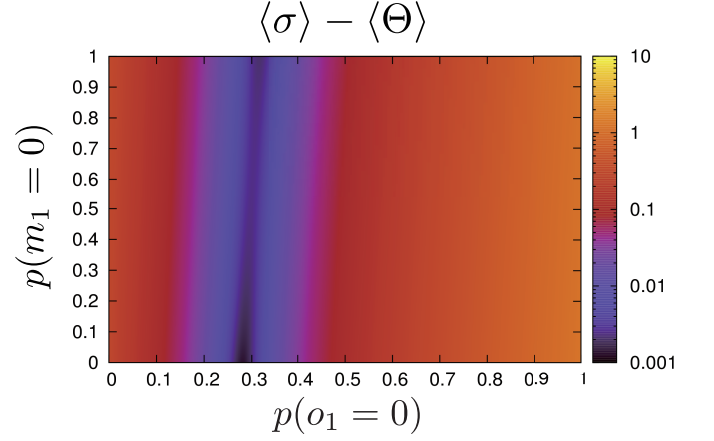
free-energy of the state μ at time t, $\Delta_{\mu\nu}^X$ is a barrier that satisfies $\Delta_{\mu\nu}^X = \Delta_{\nu\mu}^X$. This transition rate is well-established in chemical reaction models [1].

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 $k\delta \leq t \leq (k+1)\delta$. m_k-dependence of $F_\mu^O(t)$ describes the effect of time-delayed feedback.

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 Supplemental Material). The right hand sides on Eq. (16) and Eq. (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

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

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

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

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

Conclusion. In general causal networks, we have derived a novel generalization of 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.

SUPPLEMENTARY INFORMATION

A: Detailed properties of Bayesian networks

Let $\mathcal{A} = \{a_j|j = 1,2,\ldots,N_{\mathcal{A}}\}$ be the set of random variables on a BN, where $a_1, a_2,\ldots$ is in the topological ordering. The conditional probability is given by $p(a_j|a_{j-1},\ldots,a_1) = p(a_j|\mathrm{pa}(a_j))$, where $\mathrm{pa}(a_j)\subseteq\{a_1,a_2,\ldots,a_{j-1}\}$ is the set of parents of a_j. In this section, we prove two theorems [55] that has been used in the derivation of the main result in the main manuscript.

Theorem 1 (The chain rule for Bayesian networks). *For any index j, we have*

$$
p(a_j,a_{j-1},\ldots,a_1) = \prod_{j'=1}^{j}p(a_{j'}|\mathrm{pa}(a_{j'})). \tag{20}
$$

Proof.

$$
\begin{aligned}
p(a_j,a_{j-1},\ldots,a_1) &= p(a_j|a_{j-1},\ldots,a_1)p(a_{j-1},\ldots,a_1) \\
&= p(a_j|a_{j-1},\ldots,a_1)p(a_{j-1}|a_{j-2},\ldots,a_1)p(a_{j-2},\ldots,a_1) \\
&= \cdots \\
&= \prod_{j'=1}^{j}p(a_{j'}|a_{j'-1},\ldots,a_1) \\
&= \prod_{j'=1}^{j}p(a_{j'}|\mathrm{pa}(a_{j'})).\square
\end{aligned} \tag{21}
$$

In the derivation of the main result, we used this theorem as $p(X,\mathcal{C}) = \prod_{k=1}^{N}\prod_{l=1}^{N'}p(x_k|\mathrm{pa}(x_k))p(c_l|\mathrm{pa}(c_l))$, because $\mathcal{C}\cup X = \{c_1,c_2,\ldots,c_{N'},x_1,x_2,\ldots,x_N\} = \{a_1,a_2,\ldots,a_J\}$, where a_J is chosen to satisfy $a_J = x_N$.

Theorem 2 (Consistency of the specification of BN). *If $\mathcal{A}'$ is a subset of $\{a_{j-1},a_{j-2},\ldots,a_1\}$ and $\mathrm{pa}(a_j)$ is a subset of $\mathcal{A}'$ ($\mathrm{pa}(a_j)\subseteq\mathcal{A}'\subseteq\{a_{j-1},a_{j-2},\ldots,a_1\}$), we have*

$$
p(a_j|\mathcal{A}') = p(a_j|\mathrm{pa}(a_j)). \tag{22}
$$

Proof.

$$p(a_j|\mathcal{A}') = \frac{p(a_j, \mathcal{A}')}{p(\mathcal{A}')}$$

$$= \frac{\sum_{\{a_j, a_{j-1}, \ldots, a_1\} \setminus \{a_j, \mathcal{A}'\}} p(a_j, a_{j-1}, \ldots, a_1)}{\sum_{\{a_j, a_{j-1}, \ldots, a_1\} \setminus \{\mathcal{A}'\}} p(a_j, a_{j-1}, \ldots, a_1)}$$

$$= \frac{\sum_{\{a_j, a_{j-1}, \ldots, a_1\} \setminus \{a_j, \mathcal{A}'\}} \prod_{j'=1}^{j} p(a_{j'}|\mathrm{pa}(a_{j'}))}{\sum_{\{a_{j-1}, \ldots, a_1\} \setminus \{\mathcal{A}'\}} p(a_{j-1}, a_{j-2}, \ldots, a_1)}$$

$$= p(a_j|\mathrm{pa}(a_j)) \frac{\sum_{\{a_{j-1}, \ldots, a_1\} \setminus \{\mathcal{A}'\}} \prod_{j'=1}^{j-1} p(a_{j'}|\mathrm{pa}(a_{j'}))}{\sum_{\{a_{j-1}, \ldots, a_1\} \setminus \{\mathcal{A}'\}} p(a_{j-1}, a_{j-2}, \ldots, a_1)}$$

$$= p(a_j|\mathrm{pa}(a_j)).\square \tag{23}$$

In the derivation of the main result, we used this theorem as $p(c_l|\mathrm{pa}_X(c_l), \mathcal{C}_{l-1}) = p(c_l|\mathrm{pa}(c_l))$, because $\mathrm{pa}(a_{J'}) \subseteq \{\mathrm{pa}_X(c_l), \mathcal{C}_{l-1}\} \subseteq \{a_{J'-1}, a_{J'-2}, \ldots, a_1\}$, where $a_{J'}$ is chosen to satisfy $a_{J'} = c_l$.

B: Physical meaning of the transfer entropy

In Ref. [56], Schreiber introduced the transfer entropy for stochastic dynamics with two variables $I = \{i_1, i_2, \ldots, i_n, \ldots\}$ and $J = \{j_1, j_2, \ldots, j_n, \ldots\}$, where i_n (j_n) denotes the state of the system I (J) at time n. The transfer entropy from J to I is defined by

$$T_{J \to I} \equiv \sum p(I, J) \ln \frac{p(i_{n+1}, j_n, j_{n-1}, \ldots, j_{n-l}|i_n, i_{n-1} \ldots, i_{n-k})}{p(i_{n+1}|i_n, i_{n-1} \ldots, i_{n-k}) p(j_n, j_{n-1}, \ldots, j_{n-l}|i_n, i_{n-1} \ldots, i_{n-k})}, \tag{24}$$

Here, $T_{I \to J}$ characterizes the information flow from I to J; in fact, $T_{I \to J}$ is given by the difference between the entropy rate in I and that under the condition of J:

$$T_{J \to I} \equiv \Delta s_{I|J} - \Delta s_I, \tag{25}$$

where the entropy rate in I and that under the condition of J, Δs_I and $\Delta s_{I|J}$, are defined as $\Delta s_I \equiv \sum p(I)[\ln p(i_{n+1}, i_n, i_{n-1} \ldots, i_{n-k}) - \ln p(i_n, i_{n-1} \ldots, i_{n-k})]$ and $\Delta s_{I|J} \equiv \sum p(I, J)[\ln p(i_{n+1}, i_n, i_{n-1} \ldots, i_{n-k}|j_n, j_{n-1}, \ldots, j_{n-l}) - \ln p(i_n, i_{n-1} \ldots, i_{n-k}|j_n, j_{n-1}, \ldots, j_{n-l})]$, respectively.

The quantity $\langle I_{\mathrm{tr}}^l \rangle$ in our main result is defined as

$$\langle I_{\mathrm{tr}}^l \rangle \equiv \sum_{\mathcal{C}, X} p(\mathcal{C}, X) \ln \frac{p(c_l, \mathrm{pa}_X(c_l)|c_{l-1}, \ldots, c_1)}{p(c_l|c_{l-1}, \ldots, c_1) p(\mathrm{pa}_X(c_l)|c_{l-1}, \ldots, c_1)}, \tag{26}$$

which equals the transfer entropy $T_{X \to \mathcal{C}}$.

C: Multidimensional Langevin systems

We consider the following multidimensional over-damped Langevin equation:

$$\gamma^{(\mu')} \dot{x}^{(\mu')}(t) = f^{(\mu')}(x^{(1)}(t), \ldots, x^{(n')}(t)) + \xi^{(\mu')}(t), \tag{27}$$

$$\left\langle \xi^{(\mu')}(t) \xi^{(\nu')}(t') \right\rangle = 2\gamma^{(\mu')} k_B T^{(\mu')} \delta_{\mu'\nu'} \delta(t - t') \tag{28}$$

$$\left\langle \xi^{(\mu')}(t) \right\rangle = 0, \tag{29}$$

where $x^{(\mu')}$ ($\mu' = 1, \ldots, n'$) denotes a dynamical variable. With small time interval Δt, we discretize the dynamical variables as $x_k^{(\mu')} \equiv x^{(\mu')}(k\Delta t)$. We write $x_k^{(1)} \equiv x_k$. When $\boldsymbol{x}_k \equiv \{x_k^{(2)}, \ldots, x_k^{(n')}\}$ is fixed, we obtain the conditional
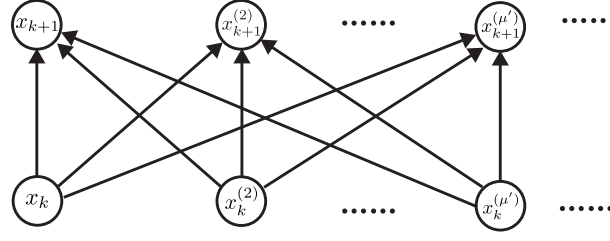
FIG. 7: BN corresponding to the multidimensional Langevin equation.

probability $p(x_{k+1}|x_k, \boldsymbol{x}_k)$ in terms of the Stratonovich product:

$$p(x_{k+1}|x_k, \boldsymbol{x}_k) = \mathcal{N} \exp\left[-\frac{\Delta t}{4\gamma^{(1)}k_B T^{(1)}}\left(\gamma^{(1)}\frac{\epsilon_k^{(1)}}{\Delta t} - f^{(1)}(\bar{x}_k^{(1)}, \boldsymbol{x}_k)\right)^2 - \frac{\Delta t}{2}\frac{\partial}{\partial x^{(1)}}f^{(1)}(\bar{x}_k^{(1)}, \boldsymbol{x}_k)\right], \quad (30)$$

where $\bar{x}_k^{(\mu')} \equiv (x_k^{(\mu')} + x_{k+1}^{(\mu')})/2$, $\epsilon_k^{(\mu')} \equiv x_{k+1}^{(\mu')} - x_k^{(\mu')}$, $f^{(1)}(\bar{x}_k, \boldsymbol{x}_k) \equiv f^{(1)}(\bar{x}_k, x_k^{(2)}, \ldots, x_k^{(n')})$, and $\mathcal{N}$ is the prefactor which does not depend on $f^{(\mu')}$ [66]. We stress that we use the mid-point rule only for $x^{(1)}$. We define the conditional probability of the backward process $p_B(x_k|x_{k+1}, \boldsymbol{x}_k)$ as

$$p_B(x_k|x_{k+1}, \boldsymbol{x}_k) = \mathcal{N} \exp\left[-\frac{\Delta t}{4\gamma^{(1)}k_B T^{(1)}}\left(-\gamma^{(1)}\frac{\epsilon_k^{(1)}}{\Delta t} - f^{(1)}(\bar{x}_k^{(1)}, \boldsymbol{x}_k)\right)^2 - \frac{\Delta t}{2}\frac{\partial}{\partial x^{(1)}}f^{(1)}(\bar{x}_k^{(1)}, \boldsymbol{x}_k)\right]. \quad (31)$$

Figure 7 shows the Bayesian network (BN) corresponding to the multidimensional Langevin equation [Eqs. (27), (28) and (29)] for the time interval between $k\Delta t$ and $(k+1)\Delta t$. Thus we have $\mathcal{B}^{k+1} = \boldsymbol{x}_k$. From Eqs. (30) and (31), we obtain $\Delta s_{\text{bath}}^{k+1}$:

$$\Delta s_{\text{bath}}^{k+1} = \ln \frac{p(x_{k+1}|x_k, \boldsymbol{x}_k)}{p_B(x_k|x_{k+1}, \boldsymbol{x}_k)} \quad (32)$$

$$= -\frac{1}{k_B T^{(1)}}f^{(1)}(\bar{x}_k^{(1)}, \boldsymbol{x}_k)\epsilon_k^{(1)}. \quad (33)$$

The definition of the heat flux in system $x^{(1)}$ by Sekimoto [57, 67] is given by $J^{(1)} \equiv f^{(1)}(\bar{x}_k^{(1)}, \bar{x}_k^{(2)}, \ldots, \bar{x}_k^{(n')})\epsilon_k^{(1)}$. We then compare $\Delta s_{\text{bath}}' \equiv -J^{(1)}/(k_B T^{(1)})$ with $\Delta s_{\text{bath}}^{k+1}$ as

$$\Delta s_{\text{bath}}' - \Delta s_{\text{bath}}^{k+1} = -\frac{1}{k_B T^{(1)}}\left[\sum_{\mu'=2}^{n'}\frac{\partial f^{(1)}}{\partial x^{(\mu')}}(\bar{x}_k^{(1)}, x_k^{(2)}, \ldots, x_k^{(\mu')}, \bar{x}_k^{(\mu'+1)}, \ldots, \bar{x}_k^{(n')})\epsilon_k^{(1)}\epsilon_k^{(\mu')}\right] \quad (34)$$

$$= o(\Delta t), \quad (35)$$

where we used $\epsilon_k^{(1)}\epsilon_k^{(\mu')} = o(\Delta t)$ with $\mu' \neq 1$ because of the independence of the noises [Eq. (28)]. Therefore, our definition of the entropy change in the heat baths on the BN (i.e., $\Delta s_{\text{bath}}^{k+1}$) is equivalent to the Sekimoto's definition (i.e., $\Delta s_{\text{bath}}'$) up to $o(\Delta t)$.

D: Repeated feedback control

We consider systems under repeated feedback control. Figure 8 shows the BN corresponding to the repeated feedback control discussed by Horowitz and Vaikuntanathan [24]. There are system X and memories $M^{(\mu')}$ with $\mu' = 1, \ldots, N'$ ($N' \leq N$). Measurements are performed on system X at time $T(\mu')$, where $T(\mu')$ is the natural number such as $1 = T(1) < T(2) < \cdots < T(N') < N$. The state of X at time $T(\mu')$ is given by $x_{T(\mu')}$, where the measurement outcome is stored in $m_1^{(\mu')}$. The states of X under feedback control can then depend on $m_1^{(\mu')}$ after time $T(\mu')$.
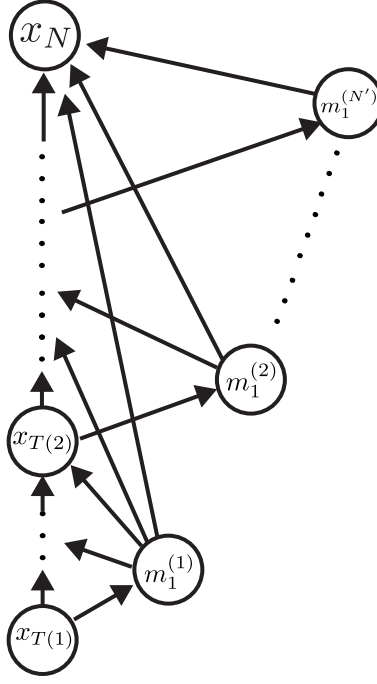
FIG. 8: BN corresponding to the repeated feedback control.

We have $\mathcal{C} = \{m_1^{(1)}, m_1^{(2)}, \ldots, m_1^{(N')}\}$ and $\mathrm{pa}(x_1) = \emptyset$, and therefore $I_{\mathrm{fin}} = I(x_N : \{m_1^{(1)}, \ldots, m_1^{(N')}\})$, $I_{\mathrm{ini}} = 0$, $I_{\mathrm{tr}}^l = I(x_{T(l)} : m_1^{(l)}|m_1^{(l-1)}, \ldots, m_1^{(1)})$, and

$$\Theta = I(x_N : \{m_1^{(1)}, \ldots, m_1^{(N')}\}) - \sum_{l=1}^{N'} I(x_{T(l)} : m_1^{(l)}|m_1^{(l-1)}, \ldots, m_1^{(1)}). \tag{36}$$

According to the main result, we obtain the following generalized Jarzynski equality:

$$\langle \exp[-\sigma + \Theta] \rangle = 1. \tag{37}$$

On the other hand, the equality derived by Horowitz and Vaikuntanathan [24] is given by

$$\left\langle \exp\left[-\beta W_d - \sum_{l=1}^{N'} I_{\mathrm{tr}}^l \right] \right\rangle = 1, \tag{38}$$

where I_{tr}^l is our definition of the transfer entropy that is given by $I_{\mathrm{tr}}^l = I(x_{T(l)} : m_1^{(l)}|m_1^{(l-1)}, \ldots, m_1^{(1)})$ and β is the inverse temperature of the heat bath. W_d is the dissipated work that is given by $\beta W_d \equiv \Delta s_{\mathrm{bath}} + \ln p_{\mathrm{eq}}(x_1) - \ln p_{\mathrm{eq}}(x_N|m_1^{(1)}, \ldots, m_1^{(N')})$, where p_{eq} is the canonical equilibrium distribution for fixed control parameter. βW_d is equivalent to $\sigma - I_{\mathrm{fin}}$ such that $\sigma - I_{\mathrm{fin}} = \Delta s_{\mathrm{bath}} + \ln p(x_1) - \ln p(x_N|m_1^{(1)}, \ldots, m_1^{(N')})$.

Therefore, our result can reproduce the result obtained by Horowitz and Vaikuntanathan in Ref. [24], when the initial and final states of the system are in thermal equilibrium.

E: Detailed calculations in the adaptation model

In the adaptation model in the main manuscript, we consider the following master equations:

$$\frac{dp_0^X}{dt}(t) = -\omega_{0,1}^X(F_0^X(t))p_0^X(t) + \omega_{1,0}^X(F_1^X(t))p_1^X(t), \tag{39}$$

$$\frac{dp_1^X}{dt}(t) = -\omega_{1,0}^X(F_1^X(t))p_1^X(t) + \omega_{0,1}^X(F_0^X(t))p_0^X(t). \tag{40}$$

where the transition rate is given by

$$\omega_{\mu,\nu}^X(F_\mu^X(t)) = \frac{1}{\tau^X} \exp\left[-\beta^X(\Delta_{\mu\nu}^X - F_\mu^X(t))\right]. \tag{41}$$

In the following, we show that $\Delta s_{\text{bath}}^{k+1}$ is equal to $-\beta^X \Delta F^X$.

We note that $p_0^X(t) + p_1^X(t) = 1$ holds because of the normalization of the probability distribution. We rewrite Eq. (39) as

$$\frac{dp_0^X}{dt}(t) = -[\omega_{0,1}^X(F_0^X(t)) + \omega_{1,0}^X(F_1^X(t))]p_0^X(t) + \omega_{1,0}^X(F_1^X(t)). \tag{42}$$

When F_0^X and F_1^X are constants, we get the solution of Eq. (42) as

$$p_0^X(t) = p_{0,\text{eq}}^X + (p_0^X(0) - p_{0,\text{eq}}^X)\exp\left[-(\omega_{0,1}^X(F_0^X) + \omega_{1,0}^X(F_1^X))t\right], \tag{43}$$

where $p_{0,\text{eq}}^X$ is defined as

$$p_{0,\text{eq}}^X(F_0^X, F_1^X) \equiv \frac{\omega_{1,0}^X(F_1^X)}{\omega_{0,1}^X(F_0^X) + \omega_{1,0}^X(F_1^X)} = \frac{\exp(-\beta^X F_0^X)}{\exp(-\beta^X F_0^X) + \exp(-\beta^X F_1^X)}. \tag{44}$$

The state of O (M) at time $t = k\delta$ ($t = k\delta - \delta'$) describes o_k (m_k) with $\delta > \delta'$. We set the interaction between the memory $X = M$ and the output system $X = O$ as follow. Let $F_\mu^M(t)$ at time $k\delta - \delta' \le t \le (k+1)\delta - \delta'$ be

$$F_\mu^M(t) = F_{\mu,j'} \quad (o_k = j'), \tag{45}$$

and let $F_\mu^O(t)$ at time $k\delta \le t \le (k+1)\delta$ be

$$F_\mu^O(t) = F_{\mu,j'k'}' \quad (m_k = j', m_{k+1} = k'), \tag{46}$$

where $j', k' = 0, 1$.

Substituting $p_0^M(0) = 0, 1$ into the solution of Eq. (43), we have the conditional probabilities $p(m_{k+1}|m_k, o_k)$:

$$p(m_{k+1} = 0|m_k = 0, o_k = j') = q_{j'} + (1 - q_{j'})\exp\left[-\omega_{j'}\delta\right], \tag{47}$$
$$p(m_{k+1} = 0|m_k = 1, o_k = j') = q_{j'} - q_{j'}\exp\left[-\omega_{j'}\delta\right], \tag{48}$$
$$p(m_{k+1} = 1|m_k = i', o_k = j') = 1 - p(m_{k+1} = 0|m_k = i', o_k = j'), \tag{49}$$

where $i' = 0, 1$, $q_{j'} \equiv p_{0,\text{eq}}^M(F_{0,j'}, F_{1,j'})$ and $\omega_{j'} \equiv \omega_{0,1}^M(F_{0,j'}) + \omega_{1,0}^M(F_{1,j'})$. Substituting $p_0^O(0) = 0, 1$ into Eq. (43), we also have the conditional probabilities $p(o_{k+1}|o_k, m_k, m_{k+1})$:

$$p(o_{k+1} = 0|o_k = 0, m_k = j', m_{k+1} = k') = q_{j'k'}' + \left(1 - q_{j'k'}'\right)\exp\left[-\omega_{j'k'}'\delta\right] \tag{50}$$
$$p(o_{k+1} = 0|o_k = 1, m_k = j', m_{k+1} = k') = q_{j'k'}' - q_{j'k'}'\exp\left[-\omega_{j'k'}'\delta\right] \tag{51}$$
$$p(o_{k+1} = 1|o_k = i', m_k = j', m_{k+1} = k') = 1 - p(o_{k+1} = 0|o_k = i', m_k = j', m_{k+1} = k'), \tag{52}$$

where $q_{j'k'}' \equiv p_{0,\text{eq}}^O(F_{0,j'k'}', F_{1,j'k'}')$ and $\omega_{j'k'}' \equiv \omega_{0,1}^O(F_{0,j'k'}') + \omega_{1,0}^O(F_{1,j'k'}')$.

We assume that the conditional probabilities of backward process $p_B(m_k|m_{k+1}, o_k)$ and $p_B(o_k|o_{k+1}, m_k, m_{k+1})$ are defined as $p_B(m_k = l'|m_{k+1} = i', o_k = j') \equiv p(m_{k+1} = l'|m_k = i', o_k = j')$ and $p_B(o_k = l'|o_{k+1} = i', m_k = j', m_{k+1} = k') \equiv p(o_{k+1} = l'|o_k = i', m_k = j', m_{k+1} = k')$ with $l' = 0, 1$, respectively.

From Eqs. (41), (47), (48) and (49), we have $\Delta s_{\text{bath}}^{k+1}$ with $X = M$:

$$\Delta s_{\text{bath}}^{k+1} = \ln\left[\frac{p(m_{k+1}|m_k, o_k)}{p_B(m_k|m_{k+1}, o_k)}\right] \tag{53}$$

$$= \begin{cases} 0 & (m_{k+1} = 0, m_k = 0, o_k = j')) \\ \ln q_{j'} - \ln(1 - q_{j'}) & (m_{k+1} = 0, m_k = 1, o_k = j') \\ \ln(1 - q_{j'}) - \ln q_{j'} & (m_{k+1} = 1, m_k = 0, o_k = j') \\ 0 & (m_{k+1} = 1, m_k = 1, o_k = j') \end{cases} \tag{54}$$

$$= -\beta^M(F_{l',j'} - F_{i',j'}) \quad (m_{k+1} = l', m_k = i', o_k = j'), \tag{55}$$

where $\mathcal{B}^{k+1} = \{o_k\}$. From Eqs. (41), (50), (51) and (52), we have $\Delta s_{\text{bath}}^{k+1}$ with $X = O$:

$$\Delta s_{\text{bath}}^{k+1} = \ln\left[\frac{p(o_{k+1}|o_k, m_k, m_{k+1})}{p_B(o_k|o_{k+1}, m_k, m_{k+1})}\right] \tag{56}$$

$$= \begin{cases} 0 & (o_{k+1} = 0, o_k = 0, m_k = j', m_{k+1} = k') \\ \ln q'_{j'k'} - \ln(1 - q'_{j'k'}) & (o_{k+1} = 0, o_k = 1, m_k = j', m_{k+1} = k') \\ \ln(1 - q'_{j'k'}) - \ln q'_{j'k'} & (o_{k+1} = 1, o_k = 0, m_k = j', m_{k+1} = k') \\ 0 & (o_{k+1} = 1, o_k = 1, m_k = j', m_{k+1} = k') \end{cases} \tag{57}$$

$$= -\beta^O(F'_{l', j'k'} - F'_{i', j'k'}) \quad (o_{k+1} = l', o_k = i', m_k = j', m_{k+1} = k'), \tag{58}$$

where $\mathcal{B}^{k+1} = \{m_k, m_{k+1}\}$, we reach the conclusion that $\Delta s_{\text{bath}}^{k+1}$ is given by the effective free-energy difference.

F: The parameter set of the numerical illustration in the adaptation model

We set the parameters of the numerical illustration in Fig. 5 of the main manuscript as follows: $\delta = 0.5$, $\beta^M = \beta^O = 0.01$, $\tau^O = \tau^M = 0.001$, $\Delta_{01}^M = \Delta_{01}^O = 100$, $F_{0,0} = F_{0,1} = 100$, $F_{1,0} = 10$, $F_{1,1} = 30$, $F'_{0,00} = F'_{0,01} = F'_{0,10} = F'_{0,11} = 100$, $F'_{1,00} = 30$, $F'_{1,01} = 20$, $F'_{1,10} = 10$ and $F'_{1,11} = 5$. In this case, we have $q'_{00} = 0.332$, $q'_{01} = 0.310$, $q'_{10} = 0.289$ and $q'_{11} = 0.278$. We note that the value of $\langle\sigma\rangle - \langle\Theta\rangle$ in Fig. 5 of the main manuscript is close to 0 when the initial states are close to the stationary distribution of the output system, which is similar to the probabilities q'_{00}, q'_{01}, q'_{10} and q'_{11}.

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