Information-geometric Legendre duality in stochastic thermodynamics

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We propose a new Legendre transformation on the space of probability distributions for stochastic thermodynamics, inspired by a Legendre duality in information geometry. It transforms between two convex functions, that is, the total entropy and a new thermodynamic potential for stochastic thermodynamics. Two coordinate systems associated with respective functions are a set of probabilities and a set of thermodynamic forces. Both convex functions are monotonically decreasing in time, serving as Lyapunov functions to describe the relaxation to equilibrium. While the monotonicity of total entropy means the second law of thermodynamics, that of the new thermodynamic potential provides a new complementary thermodynamic law. We illustrate the new potential, the coordinate system of thermodynamic forces, and the new thermodynamic law using a relaxation process of a three-state model and demonstrate that these introduced concepts provide a new insight into the process.

Legendre transformation on thermodynamic state space plays a crucial role in classical equilibrium thermodynamics [1, 2]. It provides various thermodynamic descriptions, each consisting of a coordinate system and a thermodynamic potential. While each of them conveys the complete information on the equilibrium-thermodynamic properties of the system, they admit different operations to specify thermodynamic states. This can be advantageous in a physical setting. For example, while specifying the states by the original coordinates, such as the entropy or the internal energy, can be operationally hard, specification by the temperature is realized by immersing the system in a heat bath. Moreover, such changes of description provide new theoretical perspectives. For example, the Helmholtz free energy serves as the primary quantity calculated in statistical mechanics.

The contemporary formulation of thermodynamics for stochastic process [3, 4], called stochastic thermodynamics [5–10], covers the far-from-equilibrium regime. It also discusses Legendre transformations in the definition of the free energy [11] and for the large deviation functions of thermodynamic quantities [12–23]. However, these Legendre transformations are mainly based on the expected values and do not produce a new thermodynamic description at the stochastic level with a new coordinate system of probability distributions.

A Legendre duality for probability distributions has been discussed in information geometry [24–28], namely the differential geometry for information theory. Based on informational quantities [29], geometry introduces a quadruplet of Legendre duality, consisting of two coordinate systems $\eta^G$, $\theta^G$, called dual coordinate systems, and two convex functions $\varphi^G(\eta^G)$, $\psi^G(\theta^G)$, called dual convex functions, on a space of probability distributions. Here, the pair $(\eta^G, \varphi^G(\eta^G))$ is a Legendre transform of $(\theta^G, \psi^G(\theta^G))$. On the other hand, connections between the informational quantities and stochastic-thermodynamic quantities have been established [5, 30–35], and information geometry as a differential geometry for stochastic thermodynamics [36–48] has been recently discussed in analogy with differential geometry for classical thermodynamics [49–52] and statistical mechanics [53–62]. The success of information-geometric approaches in stochastic thermodynamics might raise the question of whether the information-geometric Legendre duality can be naturally introduced to stochastic thermodynamics.

In this Letter, we construct a new quadruplet of Legendre duality $(\eta, \varphi(\eta), \theta, \psi(\theta))$ using stochastic-thermodynamic quantities on the space of probability distributions. This quadruplet is an affine transformation of the information-geometric quadruplet $(\eta^G, \varphi^G(\eta^G), \theta^G, \psi^G(\theta^G))$. The quadruplet gives two thermodynamic descriptions, mutually connected by a Legendre transformation. The first description with $(\eta, \varphi(\eta))$ is similar to the conventional description of stochastic thermodynamics, using probability distributions as the coordinates and the total entropy as the potential. The second description with $(\theta, \psi(\theta))$ is novel, using thermodynamic forces as the coordinates and a newly introduced potential. From an analogy with classical-thermodynamic transformations, the second description is also understood as designating the probability distribution by an external field needed to reproduce the distribution as an equilibrium, and the potential $\psi$ is the equilibrium free energy thereof. We also find that our dual convex functions $\varphi$, $\psi$ are Lyapunov functions of relaxation processes. This property for $\varphi$ reproduces the second law of thermodynamics, and that for $\psi$ provides a new bound of irreversibility complementary to the second law of thermodynamics. We demonstrate the two thermodynamic descriptions and the new bound using a time evolution of a three-state system. The second description captures a feature of the time trajectory unobtainable in the first description. We explain the feature using our new bound of irreversibility.

Setup.—Consider a physical system in contact with a single heat bath at a constant temperature $T$. The system stochastically jumps among $N + 1$ states $i = 0, 1, \ldots, N$ with energy $\epsilon_i$. We focus on the probability distribution $p(i) \equiv \langle p_i(t) \rangle_{i=0}^N$, where $p_i(t)$ denotes the probability to find the system in the $i$th state at time $t$. The equilibrium distri-
bution $p_{\text{eq}}$ is given by $p_{\text{eq}} \propto \exp(-\varepsilon/k_B T)$.

The time evolution obeys the master equation

$$d_t p_i(t) = \sum_{j \neq i} \left[ W_{ij} p_j(t) - W_{ji} p_i(t) \right],$$

where $d_t \equiv d/dt$ is the time derivative, and $W_{ij}$ is the transition rate from state $j$ to $i$ per unit time. We impose the detailed balance condition $W_{ij} p_{\text{eq}} = W_{ji} p_{\text{eq}}$ on the rates. We also assume their irreducibility, namely, that the system reaches from any state to any other either directly or via other states with a nonzero probability. These conditions ensure that, for any initial distributions at $t = 0$, the distribution satisfies $p_i(t) \neq 0$ for all $i$ at $t > 0$ and relaxes to the unique fixed point $p_{\text{eq}}$ as $t \to \infty$ [5].

We associate each state with the system entropy $S_{\text{sys}}(p) = -k_B \ln p_i$ based on probabilities and the bath entropy $S_{\text{bath}} = -\varepsilon_i/T + \text{const}$. Based on classical thermodynamics, as usual in stochastic thermodynamics [9]. Their sum gives the total entropy $\bar{S}(p)$ when the system is in the $i$th state,

$$\bar{S}(p) := S_{\text{sys}}(p) + S_{\text{bath}} = -k_B \ln p_i - \frac{\varepsilon_i}{T},$$

where $k_B$ is the Boltzmann constant. We set the $i$-independent constant in $S_{\text{bath}}$ to zero for simplicity. The average $\bar{S}(p) \equiv \sum_i p_i \bar{S}(p)$ is a concave function of $p$ and takes the maximum at $p_{\text{eq}}$. The time derivative $d_t \bar{S}$ gives the entropy production rate.

We can generalize all our results to incorporate internal entropy of the states [35] and exchange of particles with a single particle reservoir by replacing $\varepsilon_i$ with an appropriate state quantity. See Supplemental Material (SM) [63] for detail. SM also discusses generalization for systems without detailed balance [64, 65].

**Coordinate systems and Legendre duality.**—Following information geometry, we introduce the space consisting of the $(N+1)$-component nonzero probability distributions [24],

$$S_N := \left\{ p \in \mathbb{R}^{N+1}_{>0} \mid \sum_{i=0}^N p_i = 1 \right\}.$$  

We regard $S_N$ as the state space of stochastic thermodynamics in analogy with classical thermodynamics [Fig. 1(a)]. A moving point on $S_N$ expresses a time evolution of the distribution.

The potential $\bar{S}(p)$ and the $(N+1)$-component coordinate system $p \equiv (p_i)_{i=0}^N$ on $S_N$ constitute a thermodynamic description of stochastic thermodynamics. However, this coordinate system is redundant since the space is $N$-dimensional. We instead use redundancy-free $N$-component coordinate systems $\eta$ and $\theta$, inspired by information geometry.

We define the $\eta$-coordinates $\eta(p) \equiv (\eta_{\alpha}(p))_{\alpha=1}^N$ by a linear relation $p_i = p_{\text{eq}} + \sum_{\alpha} A_{\alpha}^i \eta_{\alpha}$. Here, $A \equiv (A_{\alpha}^i)_{\alpha=1}^N$ is an arbitrary $(N+1) \times N$ constant matrix of rank $N$ satisfying $\sum_{\alpha} A_{\alpha}^i \eta_{\alpha} = 0$ for all $\alpha$. The former condition ensures that $\eta$ spans the whole $S_N$, and the latter imposes the normalization of probabilities. The range of $\eta$ is an appropriate subset of $\mathbb{R}^N$ so that $\eta$ and $p \in S_N$ have a one-to-one correspondence, denoted by $\eta(p)$ and $p(\eta)$. Using the $\eta$-coordinates, we regard $\bar{S}(p)$ as a function of $\eta$, denoted by $\bar{S}(\eta) \equiv -\bar{S}(p(\eta))$. It is a strictly convex function of $\eta$ [Fig. 1(b)].

We perform the complete Legendre transformation of $\bar{S}(\eta)$ by $\eta$ to construct the $\theta$-coordinates $\theta(p) \equiv (\theta_{\alpha}(p))_{\alpha=1}^N$ and a new strictly convex potential function $\psi(\theta)$ [Fig. 1(c)]. We call the thermodynamic description with $(\theta, \psi(\theta))$ the dual description. The transformation and its inverse, together called the Legendre duality, are summarized as

$$\theta(\eta) = \frac{\partial \psi}{\partial \eta_\alpha}, \quad \eta_\alpha(\theta) = \frac{\partial \psi}{\partial \theta_\alpha},$$

$$\psi(p) = \eta(p) \cdot \theta(p) - \bar{S}(p),$$

where $\varphi(p) \equiv \varphi(\eta(p))$, $\psi(p) \equiv \psi(\theta(p))$, and $\eta \cdot \theta = \sum_{\alpha=1}^N \eta_\alpha \theta_\alpha$. The resulting quadruplet $(\eta, \varphi(\eta), \theta, \psi(\theta))$ reads

$$\eta_\alpha(p) = \sum_{i=0}^N (A_-)^{\alpha}_i (p_i - p_{\text{eq}}^i) \quad (\alpha = 1, \ldots, N),$$

$$\varphi(p) = -\bar{S}(p) = -\sum_{i=0}^N p_i \bar{S}(p),$$

$$\theta(\eta) = -\sum_{i=0}^N \bar{S}(p) A_{\alpha}^i \quad (\alpha = 1, \ldots, N),$$

$$\psi(\theta(p)) = \sum_{i=0}^N p_i \bar{S}(p).$$

Here, $A_- \equiv (A_-)^{\alpha}_i$ is a pseudo-inverse matrix of $A$, defined as a matrix satisfying $\sum_{\beta} A_{\beta}^\alpha (A_-)^{\beta}_j A_{\gamma}^j = 0$. 

![FIG. 1. Schematics of the main concepts [Eqs. (3) and (6)] illustrated for a three-state ($N = 2$) case. (a) The state space $S_2$, the $\eta$-coordinate system (blue), and the $\theta$-coordinate system (red). Contour lines are for $\eta_\alpha = 0.1 n$ and $\theta^\alpha = n$ $(\alpha = 1, 2; n = 0, \pm 1, \ldots)$ with bold lines representing $n = 0$. (b) The $\eta$-coordinate space and the corresponding potential $\varphi(\eta)$. They constitute a thermodynamic description of stochastic thermodynamics. (c) The $\theta$-coordinate space and the corresponding potential $\psi(\theta)$, constituting another thermodynamic description. They are the Legendre transformation of $(\varphi(\eta), \theta(\eta))$. The range of $\theta$ is the whole $\mathbb{R}^2$. Parameters: $\varepsilon^1 = \varepsilon^2 = \varepsilon$ and $A$ in Eq. (15).](image-url)
Although $A^-$ is not unique for a given $A$, the right-hand side of (6a) does not depend on its choice (see also SM for mathematical properties of $A^-$). The range of $\theta$ is the whole $\mathbb{R}^N$. A distribution with a zero entry, which we exclude from $S_N$, corresponds to $\theta^i = \infty$ or $\theta^i = -\infty$ for some $i$. The correspondence between $\theta \in \mathbb{R}^N$ and $p \in S_N$ is one-to-one, denoted by $\theta(p)$ and $p(\theta)$. This property is the consequence of the use of $N$-component coordinate systems rather than $(N+1)$-component ones (see also SM).

A different choice of $A$ leads to different coordinate systems while keeping $\varphi(p)$ and $\psi(p)$ unchanged as the functions of $p$. The new $\eta$-coordinate system is related to the old one by an invertible linear transformation, and so is the $\theta$-coordinate system. The difference is not essential in the scope of this Letter, and therefore one can choose an arbitrary $\bar{A}$ suitable for their purpose. One of the simplest choices is $A^{\alpha}_i = \delta_i^\alpha - \delta_i^0$ with $(A^-)_\alpha^i = \delta_i^\alpha$, where $\delta$ denotes the Kronecker delta. It leads to $\eta_\alpha(p) = p_\alpha - p^\alpha_\alpha$ and $\theta^\alpha(p) = -\bar{s}^\alpha(p) + \bar{s}^\alpha(p)$ for $\alpha = 1, \ldots, N$. We fix a choice of $\bar{A}$ and $A^-$ throughout the Letter.

The origins of both the coordinates correspond to the equilibriums:

$$\eta_\alpha(p^{eq}) = 0, \quad \theta^\alpha(p^{eq}) = 0.$$  \hspace{1cm} (7)

This follows from (6a), (6c), $\sum_i A^{\alpha}_i = 0$, and that $\bar{s}^\alpha(p^{eq})$ is independent of $i$. From the Legendre duality (4), Eq. (7) also implies that $\varphi$ and $\psi$ attain their minima at the equilibrium, which we write as $\varphi^{eq} \equiv \varphi(p^{eq})$ and $\psi^{eq} \equiv \psi(p^{eq})$. Due to Eq. (5), the minima satisfy $\varphi^{eq} = -\psi^{eq}$.

Relation to information geometry.—We discuss information-geometric understandings of the quadruplet (6) through the mathematical framework of dually flat geometry [27]. Generically, given a space equipped with a quadruplet of Legendre duality (such as (6)), one can construct a dually flat geometry on the space. We can do this for our state space $S_N$ and our quadruplet $(\eta, \varphi(\eta), \theta, \psi(\theta))$. On the other hand, information geometry equips the same state space $S_N$ with various quadruplets to obtain various dually flat geometries on $S_N$. Although the quadruplets in information geometry differ from ours, one of them, denoted by $(\eta^{\tilde{\eta}}, \varphi^{\tilde{\eta}}(\eta^{\tilde{\eta}}), \theta^{\tilde{\theta}}, \psi^{\tilde{\theta}}(\theta^{\tilde{\theta}}))$, is affine equivalent to ours up to a scale change by $k_8$. Since two affine equivalent quadruplets induce the same geometric structure, our quadruplet also designates the information-geometric structure on $S_N$ (see SM for details).

Due to the affine equivalence, we can express information-geometric quantities and notions using our quadruplet. For example, the Kullback–Leibler divergence between arbitrary two points $p, q \in S_N$, defined by $D_{KL}(p||q) = \sum_i p_i \ln(p_i/q_i)$ [27–29], is related to the quadruplet by $k_8 D_{KL}(p||q) = \varphi(p) + \psi(q) - \eta(p) \cdot \theta(q)$. In particular, setting either $p$ or $q$ to the equilibrium gives

$$\varphi(p) - \varphi^{eq} = k_8 D_{KL}(p||p^{eq}), \quad \psi(p) - \psi^{eq} = k_8 D_{KL}(p^{eq}||p),$$  \hspace{1cm} (8)

where we used (7) and $\varphi^{eq} = -\psi^{eq}$. These are information-geometric expressions of the potential functions.

Kullback–Leibler divergence has the contraction property [3, 8] under the time evolution (1). It states $d_i D_{KL}(p(t)||q(t)) \leq 0$ for arbitrary two points $p(t), q(t) \in S_N$ obeying the same master equation. The inequality is saturated only when $p(t) = q(t)$ if the transition rates are irreducible [63]. Consequently, we obtain

$$d_i \left[ \varphi(p) + \psi(q) - \eta(p) \cdot \theta(q) \right] < 0, \quad (p \neq q),$$  \hspace{1cm} (9)

where we omitted the time dependence $t$. Since $p^{eq}$ is the fixed point of the time evolution, we reach using (7) (see also SM)

$$d_i \varphi(p) < 0, \quad d_i \psi(p) < 0, \quad (p \neq p^{eq}).$$  \hspace{1cm} (10)

Eq. (10) states that both the potentials monotonically decrease in time. Namely, $\varphi(p) - \varphi^{eq}$ and $\psi(p) - \psi^{eq}$ are both Lyapunov functions for the time evolution (1).

That $\theta$-coordinates span the whole $S_N$ without redundancy and the monotonicity of $\psi$ are the main claims so far. We investigate their thermodynamic implications below.

Stochastic-thermodynamic interpretation.—We begin with interpretations immediate from the expressions (6).

First, since $\varphi$ is the negative of the total entropy, its time derivative gives the entropy production rate $\Sigma$:

$$\Sigma = d_i S = -d_i \varphi = -\sum_{\alpha=1}^N \theta^\alpha d_i \eta_\alpha,$$  \hspace{1cm} (11)

where we used (4). Its monotonicity is the well-known second law of thermodynamics [5, 9].

On the other hand, the monotonicity of $\psi$ is novel and contrasts with the second law. The function $\psi$ (6d) is the total entropy $\bar{s}$ averaged over the equilibrium distribution. This average is monotonically decreasing $d_i(\bar{s}(p))_{p^{eq}} = d_i \psi(p) < 0$, where $\bar{s}(p) := \sum_i q_i \bar{s}^\alpha(p)$ denotes the average over $q$. This property is seemingly opposite to the second law of thermodynamics, i.e., the increase of the average $d_i(\bar{s}(p))_{p} = -d_i \varphi(p) > 0$. Therefore, the monotonicities of the two functions reflect different aspects of the change in $\bar{s}$.

The $\theta$-coordinate ($-\theta^\alpha$) is the thermodynamic force conjugate to the probability flow $d_i \eta_\alpha$. Consider the decomposition of probability change $d_i p_i = \sum_i A^{\alpha}_i d_i \eta_\alpha$. Here, $d_i \eta_\alpha$ designates the probability flow proportional to $(A^{\alpha}_i)_N$.

In Eq. (11), we decompose the entropy production rate into the contributions from each flow $d_i \eta_\alpha$. Since the coefficient ($-\theta^\alpha$) expresses the entropy production rate per unit flow of $d_i \eta_\alpha$, ($-\theta^\alpha$) is the thermodynamic force conjugate to $d_i \eta_\alpha$. Thermodynamic forces vanish at the equilibrium, consistent with (7). Since $\theta$ is a coordinate system on $S_N$, we can use these thermodynamic forces to designate a distribution on $S_N$.

Equilibrium-thermodynamic interpretation.—Next, we interpret the dual description $(\theta, \psi(\theta))$ by an analogy with
classical-thermodynamic Legendre transformations. Concretely, we obtain the following expressions (see also SM):

\[ p_i(\theta) = \exp\left(-\frac{\epsilon^i - v^i_\theta(\theta) + T\psi(\theta)}{k_B T}\right) \quad (12) \]

\[ T\psi(\theta) = k_B T \ln \left[ \sum_{i=0}^{N} \exp\left(-\frac{\epsilon^i - v^i_\theta(\theta)}{k_B T}\right) \right] \quad (13) \]

with

\[ v^i_\theta(\theta) := T \sum_{a=1}^{N} (\tilde{A}^-)^i_a \theta^a, \quad \theta^a = \frac{1}{T} \sum_{i=0}^{N} A^i_v v^i_\theta(\theta) \quad (14) \]

where \((\tilde{A}^-)^i_a := (A^-)^i_a - \sum_j (A^-)^i_j p^eq_j\) is independent of the choice of \(A^-\) and itself a pseudo-inverse of \(A\). Equation (12) states that \(p(\theta)\) is reproduced as an equilibrium distribution under the external field \(v_\theta(\theta) \equiv (v^i_\theta(\theta))_{i=0}^{N}\), which modifies the state energy \(\epsilon^i\) to \(\epsilon^i - v^i_\theta\). The potential function \(T\psi(\theta)\) is the negative of the corresponding equilibrium free energy [Eq. (13)]. As in Eq. (14), \(\theta\) is linearly related to the field. The \(\theta^a\) coordinate \(T\theta^a\) specifies the component of the field proportional to \((\tilde{A}^-)^i_a\) \(0 \leq a \leq N\). In other words, \(T\theta^a\) is the strength of the field conjugate to the observable \(i \mapsto (\tilde{A}^-)^i_a\). We can use these external fields to designate a distribution on \(S_N\).

The field \(v_\theta(\theta)\) satisfies \(\sum_i v^i_\theta p^eq_i = 0\) due to \(\sum_i (\tilde{A}^-)^i_a p^eq_i = 0\). Although any field \(v \equiv (v^i)_{i=0}^{N}\) of the form \(v = v^i_\theta(\theta) + \text{const}\) reproduces the same distribution \(p(\theta)\) as an equilibrium, we need to fix this ambiguity by imposing \(\sum_i v^i_\theta p^eq_i = 0\) to obtain (13).

Equation (13) implies an operational interpretation of the potential \(\psi(\theta)\). Since the potential is regarded as the equilibrium free energy, the difference \(T\psi(\theta) - T\psi^eq\) is extracted as the work in the quasistatic process from \(p^eq\) to \(p(\theta)\) by applying the external field \(v_\theta(\theta)\).

To verify Eqs. (12)–(14) intuitively, recall that the physical picture of classical-thermodynamic Legendre transformations is to externally fix the Legendre-transformed degrees of freedom (e.g., temperature) and equilibrate the system accordingly [2]. Since we transform all the degrees of freedom, our transformation corresponds to fixing all the degrees of freedom by applying \(v_\theta\) and equilibrating the system. This intuition is formally expressed with the variational formula of Legendre transformation (e.g., Ref. [12]) to prove (12)–(14) (see SM).

Combined with the monotonicity, the equilibrium free energy under the external field \(v_\theta\) is monotonically increasing. In other words, the sum of the Boltzmann factors \([\exp \left(-(\epsilon^i - v^i_\theta) / k_B T\right)]\) must increase. This gives an equilibrium-thermodynamic interpretation of the constraint. We remark that this monotonicity has no counterpart in classical thermodynamics, in which we do not consider processes involving changes in Legendre-transformed degrees of freedom.

**Example:**—We demonstrate the dual description with the interpretation (12)–(14) using a three-state \((N = 2)\) model.

Consider a system with one unstable state \((i = 0)\) and two stable states \((i = 1, 2)\) with energies \((\epsilon^0, \epsilon^1, \epsilon^2) = (5k_B T, 0, 0)\) [Fig. 2(a)]. We set the transition rates \(W_{ij} = k_{ji} \exp\left((\epsilon^i - \epsilon^j) / 2k_B T\right)\) with \(k_{ij} = k_{ji}\) and \((k_{01}, k_{02}, k_{12}) = (1, 0.25, 0)\). Namely, relaxation from the state 0 to 1 is faster than that to the state 2. We set the initial distribution to \((p_0, p_1, p_2) = (0.8, 0.1, 0.1)\). Thus, the probability first flows into state 1 and then slowly relaxes to the equilibrium, reducing the imbalance in probabilities between states 1 and 2. Figure 2(b) shows the time change of the potentials, confirming the monotonicity (10).

We introduce our coordinates with

\[ A = \begin{pmatrix} 0 & 1 & -1 \\ 1 & -\frac{1}{2} & -\frac{1}{2} \\ -1 & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix}, \quad A^- = \begin{pmatrix} 0 & \frac{1}{2} & -\frac{1}{2} \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (15) \]

We can interpret \(\eta_1 = (p_1 - p_2) / 2\) and \(\theta^1 = \tilde{s}^2 - \tilde{s}^3\) as quantifying the imbalance in probabilities between the two stable states, while \(\eta_2 = p_0 - p_0^{eq}\) and \(\theta^2 = (\tilde{s}^1 + \tilde{s}^3) / 2 - \tilde{s}^0\) reflect the excess probability of the unstable state.
Figure 2(c) illustrates the time evolution in the η-coordinates. The process consists of two stages. The first stage is characterized by the growth of the imbalance η₁, whereas the second stage is by its decrease. This behavior matches our intuition about the separation of stages. The separation of stages is distinct because of the time-scale separation, i.e., the large discrepancy between the two nonzero eigenvalues of the rate matrix (W_{ij}), about −15 and −0.033. Here, \( (W_{ij}) \) is defined by rewriting the master equation (1) as \( d_p = \sum_j W_{ij} p_j \) [5].

On the other hand, the time evolution presented in θ-coordinates [Fig. 2(d)] appears to consist of three stages, colored separately in the figures. Namely, the earlier stage observed in the η-coordinates is further divided into two stages, one with increasing θ� and the other with almost constant θ₁. Thus, the θ-coordinates reveal the feature of the trajectory unobtainable in the η-coordinates.

To capture the insight behind this additional separation, we examine the constraint \( d_i \psi < 0 \) with the expression of \( \psi(\theta) \) in (13). First, we calculate the virtual external field \( v_\ast(\theta) \). Since \( p_{\theta}^{\text{eq}} < p_\theta^1 = p_\theta^2 \), the condition \( \sum_i v_\ast p_\theta^{\text{eq}} = 0 \) reduces to \( v_\ast^1 = -v_\ast^2 \). Thus, the second equation in (14) leads to \( v_\ast^1 = -v_\ast^2 \approx T\theta^2/2 \) and \( v_\ast^2 \approx T\theta^2 \). Figure 2(e) shows the time evolution of the modified state energy \( \epsilon^1 - v_\ast^1 \). Letting \( z^1(\theta) = \exp[-(\epsilon^1 - v_\ast^1)/k_B T] \) be the Boltzmann factor of the \( i \)th state, we obtain \( z^1(\theta) \approx \exp[(\theta^2/k_B - 5)] \) and \( z^1(\theta) + z^2(\theta) \approx 2\cosh(\theta^1/2k_B) \). In particular, \( z_1^1 + z_1^2 \) increases as the imbalance \( \theta^1 \) grows. Since the sum of these factors must decrease in time, this increase must be compensated by a decrease in \( \theta^2 \). When \( \theta^2 \) is large, this compensation is easy since \( z_1^0 \) is large enough. However, when \( \theta^2 \) decreases to some extent, \( z_1^0 \) becomes exponentially small and can no longer compensate for the increase. This suppresses the growth of \( \theta^1 \) and separates the first and the second stages.

Conclusion.—In this Letter, we introduce the quadruplet of Legendre duality (6) on \( S_\eta \) to obtain two descriptions of stochastic thermodynamics, the one with \( (\eta, \varphi(\eta)) \) and the dual description with \( (\theta, \psi(\theta)) \). Its affine equivalence to the information-geometric quadruplet leads to the monotonically increasing connections, namely the constraint \( d_i \psi < 0 \) and the Legendre transformation between total entropy and equilibrium free energy, might translate back and forth between such equilibrium properties and the nonequilibrium properties of the system. Also, the connection may bring existing approximating methods of free energy in equilibrium statistical mechanics into stochastic thermodynamics. Another possible direction is to formulate similar quadruplets in other nonequilibrium thermodynamics, including quantum thermodynamics [68–71] and nonlinear chemical thermodynamics [1, 72–76] based on quantum information geometry [77–79] and chemical information geometry [75].

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[1] E. Fermi, *Thermodynamics* (Dover, New York, 1956).
[2] H. B. Callen, *Thermodynamics and an Introduction to Thermostatistics*, 2nd ed. (Wiley, New York, 1985).
[3] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry*, 3rd ed. (North-Holland, Amsterdam, 2007).
[4] C. W. Gardiner, *Stochastic methods: a handbook for the natural and social sciences*, 4th ed. (Springer, Berlin Heidelberg, 2009).
[5] J. Schnakenberg, Network theory of microscopic and macroscopic behavior of master equation systems, *Rev. Mod. Phys.* **48**, 571 (1976).
[6] U. Seifert, Stochastic thermodynamics: principles and perspectives, *Eur. Phys. J. B* **64**, 423 (2008).
[7] U. Seifert, Stochastic thermodynamics, fluctuation theorems and molecular machines, *Rep. Prog. Phys.* **75**, 126001 (2012).
[8] K. Sekimoto, *Stochastic Energetics* (Springer, Berlin Heidelberg, 2010).
[9] C. Van den Broeck and M. Esposito, Ensemble and trajectory thermodynamics: A brief introduction, *Physica (Amsterdam)* **418A**, 6 (2015).
[10] S. Ciliberto, Experiments in stochastic thermodynamics: Short history and perspectives, *Phys. Rev. X* **7**, 021051 (2017).
[11] M. Esposito and C. Van den Broeck, Second law and Landauer principle far from equilibrium, *EPL* **95**, 40004 (2011).
[12] H. Touchette, The large deviation approach to statistical mechanics, *Phys. Rep.* **478**, 1 (2009).
[13] J. L. Lebowitz and H. Spohn, A Gallavotti–Cohen-type symmetry in the large deviation functional for stochastic dynamics, *J. Stat. Phys.* **95**, 333 (1999).
[14] P. Gaspard, Fluctuation theorem for nonequilibrium reactions, *J. Chem. Phys.* **120**, 8898 (2004).
[15] D. Andrieux and P. Gaspard, Fluctuation theorem for transport in mesoscopic systems, *J. Stat. Mech.: Theory Exp.* (2006), P01011.
[16] C. Giardinà, J. Kurchan, and L. Peliti, Direct evaluation of large-deviation functions, *Phys. Rev. Lett.* **96**, 120603 (2006).
[17] V. Lecomte and J. Tailleur, A numerical approach to large devi-
ations in continuous time, J. Stat. Mech.: Theory Exp. (2007), P03004.

[18] A. Imparato and L. Peliti, The distribution function of entropy flow in stochastic systems, J. Stat. Mech.: Theory Exp. (2007), L02001.

[19] J. Mehlf, T. Speck, and U. Seifert, Large deviation function for entropy production in driven one-dimensional systems, Phys. Rev. E 78, 011123 (2008).

[20] T. Nemoto and S.-i. Sasa, Thermodynamic formula for the cumulant generating function of time-averaged current, Phys. Rev. E 84, 061113 (2011).

[21] T. Nemoto and S.-i. Sasa, Computation of large deviation statistics via iterative measurement-and-feedback procedure, Phys. Rev. Lett. 112, 090602 (2014).

[22] P. T. Nyawo and H. Touchette, Large deviations of the current for driven periodic diffusions, Phys. Rev. E 94, 032101 (2016).

[23] M. L. Rosinberg, G. Tarjus, and T. Munakata, Stochastic thermodynamics of Langevin systems under time-delayed feedback control. II. Nonequilibrium steady-state fluctuations, Phys. Rev. E 95, 022123 (2017).

[24] N. N. Chentsov, Statistical decision rules and optimal inference (American Mathematical Society, Providence, 1982) (Originally published in Russian, Nauka, Moscow, 1972).

[25] S.-i. Amari, Differential geometry of curved exponential families—curvatures and information loss, Ann. Stat. 10, 357 (1982).

[26] S.-i. Amari, Information geometry of the EM and em algorithms for neural networks, Neural Netw. 8, 1379 (1995).

[27] S.-i. Amari and H. Nagaoka, Methods of information geometry (American Mathematical Society/Oxford University Press, Providence, 2000) (Originally published in Japanese, Iwanami, Tokyo, 1993).

[28] S.-i. Amari, Information geometry and its applications (Springer, Japan, 2016).

[29] T. M. Cover and J. A. Thomas, Elements of information theory (Wiley-Interscience, Hoboken, NJ, 2006).

[30] A. Wehr, General properties of entropy, Rev. Mod. Phys. 50, 221 (1978).

[31] J. M. R. Parrondo, J. M. Horowitz, and T. Sagawa, Thermodynamics of information, Nat. Phys. 11, 131 (2015).

[32] S. Ito, Backward transfer entropy: Informational measure for detecting hidden Markov models and its interpretations in thermodynamics, gambling and causality, Sci. Rep. 6, 36831 (2016).

[33] R. Kawai, J. M. R. Parrondo, and C. Van den Broeck, Dissipation: The phase-space perspective, Phys. Rev. Lett. 98, 080602 (2007).

[34] A. N. Gorban, P. A. Gorban, and G. Judge, Entropy: The Markov ordering approach, Entropy 12, 1145 (2010).

[35] M. Esposito, Stochastic thermodynamics under coarse graining, Phys. Rev. E 85, 041125 (2012).

[36] S. Ito, Stochastic thermodynamic interpretation of information geometry, Phys. Rev. Lett. 121, 030605 (2018).

[37] N. Shiraiishi and K. Saito, Information-theoretical bound of the irreversibility in thermal relaxation processes, Phys. Rev. Lett. 123, 110603 (2019).

[38] T. Nakamura, H. H. Hasegawa, and D. J. Driebe, Reconsideration of the generalized second law based on information geometry, J. Phys. Commun. 3, 015015 (2019).

[39] D. Gupta and D. M. Busiello, Tighter thermodynamic bound on the speed limit in systems with unidirectional transitions, Phys. Rev. E 102, 062121 (2020).

[40] Z. Zhang, S. Guan, and H. Shi, Information geometry in the population dynamics of bacteria, J. Stat. Mech.: Theory Exp. (2020), 073501.

[41] S. J. Bryant and B. B. Machta, Energy dissipation bounds for autonomous thermodynamic cycles, Proc. Natl. Acad. Sci. 117, 3478 (2020).

[42] S. Ito and A. Dechant, Stochastic time evolution, information geometry, and the Cramér-Rao bound, Phys. Rev. X 10, 021056 (2020).

[43] S. Ito, M. Oizumi, and S.-i. Amari, Unified framework for the entropy production and the stochastic interaction based on information geometry, Phys. Rev. Research 2, 033048 (2020).

[44] S. B. Nicholson, L. P. García-Pintos, A. del Campo, and J. R. Green, Time—information uncertainty relations in thermodynamics, Nat. Phys. 16, 1211 (2020).

[45] A. Kolchinsky and D. H. Wolpert, Entropy production given constraints on the energy functions, Phys. Rev. E 104, 034129 (2021).

[46] A. Kolchinsky and D. H. Wolpert, Dependence of integrated, instantaneous, and fluctuating entropy production on the initial state in quantum and classical processes, Phys. Rev. E 104, 054107 (2021).

[47] A. Kolchinsky and D. H. Wolpert, Work, entropy production, and thermodynamics of information under protocol constraints, Phys. Rev. X 11, 041024 (2021).

[48] S. Ito, Information geometry, trade-off relations, and generalized glansdorff-prigogine criterion for stability, J. Phys. A: Math. Theor. (2021), in press.

[49] F. Weinhold, Metric geometry of equilibrium thermodynamics, J. Chem. Phys. 63, 2479 (1975).

[50] G. Ruppeiner, Thermodynamics: A Riemannian geometric model, Phys. Rev. A 20, 1608 (1979).

[51] P. Salamon and R. S. Berry, Thermodynamic length and dissipated availability, Phys. Rev. Lett. 51, 1127 (1983).

[52] G. Ruppeiner, Riemannian geometry in thermodynamic fluctuation theory, Rev. Mod. Phys. 67, 605 (1995).

[53] G. E. Crooks, Measuring thermodynamic length, Phys. Rev. Lett. 99, 100602 (2007).

[54] E. H. Feng and G. E. Crooks, Length of time’s arrow, Phys. Rev. Lett. 101, 090602 (2008).

[55] D. C. Brody and D. W. Hook, Information geometry in vapour–liquid equilibrium, J. Phys. A 42, 023001 (2008).

[56] D. A. Sivak and G. E. Crooks, Thermodynamic metrics and optimal paths, Phys. Rev. Lett. 108, 190602 (2012).

[57] M. Polettini and M. Esposito, Nonconvexity of the relative entropy for Markov dynamics: A Fisher information approach, Phys. Rev. E 88, 012112 (2013).

[58] B. B. Machta, Dissipation bound for thermodynamic control, Phys. Rev. Lett. 115, 260603 (2015).

[59] K. Takahashi, Shortcuts to adiabaticity applied to nonequilibrium entropy production: an information geometry viewpoint, New J. Phys. 19, 115007 (2017).

[60] G. M. Rotskoff, G. E. Crooks, and E. Vanden-Eijnden, Geometric approach to optimal nonequilibrium control: Minimizing dissipation in nanomagnetic spin systems, Phys. Rev. E 95, 012148 (2017).

[61] J. Korbel, R. Hanel, and S. Thurner, Information geometry of scaling expansions of non-exponentially growing configuration spaces, Eur. Phys. J.: Spec. Top. 229, 787 (2020).

[62] M. Aguiler, S. A. Moosavi, and H. Shimazaki, A unifying framework for mean-field theories of asymmetric kinetic Ising systems, Nat. Commun. 12, 1 (2021).

[63] See Supplemental Material on [url] for the proofs and related discussions.

[64] T. Hatano and S.-i. Sasa, Steady-state thermodynamics of Langevin systems, Phys. Rev. Lett. 86, 3463 (2001).
[65] M. Esposito and C. Van den Broeck, Three faces of the second law. I. master equation formulation, Phys. Rev. E 82, 011143 (2010).
[66] L. D. Landau and E. M. Lifshiz, Statistical Physics, Part I (Butterworth-Heinemann, Oxford, 1980).
[67] D. Ruelle, Statistical Mechanics (W. A. Benjamin, New York, 1969).
[68] S. Vinjanampathy and J. Anders, Quantum thermodynamics, Contemp. Phys. 57, 545 (2016).
[69] S. Deffner and S. Campbell, Quantum thermodynamics: an introduction to the thermodynamics of quantum information (Morgan & Claypool, San Rafael, CA, 2019).
[70] P. Strasberg and A. Winter, First and second law of quantum thermodynamics: A consistent derivation based on a microscopic definition of entropy, PRX Quantum 2, 030202 (2021).
[71] M. Scandi and M. Perarnau-Llobet, Thermodynamic length in open quantum systems, Quantum 3, 197 (2019).
[72] H. Ge and H. Qian, Nonequilibrium thermodynamic formalism of nonlinear chemical reaction systems with Waage–Guldberg’s law of mass action, Chem. Phys. 472, 241 (2016).
[73] R. Rao and M. Esposito, Nonequilibrium thermodynamics of chemical reaction networks: wisdom from stochastic thermodynamics, Phys. Rev. X 6, 041064 (2016).
[74] G. Falasco, R. Rao, and M. Esposito, Information thermodynamics of tumbling patterns, Phys. Rev. Lett. 121, 108301 (2018).
[75] K. Yoshimura and S. Ito, Information geometric inequalities of chemical thermodynamics, Phys. Rev. Research 3, 013175 (2021).
[76] F. Avanzini, E. Penocchio, G. Falasco, and M. Esposito, Nonequilibrium thermodynamics of non-ideal chemical reaction networks, J. Chem. Phys. 154, 094114 (2021).
[77] H. Nagaoka, Differential geometrical aspects of quantum state estimation and relative entropy, in Quantum Communications and Measurement (Springer, Boston, MA, 1995) pp. 449–452.
[78] D. Petz and C. Sudár, Geometries of quantum states, J. Math. Phys. 37, 2662 (1996).
[79] M. R. Grasselli and R. F. Streater, On the uniqueness of the Chentsov metric in quantum information geometry, Infin. Dimens. Anal. Quantum Probab. Relat. Top. 4, 173 (2001).
Supplemental Material for
Information-geometric Legendre duality in stochastic thermodynamics
Naruo Ohga and Sosuke Ito

Sections A–D are supplemental discussions related to the overall setup, including possible generalizations, mathematical properties of the pseudo-inverse matrix $A^{-}$, and a comparison between $N$-component and $(N + 1)$-component coordinate systems. Sections E–G contain the details of the connection of our quadruplet with information geometry and comments on the proof of the monotonicity (10). Sections H proves the equilibrium-thermodynamic interpretation (12)–(14).

A. Generalization for systems with internal entropy and a particle reservoir

We can generalize all our results for systems with internal entropy and in contact with a single particle reservoir. Internal entropy $s'_{\text{int}}$ is a contribution to the system entropy independent of the probability distribution. It enters the system entropy as $s'_{\text{sys}}(p) = -k_B \ln p_i + s'_{\text{int}}$. Such contribution arises, for example, when the states of the system are already coarse-grained [35]. Next, suppose the system exchanges particles with a single particle reservoir of chemical potential $\mu$. Let $n^i$ denote the particle number of the system when in the $i$th state. Then, the entropy of the bath (the heat bath and the particle reservoir together) becomes $s'_{\text{bath}} = -(\epsilon^i - \mu n^i)/T$. Summing them up, the total entropy (2) is generalized to

$$\bar{s}'(p) \equiv s'_{\text{sys}}(p) + s'_{\text{bath}} = -k_B \ln p_i + s'_{\text{int}} - \frac{\epsilon^i - \mu n^i}{T} = -k_B \ln p_i - \frac{\omega^i}{T}$$

with $\omega^i := \epsilon^i - \mu n^i - T s'_{\text{int}}$. All the results in the main text remain valid with the substitution of $\epsilon^i$ for $\omega^i$. For example, statements involving no explicit expression of $\bar{s}'$ immediately hold. The equilibrium distribution changes into $p_{\text{eq}}^i \propto \exp\left(-\omega^i/k_B T\right)$. An external field $\psi^i$ modifying the energy $\epsilon^i$ to $\epsilon^i - \psi^i$ is equivalently interpreted as modifying $\omega^i$ to $\omega^i - \psi^i$.

B. Generalization for systems without detailed balance

We can also generalize the results formally for systems without detailed balance. Consider a system with a unique steady distribution $p^\Omega \equiv (p^\Omega)_i \in S_N$ breaking the detailed balance condition. This situation occurs for a broad class of systems, such as in contact with multiple heat baths or multiple particle reservoirs [9]. In this situation, the total entropy of the system and the baths together is no longer determined solely by the probability distribution of the system. For example, it can continuously increase even if the system stays in the steady distribution. Therefore, we cannot introduce a quantity like $\bar{s}'(p)$ in the main text.

Instead, we define $\phi^i$ by $p_{\text{eq}}^i = \exp(-\phi^i)$ and use the following $\bar{s}'$ in place of $\bar{s}'$ [7]:

$$\bar{s}'(p) := -k_B \ln p_i - k_B \phi^i.$$  

(S2)

The average is $\bar{s}'(p) = \sum_i \bar{s}'(p)_i p_i$. Its time derivative is the Hatano–Sasa excess entropy production rate [64]. By replacing $p_{\text{eq}}^i$ with $p_{\text{eq}}^i$, $\epsilon^i/k_B T$ with $\phi^i$, and $\bar{s}'$ with $\bar{s}'$, we can formally reproduce our results in the main text to these cases. For example, the quadruplet (6) becomes

$$\eta_a(p) = \sum_i (A^{-})_{ai} (p_i - p_{\text{eq}}^i), \quad \varphi(\eta(p)) = -\bar{s}'(p) = -\sum_i p_i \bar{s}'(p),$$

$$\theta^a(p) = -\sum_i \bar{s}'(p) A_{ai}, \quad \psi(\theta(p)) = \sum_i p_{\text{eq}}^i \bar{s}'(p).$$

(S3)

The origins of the coordinates correspond to $p^\Omega$. The information-geometric interpretations of the potential functions are

$$k_B D_{KL}(p||q) = \varphi(p) + \psi(q) - \eta(p) \cdot \theta(q),$$

$$\varphi(p) - \varphi(p^\Omega) = k_B D_{KL}(p||p^\Omega), \quad \psi(p) - \psi(p^\Omega) = k_B D_{KL}(p||p^\Omega).$$

(S4) (S5)

As in detailed-balanced systems, this interpretation and the contraction property of the Kullback–Leibler divergence lead to the monotonicity $d_i \varphi(p(i)) < 0$ and $d_i \psi(p(i)) < 0$ for $p(i) \neq p^\Omega$. The former is the nonnegativity of the Hatano–Sasa
excess entropy production rate; the latter gives a new constraint on the time evolution. The equilibrium-thermodynamic interpretation of $\theta$ and $\psi(\theta)$ is also formally obtained, but the modification from $\phi^i$ to $\phi^i - v_i/k_B T$ does not seem to allow a clear and general physical interpretation as in detailed-balanced systems.

C. Properties of the pseudo-inverse matrix $A^-$

An $(N + 1) \times N$ matrix $A \equiv (A_i^a)_{i=0}^N$ is defined in the main text as an arbitrary matrix that satisfies $\sum_i A_i^a = 0$ and rank $A = N$. We fix one choice of $A$ in this section. Its pseudo inverse $A^- \equiv ((A^-)_i^a)_{i=0}^N$ is an arbitrary matrix satisfying $\sum_{i,j} A_i^\beta (A^-)_j^\beta / A_j^\beta = A_i^a$. It is not unique for the fixed $A$. For any choice of $A^-$, the following properties hold:

\[
\sum_i (A^-)^\beta_i A_i^\alpha = \delta^\beta_\alpha, \quad (S6)
\]

\[
\sum_{\alpha} A_i^\alpha (A^-)_\alpha^a = \delta_i^a + h_i, \quad (S7)
\]

\[
\sum_{\alpha,j} A_i^\alpha (A^-)_\alpha^j (p_j - q_i) = p_i - q_i, \quad (S8)
\]

where $(h_i)_{i=0}^N$ is a set of constants dependent on the choice of $A^-$, and $(p_i)_{i=0}^N$ and $(q_i)_{i=0}^N$ are arbitrary two probability distributions. These relations help calculation in the main text. To prove (S6), subtract the obvious relation $\sum_\beta A_i^\beta \delta^\beta_\alpha = A_i^\alpha$ from the definition of $A^-$ to obtain $\sum_{\beta,j} A_i^\beta [\sum_{\alpha} (A^-)_\beta^\alpha A_j^\alpha - \delta^\beta_\alpha] = 0$. Since rank $A = N$, the kernel of $A$ is the null space. Therefore, we obtain $\sum_{\beta} (A^-)_\beta^\alpha A_j^\beta - \delta^\beta_\alpha = 0$. To prove (S7), subtract $\sum_i \delta_i^a A_j^\alpha = A_j^\alpha$ from the definition of $A^-$ to reach $\sum_i [\sum_{\beta} A_i^\beta (A^-)_\beta^\alpha - \delta_i^\alpha] A_j^\alpha = 0$. From rank $A = N$ and $\sum_i A_i^\alpha = 0$, the cokernel (left kernel) of $A$ is one-dimensional and spanned by $(1)_{i=0}^N$. Thus we find that $[\sum_{\beta} A_i^\beta (A^-)_\beta^\alpha - \delta_i^\alpha]_{j=0}^N$ for each $i$ is proportional to the vector $(1)_{i=0}^N$. Namely, we can write $\sum_{\beta} A_i^\beta (A^-)_\beta^\alpha - \delta_i^\alpha = h_i$ using some $j$-independent constants $(h_i)_{i=0}^N$. Eq. (S8) easily follows from (S7) and $\sum_i p_i = \sum_i q_i = 1$.

Next, let $(A^-)_\alpha^i$ and $(A^-')_\alpha^i$ be any two choices of the pseudo inverse for a fixed $A$. Then, there exists a set of $i$-independent constants $(c^a_{i,a})_{i=0}^N$ such that

\[
(A^-')_\alpha^i = (A^-)_\alpha^i + c^a_{i,a} \quad (S9)
\]

holds. Conversely, let $(A^-)_\alpha^i$ be one choice and define $(A^-')_\alpha^i$ by (S9) using an arbitrary $(c^a_{i,a})_{i=0}^N$. Then, $(A^-')_\alpha^i$ is also a pseudo inverse. To prove the first statement, obtain $\sum_{\beta} [(A^-)^\beta_\alpha = (A^-')^\beta_\alpha] A_j^\alpha = 0$ from (S6). Since the cokernel of $A$ is spanned by $(1)_{i=0}^N$, $(A^-)^\beta_\alpha - (A^-')^\beta_\alpha|_{j=0}^N$ for each $\beta$ is proportional to $(1)_{i=0}^N$. This is equivalent to the desired statement. To prove the converse, just substitute (S9) into the definition of the pseudo inverse and use $\sum_i A_i^\alpha = 0$. The converse property helps calculate a pseudo-inverse matrix: one can first calculate the unique Moore–Penrose pseudo inverse using existing programs and then exploit (S9) to find a more tractable choice.

D. Comparison between $N$-component and $(N + 1)$-component coordinate systems

We use redundancy-free $N$-component coordinate systems on $S_N$ in the main text. Here we discuss the necessity of this choice. If we used an $(N + 1)$-component coordinates system, the introduced coordinates via a Legendre transformation would not admit a one-to-one correspondence with $p \in S_N$ and would be much less convenient. For example, the Legendre transformation of the convex function $-\tilde{S}(p)$ by the coordinate system $\tilde{\eta}(p) = (p_i - p_i^{eq})_{i=0}^N$ leads to the following quadruplet:

\[
\tilde{\eta}(p) = p_i - p_i^{eq}, \quad \tilde{\phi}(\tilde{\eta}(p)) = -\tilde{S}(p) = -\sum_i p_i \tilde{s}^i(p), \quad \tilde{\theta}(p) = -\tilde{s}^i(p) + k_B, \quad \tilde{\psi}(\tilde{\theta}(p)) = \sum_i p_i^{eq} \tilde{s}_i(p) \quad (S10)
\]

for $i = 0, \ldots, N$. Here, we extend the definitions of $\tilde{s}^i(p)$ and $\tilde{S}(p)$ naturally for all $p \in \mathbb{R}^{N+1}$. Within the $(N+1)$-dimensional space spanned by $\tilde{\theta}$, only a $N$-dimensional subspace is a physical space that admits the normalization of probability. The subspace, specified by $\sum_i p_i(\tilde{\theta}) = \sum_i \exp(\tilde{\theta}/k_B - e_i/k_B T - 1) = 1$, is curved in $\mathbb{R}^{N+1}$ and nontrivial.
E. Dually flat geometry

This section provides a brief introduction to dually flat geometry based on Ref. [27]. Dually flat geometry is a differential-geometrical framework, regarded as a generalization of Riemannian geometry. It consists of several geometric concepts, including a divergence, a metric, and two connections. These concepts are defined coherently to form a unified geometric structure on a space (manifold), which we write as $M$. Points on the manifold $M$ are written as $P, Q, \cdots \in M$. In the main text, we consider the dually flat geometry on the space consisting of the $(N+1)$-component nonzero probability distributions $S_N$. The space $S_N$ corresponds to the manifold $M$ here, and probability distributions $p, q, \cdots \in S_N$ correspond to points $P, Q, \cdots \in M$. We remark that concepts of dually flat manifold are not necessarily based on the probability distributions, and here we will explain these concepts without using properties specific to probability distributions.

To give a concrete expression to the geometric concepts of dually flat geometry on $M$, we introduce a quadruplet of Legendre duality. Let $K$ denote the dimensionality of $M$. We introduce two coordinate systems $\eta(P) \equiv (\eta_a(P))_{a=1}^K$, $\theta(P) \equiv (\theta^a(P))_{a=1}^K$ that spans $M$ and two convex functions $\varphi(\eta), \psi(\theta)$ that satisfies Legendre duality

$$\frac{\partial \varphi}{\partial \eta_a}(P) = \theta^a(P), \quad \frac{\partial \psi}{\partial \theta^a}(P) = \eta_a(P), \quad \varphi(\eta(P)) + \psi(\theta(P)) = \theta^a(P) \cdot \eta_a(P) = 0 \tag{S11}$$

at each $P \in M$. Hereafter, we regard $\eta$ as a column vector and $\theta$ as a row vector. (We do not care about this distinction in the main text, where we avoid matrix-vector product notation.)

The quadruplet $(\eta, \varphi(\eta), \theta, \psi(\theta))$ completely determines the dually flat geometric structure on $M$. For example, it defines the Bregman divergence between arbitrary two points $P, Q \in M$ by

$$D(P|Q) := \varphi(P) + \psi(Q) - \theta(Q) \cdot \eta(P) = \varphi(P) - \varphi(Q) - \theta(Q) \cdot [\eta(P) - \eta(Q)]$$

$$= \psi(Q) - \psi(P) - \eta(P) \cdot [\theta(Q) - \theta(P)], \tag{S12}$$

where the second and the third equality is due to the Legendre duality (S11). The quadruplet also induces the metric by $g^{ab} := \frac{\partial^2 \varphi}{\partial \eta_a \partial \eta_b}$ in the $\eta$-coordinates and $g_{ab} := \frac{\partial^2 \psi}{\partial \theta^a \partial \theta^b}$ in the $\theta$-coordinates. These two expressions are equivalent owing to the Legendre duality. This metric leads to the following line element (infinitesimal squared distance) associated with an infinitesimal displacement from $P \in M$ to $P+dP \in M$ (the latter is merely a symbolic notation):

$$dl^2 = \sum_{a,b} \frac{\partial^2 \varphi}{\partial \eta_a \partial \eta_b} d\eta_a d\eta_b = \sum_{a,b} \frac{\partial^2 \psi}{\partial \theta^a \partial \theta^b} d\theta^a d\theta^b = \sum_a d\theta^a d\eta_a = d\theta \cdot d\eta = 2D(P||P+dP) = 2D(P+dP||P), \tag{S13}$$

where $d\eta$ and $d\theta$ represent the same displacement expressed with each coordinate system. The quadruplet also determines other geometric entities.

Two quadruplets $(\eta, \varphi(\eta), \theta, \psi(\theta))$ and $(\eta', \varphi'(\eta'), \theta', \psi'(\theta'))$ on $M$ determine the same dually flat geometric structure if and only if they are affine equivalent to each other. Here, affine equivalence means that they are related by an affine transformation

$$\eta' = D\eta + a, \quad \varphi'(\eta') = \varphi(\eta) + bD\eta + b \cdot a + C,$$

$$\theta' = \theta D^{-1} + b, \quad \psi'(\theta') = \psi(\theta) + \theta D^{-1} a - C, \tag{S14}$$

where $D$ is a $K \times K$ regular constant matrix, $a \equiv (a_a)_{a=1}^K$ is a constant column vector, $b \equiv (b^a)_{a=1}^K$ is a constant row vector, and $C$ is a constant. Its inverse transformation also has the same form. The transformed quadruplet $(\eta', \varphi'(\eta'), \theta', \psi'(\theta'))$ also satisfies the Legendre duality (S11). To verify that they give the same geometrical structure, we need to check the invariance of the expressions of geometrical concepts under the transformation. For example, the divergence (S12) and the line element (S13) are invariant since we can prove the following equalities:

$$\varphi(P) + \psi(Q) - \theta(Q) \cdot \eta(P) = \varphi(P) + \psi'(Q) - \theta'(Q) \cdot \eta'(P), \quad d\theta \cdot d\eta = d\theta' \cdot d\eta'. \tag{S15}$$

Other geometrical entities are also proven to be invariant.

Another type of transformation for a quadruplet is a scale change

$$\eta'_a(\eta) = Q_1 \eta_a, \quad \varphi'(\eta') = Q_1 Q_2 \varphi(\eta), \quad \theta'^a(\theta) = Q_2 \theta^a, \quad \psi'(\theta') = Q_1 Q_2 \psi(\theta), \tag{S16}$$

where $Q_1$ and $Q_2$ are arbitrary positive constants. This transformation makes the line element and the divergence $Q_1 Q_2$ times larger. Therefore, the new geometry is different from the old one in the strict sense. However, they are essentially the same for most applications.
F. Dually flat geometry on the state space of stochastic thermodynamics and its relation to information geometry

Based on the general theory in the previous section, we construct a dually flat geometry on the state space \( S_N \) from our thermodynamic quadruplet in Eq. (6), which we write here as \((\eta^h, \varphi^h(\eta^h), \theta^h, \psi^h(\theta^h))\) to avoid confusion. To investigate the induced geometrical structures, we can calculate the geometrical quantities directly from their definitions such as (S12) and (S13). Alternatively, we can relate our quadruplet to an information-geometric one with an affine transformation and a scale change and investigate ours through the relation. We take the latter route to clarify the underlying mathematical structure. Our quadruplet (6) is affine equivalent to the following quadruplet \((\eta^l, \varphi^l(\eta^l), \theta^l, \psi^l(\theta^l))\),

\[
\eta^l(p) = p_s, \quad \varphi^l(\eta^l(p)) = \int_0^p \ln p_i, \quad \theta^l(p) = -\int_0^p \psi^l(\theta^l(p)) = -\ln p_0, \tag{S17}
\]

by the transformation (S14) using \( D = (A_i^0)_{i=1}^N, a = (p_i^q)_{i=1}^N, b = (\epsilon^0/T - \epsilon^1/T_{i=1})^N \), and \( C = -\epsilon^0/T \). This quadruplet is further transformed into another quadruplet \((\eta^G, \varphi^G(\eta^G), \theta^G, \psi^G(\theta^G))\) by a scale change (S16) with \( Q_1 = 1 \) and \( Q_2 = k^{-1}_N \):

\[
\eta^G(p) = p_s, \quad \varphi^G(\eta^G(p)) = \sum_{i=0}^N p_i \ln p_i, \quad \theta^G(p) = \ln \frac{p_s}{p_0}, \quad \psi^G(\theta^G(p)) = -\ln p_0. \tag{S18}
\]

The last quadruplet (S18) is one of the quadruplets used in information geometry [27]. Its corresponding Bregman divergence is the Kullback–Leibler divergence \( D_{KL} \), and the line element is the Fisher information \( I_F \), defined by \( I_F = \sum_i (d p_i)^2 / p_i \). By tracing back the successive transformations, we obtain the following relations between the divergences \( D^h(p|q) \), \( D^t(p|q) \), \( D^G(p|q) \) and line elements \((d \theta^h)^2 \), \((d \ell^t)^2 \), \((d \ell^G)^2 \) corresponding to the three quadruplets above:

\[
k_n D_{KL}(p||q) = k_n D^G(p||q) = D^t(p||q) = D^h(p||q) \equiv \varphi^h(p) + \theta^h(q) - \psi^h(q), \quad \tag{S19}
\]

\[
k_n I_F = k_n (d \ell^G)^2 = (d \ell^t)^2 = (d \theta^h)^2 \equiv d \theta^h \cdot d \eta^h. \tag{S20}
\]

Eq. (S19) certifies the expression of Kullback–Leibler divergence with the quadruplet (6) in the main text.

We can exploit Eqs. (S19)–(S20) to obtain stochastic-thermodynamic expressions of \( D_{KL} \) and \( I_F \) in (S19)–(S20) with various expressions in Eqs. (S12)–(S13) and further inserting the definitions of our quadruplet (6) yield

\[
k_n D_{KL}(p||q) = -\sum_i \left[\tilde{s}_i(p) - \tilde{s}_i(q)\right] p_i, \quad k_n I_F = -\sum_{i,j} \frac{\partial^2 \tilde{s}}{\partial p_i \partial p_j} p_i d p_j = -\sum_i d \tilde{s}_i d p_i, \tag{S21}
\]

where \( d \tilde{s}_i \) denotes the change in \( \tilde{s}_i \) due to the displacement \( d p \). These expressions clarify the connection between the state entropy \( \tilde{s} \) and the information-geometric quantities.

G. Notes on the proof of the monotonicity (10)

We discuss the equality condition for the contraction property of Kullback–Leibler divergence [3, 8]

\[
d_t D_{KL}(p(t)||q(t)) \leq 0, \tag{S22}
\]

which is used in the main text to prove the monotonicity (10). Here, we prove that the equality holds if and only if \( p(t) = q(t) \). Suppose we only consider \( p(t), q(t) \in S_N \) and assume the irreducibility of the transition rates. The proof of the inequality is as follows [3]:

\[
d_t D_{KL}(p(t)||q(t)) = d_t \sum_i p_i \ln \frac{p_i}{q_i} = \sum_{i,j} \ln \left[ \frac{W_{ij}}{q_j} \ln p_i - \frac{W_{ij}}{q_j} \ln p_i - \frac{W_{ij}q_j - W_{ij}q_i}{q_i} p_i \right] \leq 0, \tag{S23}
\]

where we used \( \ln x - x + 1 \leq 0 \) for \( x > 0 \) and omitted \( t \) for brevity. Since \( \ln x - x + 1 = 0 \) holds if and only if \( x = 1 \), the equality condition of (S23) is either \( p_j = 0, W_{ij} = 0, \) or \( p_i q_j / q_i p_j = 1 \) for each pair \( i, j (i \neq j) \). The first possibility \( p_j = 0 \)
is excluded due to the assumption \( p \in S_N \). If the system can directly jump from state \( j \) to \( i \), the second possibility \( W_{ij} = 0 \) is also denied, and we need \( p_i/q_i = p_j/q_j \) to saturate the inequality (S23). Even if the system cannot directly jump from state \( j \) to \( i \), it can reach from state \( j \) to \( i \) via other states due to the irreducibility of the transition rates. Therefore, iterative use of this equality eventually imposes \( p_i/q_i = p_j/q_j \) for all the pairs \( i, j \) (\( i \neq j \)). In other words, \( p_i/q_i \) must be equal for all the states. Together with the normalization of probability \( \sum_i p_i = \sum_i q_i = 1 \), this condition implies \( p = q \).

The main text proves the monotonicity (10) as a consequence of Eq. (S22). Alternatively, we can give a direct proof of the monotonicity. By a direct calculation of the time derivatives, we obtain

\[
\frac{d\ln p_i}{dt} = \sum_j \delta(p_i(t)) p_j(t) - \sum_j \delta(p_j(t)) p_i(t) - \frac{dW_{ij}}{dt} \sum k \ln p_k(t)
\]

(S24)

\[
\frac{d\psi}{dt} = \sum_j p_j \delta(p_i(t)) - \sum_k \ln p_k(t) - \frac{dW_{ij}}{dt} \sum k \ln p_k(t)
\]

(S25)

From the detailed balance condition \( W_{ij}/W_{ji} = p_i^\text{eq}/p_j^\text{eq} \), the three terms \( \delta(p_i) - \delta(p_j) \), \( p_j^\text{eq}/p_i - p_i^\text{eq}/p_j \), and \( W_{ij} - W_{ji}p_j \) have the same sign (zero, negative, or positive). Therefore, \( d\ln p_i < 0 \) and \( d\psi < 0 \) hold, with the equalities satisfied only when the three terms vanish identically for all the pairs \( i, j \). This situation is specific to the equilibrium distribution. Note that the proof here for \( d\ln p_i < 0 \) is essentially identical to the proof of the second law of thermodynamics found in the literature (e.g., Ref. [65]).

### H. Proofs of the equilibrium-thermodynamic interpretation Eqs. (12)–(14)

Here we prove the equilibrium-thermodynamic interpretation (12)–(14) in two routes. The first proof is a direct calculation using the definition of total entropy (2), the primary expression of the quadruplet (6c)–(6d), the definition of the matrix \( (\tilde{A}^-)_\alpha^i \), and the normalization of probability. The second proof is more concise, starting from the variational formula of Legendre transformation (e.g., Ref. [12]) in analogy with classical thermodynamics.

In preparation for both the proofs, we clarify three properties of the matrix \( (\tilde{A}^-)_\alpha^i \). First, its definition does not depend on the choice of \( \tilde{A}^- \). To check this independence, recall that any two choices of \( \tilde{A}^- \) are connected with each other as in (S9) and substitute the connection (S9) into the definition of \( (\tilde{A}^-)_\alpha^i \). Second, this matrix is a pseudo-inverse matrix of \( A \). To certify this property, recall Eq. (S9) again and replace the \( i \)-independent constant \( c^\text{eq}_\alpha \) therein with \( -\sum_j (\tilde{A}^-)_\alpha^j p_j^\text{eq} \). Third, the matrix satisfies \( \sum_j (\tilde{A}^-)_\alpha^j p_j^\text{eq} = 0 \), as calculated by \( \sum_j (\tilde{A}^-)_\alpha^j p_j^\text{eq} = \sum_j (\tilde{A}^-)_\alpha^j p_j^\text{eq} - \sum_j p_j^\text{eq} \sum_j (\tilde{A}^-)_\alpha^j p_j^\text{eq} = \sum_j (\tilde{A}^-)_\alpha^j p_j^\text{eq} - \sum_j (\tilde{A}^-)_\alpha^j p_j^\text{eq} = 0 \).

We first briefly mention Eq. (14). The first equation there is the definition of \( v_s \). The second equation is proven using the definition of \( v_s \) and \( \sum_j (\tilde{A}^-)_\alpha^j A_{ij}^\alpha = \delta_{ij}^\text{eq} + h_i \) using unknown constants \( (h_i)_{i=0} \). To determine the constants, we multiply this relation by \( p_i^\text{eq} \) and take the summation over \( j \) to obtain

\[
0 = \sum_{\alpha, j} A_{ij}^\alpha (\tilde{A}^-)_\alpha^j p_j^\text{eq} = \sum_j (\delta_{ij}^\text{eq} + h_i) p_j^\text{eq} = p_i^\text{eq} + h_i,
\]

(S26)

where the first equality is due to \( \sum_j (\tilde{A}^-)_\alpha^j p_j^\text{eq} = 0 \). Therefore, we obtain \( h_i = -p_i^\text{eq} \) and \( \sum_j A_{ij}^\alpha (\tilde{A}^-)_\alpha^j = \delta_{ij}^\text{eq} - p_i^\text{eq} \). Next, we use this result to calculate the relation between \( v_s^\text{eq} \) and \( \tilde{s}(p(\theta)) \). We start from the definition of \( v_s^\text{eq} \) to obtain

\[
\frac{1}{T} v_s^\text{eq} = \sum_{\alpha, i} \theta^\alpha (\tilde{A}^-)_\alpha^i \frac{1}{T} = -\sum_{j, i} \tilde{s}(p(\theta)) A_{ij}^\alpha (\tilde{A}^-)_\alpha^j = -\sum_{j} \delta_{ij}^\text{eq} - p_j^\text{eq} \delta \tilde{s}(p(\theta)) + \psi(\theta),
\]

(S27)

where we used (6c) for the second equality and (6d) for the last equality. We remark that we already know the relation \( \sum_i T^{-1} v_s^\text{eq} A_{i}^\alpha = -\sum_i \tilde{s}(p(\theta)) A_{i}^\alpha \) between \( v_s^\text{eq} \) and \( \tilde{s}(p(\theta)) \) from Eq. (6c) and the second equation in Eq. (14). This
relation is reproduced from (S27) by multiplying (S27) by $A_i$, taking the summation over \(i\), and using \(\sum_i A_i = 0\). We are now ready to prove the desired expressions (12)–(13). Inserting the definition of the total entropy (2) into (S27), we obtain

\[
\frac{1}{T} v'_\alpha(\theta) = k_B \ln p_i(\theta) + \frac{\epsilon_i}{T} + \psi(\theta).
\]  

(S28)

By solving (S28) with respect to \(p_i(\theta)\), we obtain Eq. (12). Finally, we substitute the obtained (12) into the normalization of probability \(\sum_i p_i(\theta) = 1\) and solve the resulting equation with respect to \(T \psi(\theta)\) to obtain Eq. (13).

The second route to prove (12)–(13) uses the variational expression of Legendre transformation:

\[
\psi(\theta) = \operatorname{max}_\eta \{ \theta \cdot \eta - \varphi(\eta) \}, \quad \eta(\theta) = \operatorname{argmax}_\eta \{ \theta \cdot \eta - \varphi(\eta) \}.
\]  

(S29)

First, we exploit the one-to-one correspondence between \(\eta\) and \(p\) to rewrite them as

\[
\psi(\theta) = \operatorname{max}_p \{ \theta \cdot \eta(p) + S(p) \}, \quad p(\theta) = \operatorname{argmax}_p \{ \theta \cdot \eta(p) + S(p) \}.
\]  

(S30)

To further rewrite the maximand in Eq. (S30), we notice \(\eta_s = \sum_i (\tilde{A}^-)_{\alpha i}^s (p_i - p_i^\text{eq})\), since the right-hand side of (6a) does not depend on the choice of a pseudo-inverse matrix of \(\tilde{A}\), and \((\tilde{A}^-)_{\alpha i}^s\) is one of the pseudo-inverse matrices. We also introduce the nonequilibrium free energy [11] by \(F(p; \epsilon) := E(p; \epsilon) - TS_{\text{sys}}(p)\) with \(E(p; \epsilon) = \sum_i p_i \epsilon_i^s\) and \(S_{\text{sys}}(p) = \sum_i p_i s_{i \text{sys}} = -k_B \sum_i p_i \ln p_i\). The free energy equals \(-T \bar{S}(p)\) in the main text for each fixed \(\epsilon\). However, we introduced it to emphasize that it is a function of both \(p\) and \(\epsilon\). For a fixed \(\epsilon\), it takes the minimum at the corresponding equilibrium distribution \(p^\text{eq}(\epsilon)\), defined by \(p^\text{eq}(\epsilon) \propto \exp(-\epsilon/k_B T)\). The minimum value is the equilibrium free energy \(F^\text{eq}(\epsilon) := F(p^\text{eq}(\epsilon); \epsilon) = -k_B T \ln \left[ \sum_i \exp \left( -\epsilon_i/k_B T \right) \right]\). Now, we use these observations to rewrite the maximand in (S30) as

\[
\theta \cdot \eta(p) + \bar{S}(p) = \sum_{\alpha \beta} \theta^\alpha (\tilde{A}^-)_{\alpha i}^s (p_i - p_i^\text{eq}) - \frac{1}{T} F(p; \epsilon)
\]

\[
= \frac{1}{T} \sum_i \nu'_\alpha(\theta) p_i - \frac{1}{T} \sum_i p_i \epsilon_i^s - k_B \sum_i p_i \ln p_i = -\frac{1}{T} F(p; \epsilon - v_\ast(\theta)),
\]  

(S31)

where we used \(\nu'_\alpha(\theta) = T \sum_{\alpha \beta} (\tilde{A}^-)_{\alpha i}^s \theta^\beta\) and \(\sum_i (\tilde{A}^-)_{\alpha i}^s p_i^\text{eq} = 0\) for the second equality. Therefore, we have only to minimize the free energy. Since the minimizer is the equilibrium distribution corresponding to the energy \(\epsilon - v_\ast(\theta)\), we obtain

\[
\psi(\theta) = -\frac{1}{T} F^\text{eq}(\epsilon - v_\ast(\theta)), \quad p(\theta) = p^\text{eq}(\epsilon - v_\ast(\theta)),
\]  

(S32)

which reproduce Eqs. (12)–(13).