Thermodynamic variational relation

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In systems far from equilibrium, the statistics of observables are connected to entropy production, leading to the thermodynamic uncertainty relation (TUR). However, the derivation of TURs often involves constraining the parity of observables, such as considering asymmetric currents, making it unsuitable for the general case. We propose a thermodynamic variational relation (TVR) between the statistics of general observables and entropy production, based on the variational representation of f divergences. From this result, we derive a universal TUR and other relations for higher-order statistics of observables.

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I. INTRODUCTION

The second law of thermodynamics posits that entropy production is non-negative. While the random nature of the entropy production, denoted as Σ, may seem insignificant in large-scale systems, it takes center stage at smaller scales due to the pronounced impact of thermal and quantum fluctuations [1–13].

In the realm of nonequilibrium thermodynamics, physical observables, such as particle currents, heat, and work, undergo fluctuations. These fluctuations are encapsulated within the probability density function (pdf) $p(\Sigma, \phi)$, where Σ represents the entropy production and ϕ the underlying observable, where the pdf typically depends on both the system and time, particularly in transient regimes.

At the heart of these fluctuations is the detailed fluctuation theorem (DFT) [6,8,14–16], which equates a random variable $\Sigma(\Gamma)$ to the asymmetry of the trajectory probabilities,

$$\Sigma(\Gamma) := \ln \frac{P_F(\Gamma)}{P_B(\Gamma^\dagger)}, \tag{1}$$

where Γ is some process and $m(\Gamma) = \Gamma^\dagger$ is a conjugate (involution), such that $m(m(\Gamma)) = \Gamma$, and P_F (P_B) is the probability of observing Γ in the forward (backward) process. In stochastic thermodynamics, when local detailed balance is assumed, the variable $\Sigma(\Gamma)$ is usually identified as the stochastic entropy production for the trajectory [3,17] with a proper choice of initial conditions and reservoirs [18–20]. As a consequence of (1), for instance, we have the integral FT, $\langle \exp(-\Sigma)\rangle_F = 1$, and the second law, $\langle \Sigma \rangle_F \geqslant 0$, from Jensen's inequality, where $\langle\,\rangle_i$ is the average with respect to $P_i(\Gamma)$, $i \in \{F, B\}$.

The broad applicability of the fluctuation theorem (1), especially when systems are far from equilibrium, renders it a useful tool in the study of nonequilibrium physics. This utility has prompted extensive theoretical and experimental investigation of these theorems within classical systems. The relevance of the detailed fluctuation theorem extends to the quantum realm [2,4,21–23], especially to account for heat exchange between quantum-correlated bipartite thermal systems [24].

A consequence of (1) is the thermodynamic uncertainty relation (TUR) [17,25–34], which reads in the case of odd currents $\phi(\Gamma^\dagger) = -\phi(\Gamma)$ and $F = B$,

$$\frac{\langle \phi^2 \rangle - \langle \phi \rangle^2}{\langle \phi \rangle^2} \geqslant \sinh^{-2}\left(\frac{g(\langle \Sigma \rangle)}{2}\right), \tag{2}$$

where $g(x)$ the inverse of $h(x) = x \tanh(x/2)$, for $x \geqslant 0$.

However, in the derivation of TURs, there is usually interest in observables $\phi(\Gamma)$ bearing a particular parity under involution, such as the current $\phi(\Gamma^\dagger) = -\phi(\Gamma)$. This specific constraint prompts the question of whether other relationships exist between the statistics of general observables and the entropy production. Such general relations were the subject of recent studies [33,35,36].

Expanding on the idea that the average entropy production is equivalent to the Kullback-Leibler (KL) divergence $\langle \Sigma \rangle_F = \sum_\Gamma P_F(\Gamma) \ln P_F(\Gamma)/P_B(\Gamma^\dagger)$, we extend this consideration to encompass any f divergence, demonstrating that it too can be represented in terms of the statistics of Σ. We then leverage a theorem from information theory [37] to elucidate our main result for any convex function f,

$$\langle \phi \circ m \rangle_B - \langle f^*(\phi) \rangle_F \leqslant \langle f(e^{-\Sigma}) \rangle_F, \tag{3}$$

where f^* represents the Legendre transform of f, ϕ is any observable within the effective domain of f^* [ensuring that $f^*(\phi)$ is finite], and $\phi \circ m(\Gamma) := \phi(\Gamma^\dagger)$. This relation, referred to as the thermodynamic variation relation (TVR), is rooted in the variational representation of f divergences. Notably, the TVR does not impose any constraints on the parity of ϕ, thereby rendering it a universally applicable relation. The choice of f determines the specific nature of the relationships, as is demonstrated in the various applications. While the TVR does not have strict limitations for specific classes of observables (such as asymmetric currents in TURs), it is a tight expression for general observables, as explained further in the formalism section.

As one example of application of the TVR (3), for a particular choice of f, we obtain a universal TUR [36],

$$\frac{(\langle \phi \circ m \rangle_B - \langle \phi \rangle_F)^2}{\langle \phi^2 \rangle_F - \langle \phi \rangle_F^2} \leqslant \langle e^{-2\Sigma} \rangle_F - 1, \tag{4}$$

which is useful as a bound for the discrepancy between the means of the forward and backward processes, $\langle\phi\rangle_F$ and $\langle\phi\circ m\rangle_B$. Note that Eq. (4) presents a unique configuration where the left-hand side (LHS) solely consists of observables, while the right-hand side (RHS) is expressed in terms of the statistics of Σ. This configuration bears a resemblance to the thermodynamic uncertainty relation (TUR). Further discussion below will reveal that Eq. (4) corresponds to the f-divergence scenario, specifically, the χ^2 case.

The paper is organized as follows. First, we present the formalism to prove our main result. Then, we discuss the result and apply it for different choices of f: Total variation case, the χ^2 case yielding the universal TUR (4) for general observables, and the α-divergence case, resulting in thermodynamic relations consisting of high-order statistics of observables.

II. FORMALISM

Our result (3) is a direct application of a stronger result from information theory for f divergences that we review and discuss below.

Let $\Gamma\in S$ and $m:S\to S$ is any involution $m(m(\Gamma))=\Gamma$, with $\Gamma^\dagger:=m(\Sigma)$. Let $P_F:S\to[0,1]$ and $P_B:S\to[0,1]$ be any probability functions. We consider P_F and P_B such that $P_F(\Gamma)=0\to P_B(\Gamma^\dagger)=0$ for any $\Gamma\in S$ (absolute continuity). Let $\phi:S\to\mathbb{R}$ be any finite observable $[\sup_\Gamma|\phi(\Gamma)|<\infty]$.

We define f-divergence $D_f(P|Q)$ as follows: Let $f:[0,\infty)\to\mathbb{R}$ be a convex function, $f(1)=0$, and $\lim_{x\to0^+}f(x)=f(0)$. The f-divergence $D(P|Q)$, for P absolute continuous with respect to Q, is defined as

$$D_f(P|Q):=\sum_\Gamma f\left(\frac{P(\Gamma)}{Q(\Gamma)}\right)Q(\Gamma). \tag{5}$$

The result from information theory is a variational representation for f divergences [37], namely

$$D_f(P|Q)=\sup_{\phi\in\mathrm{dom}(f^*)}\langle\phi\rangle_P-\langle f^*(\phi)\rangle_Q, \tag{6}$$

where we define the convex conjugate f^* as the Legendre transformation,

$$f^*(y):=\sup_x xy-f(x). \tag{7}$$

When (5) is applied to $P_B(\Gamma^\dagger)$ and $P_F(\Gamma)$, we obtain from (1),

$$D_f(P_B\circ m|P_F)=\langle f(e^{-\Sigma})\rangle_F. \tag{8}$$

We also have from the involution property

$$\langle\phi\rangle_{P_B\circ m}=\langle\phi\circ m\rangle_{P_B}. \tag{9}$$

Combining (8) and (9) in (6), we obtain (3). Actually, (6) is stronger, which makes (3) a tight bound for general ϕ. If, however, one constrains ϕ to a class of observables [for instance, asymmetric, $\phi(\Gamma^\dagger)=-\phi(\Gamma)$], then the bound might become loose as it does not considered any property of ϕ on the derivation.

III. DISCUSSION

Relation (6) is called a variational representation because it represents the maximum of the functional $d[\phi]:=\langle\phi\rangle_P-\langle f^*(\phi)\rangle_Q$ over any observable ϕ for fixed P,Q. Loosely speaking, if ϕ' is the observable that maximizes $d[\phi]$, it means the variation is zero, $\delta d[\phi]/\delta\phi=0$ at $\phi=\phi'$, and we have $D_f(P|Q)=d[\phi']$. Thus, the f divergence is the maximum value of $d[\phi]$. The proof of this statement constitutes the theorem (6), which is sufficient to prove the main result (3). However, it depends on a relatively complex theorem that might not be easily intuitive.

Alternatively, a simpler and more intuitive proof of (3) goes as follows. From (7), we have Fenchel's inequality for any $x\in\mathrm{dom}(f)$ and $y\in\mathrm{dom}(f^*)$,

$$f(x)+f^*(y)\geqslant xy. \tag{10}$$

Now let $y:=\phi(\Gamma)$, where $\phi:S\to\mathrm{effdom}(f^*)$ is an observable that takes values in the effective domain of f^* [i.e., $f^*(y)$ is finite], and let $x:=P_B(\Gamma^\dagger)/P_F(\Gamma)$ in (10), which results in

$$f\left(\frac{P_B(\Gamma^\dagger)}{P_F(\Gamma)}\right)+f^*(\phi(\Gamma))\geqslant\phi(\Gamma)\frac{P_B(\Gamma^\dagger)}{P_F(\Gamma)}. \tag{11}$$

Finally, replacing $P_B(\Gamma^\dagger)/P_F(\Gamma)=\exp[-\Sigma(\Gamma)]$ from (1), multiplying (11) by $P_F(\Gamma)$ and summing over all Γ it yields

$$\sum_\Gamma[f(e^{-\Sigma(\Gamma)})+f^*(\phi(\Gamma))]P_F(\Gamma)\geqslant\sum_\Gamma\phi(\Gamma)P_B(\Gamma^\dagger). \tag{12}$$

Now using $\sum_\Gamma\phi(\Gamma)P_B(\Gamma^\dagger)=\sum_\Gamma\phi(\Gamma^\dagger)P_B(\Gamma)$ and reordering the terms in (12), we get

$$d[\phi]=\langle\phi\circ m\rangle_B-\langle f^*(\phi)\rangle_F\leqslant\langle f(e^{-\Sigma})\rangle_F, \tag{13}$$

which is our main result (3) for any observable with $\phi(\Gamma)\in\mathrm{dom}(f^*)$ for all Γ. Thus, we have proved $d[\phi]\leqslant D_f(P_B\circ m|P_F)$ for any ϕ, which results in $d[\phi']=\max_\phi d[\phi]\leqslant D_f(P_B\circ m|P_F)$.

In the subsequent applications, we will focus on a particular $f(x)$ in (3). We then calculate $\langle f[\exp(-\Sigma)]\rangle_F$ and the Legendre transform f^* respective to the chosen f. Ultimately, we determine the specific form of the TVR corresponding to this particular case. We select examples of f that have previously been examined in information theory [37], and we translate them into the language of thermodynamics.

IV. APPLICATIONS

A. Total variation

The result of this application can also be derived using other methods, but it is a staple example of how to use the TVR (3). Consider the convex function $f(x)=|x-1|/2$. Note that f is not differentiable at $x=1$, but it is not required for the result (3). Moreover, f satisfies the conditions for the f divergence (5) and $D_f(P|Q)$ is called the total variation distance in this case. The Legendre transform (7) is given by

$$f^*(y)=y, \tag{14}$$

for $|y|\leqslant1/2$, and $f^*=\infty$, for $|y|>1/2$. Within the effective domain of f^*, we have from (3)

$$\langle\phi\circ m\rangle_B-\langle\phi\rangle_F\leqslant\langle|1-e^{-\Sigma}|/2\rangle_F, \tag{15}$$

for $|\phi(\Gamma)|\leqslant1/2$ for all Γ. We multiply both sides by $2M\geqslant0$ and redefine $2M\phi\to\phi$ to obtain

$$\langle\phi\circ m\rangle_B-\langle\phi\rangle_F\leqslant M\langle|1-e^{-\Sigma}|\rangle_F, \tag{16}$$

for any $\sup_\Gamma|\phi(\Gamma)| \leqslant M$, which can be written for any bounded ϕ if you choose $M = \sup_\Gamma[|\phi(\Gamma)|] := |\phi|_{\max}$,

$$\frac{\langle\phi\circ m\rangle_B - \langle\phi\rangle_F}{2|\phi|_{\max}} \leqslant \frac{1}{2}\langle|1-e^{-\Sigma}|\rangle_F = \Delta(P_F|P_B\circ m), \quad (17)$$

where introduced the total variation $\Delta(P,Q) = \sum_\Gamma |P(\Gamma) - Q(\Gamma)|/2$. We note that (17) has a similar form to the TUR (2), in the sense that the LHS depends on the observable and the RHS depends on the statistics of Σ. This expression is valid for any bounded observable.

On a side note, check that the bound can also be obtained by the expression

$$\sum_\Gamma \frac{\phi(\Gamma)}{|\phi|_{\max}}\frac{[P_F(\Gamma) - P_B(\Gamma^\dagger)]}{2} \leqslant \sum_\Gamma \frac{|P_F(\Gamma) - P_B(\Gamma^\dagger)|}{2}, \quad (18)$$

and it is saturated by a minimal current $\phi(\Gamma) \in \{\phi_{\max}, -\phi_{\max}\}$ defined as $\phi(\Gamma) := \mathrm{sgn}[P_F(\Gamma) - P_B(\Gamma^\dagger)]|\phi|_{\max}$, just as the TUR (2).

B. χ^2 and universal TUR

Now we consider the convex function $f(x) = (x-1)^2$. It satisfies the conditions for f divergences and $D_f(P|Q)$ is the χ^2 divergence. The Legendre transform f^* (7) is given by

$$f^*(y) = y + y^2/4, \quad (19)$$

for any y. We also have $\langle f(e^{-\Sigma})\rangle_F = \langle e^{-2\Sigma}\rangle_F - 1$, where we used $\langle e^{-\Sigma}\rangle_F = 1$ explicitly. Then, the TVR (3) reads

$$\langle\phi\circ m\rangle_B - \left\langle\phi + \frac{\phi^2}{4}\right\rangle_F \leqslant \langle e^{-2\Sigma}\rangle_F - 1. \quad (20)$$

Since (20) is valid for any ϕ, now we redefine $\phi \to a(\phi - \langle\phi\rangle_F)$ and maximize the LHS of (20) with respect to a and obtain $a' := 2(\langle\phi\rangle_F - \langle\phi\circ m\rangle_B)/(\langle\phi^2\rangle_F - \langle\phi\rangle_F^2)$. Finally, replacing $\phi = a'(\phi - \langle\phi\rangle_F)$ in (20) yields

$$\frac{(\langle\phi\circ m\rangle_B - \langle\phi\rangle_F)^2}{\langle\phi^2\rangle_F - \langle\phi\rangle_F^2} \leqslant \langle e^{-2\Sigma}\rangle_F - 1, \quad (21)$$

which is the result (4). For the specific case of asymmetric observables, $\phi\circ m = -\phi$ and $F = B$, such that $\langle\,\rangle_F = \langle\,\rangle_B = \langle\,\rangle$, we note that

$$\frac{\langle\phi^2\rangle - \langle\phi\rangle^2}{\langle\phi\rangle^2} \geqslant \sinh^{-2}\left(\frac{g(\langle\Sigma\rangle)}{2}\right) \geqslant \frac{4}{\langle e^{-2\Sigma}\rangle - 1}, \quad (22)$$

where the first inequality in (22) is the TUR (2) and the second inequality comes from the TVR (4), which is consistent with the TUR (2) and we used a recent result [38] in the last inequality.

C. α divergences

Consider $f_\alpha(x) = [x^\alpha - \alpha x - (1-\alpha)]/[\alpha(\alpha-1)]$, for $\alpha \in (-\infty, 0)\cup(0,1)$ and $x \in [0,\infty)$. In this case, $D_f(P|Q)$ is called the α divergence. The Legendre transform f^* (7) is given by

$$f^*(y) = \frac{h(y)^\alpha - 1}{\alpha}, \quad (23)$$

for $y \in [-\infty, 1/(1-\alpha)]$, where $h(y) := [(\alpha-1)y + 1]^{1/(\alpha-1)}$. We also have

$$\langle f_\alpha(e^{-\Sigma})\rangle_F = \frac{\langle e^{-\alpha\Sigma}\rangle_F - 1}{\alpha(\alpha-1)}, \quad (24)$$

and the TVR (3) reads

$$\langle\phi\circ m\rangle_B - \left\langle\frac{h(\phi)^\alpha - 1}{\alpha}\right\rangle_F \leqslant \frac{\langle e^{-\alpha\Sigma}\rangle_F - 1}{\alpha(\alpha-1)}, \quad (25)$$

for ϕ such that $\phi(\Gamma) \in [-\infty, 1/(1-\alpha)]$ for all Γ. Now we redefine $\phi \to (\phi^{\alpha-1} - 1)/(\alpha-1)$ in (25), which makes $h(\phi)^\alpha \to \phi^\alpha$ and results in

$$-\frac{\langle\phi^{\alpha-1}\circ m\rangle_B}{1-\alpha} - \frac{\langle\phi^\alpha\rangle_F}{\alpha} \leqslant \frac{\langle e^{-\alpha\Sigma}\rangle_F}{\alpha(\alpha-1)}, \quad (26)$$

for $\inf_\Gamma \phi(\Gamma) \geqslant 0$. Redefining $\phi \to a\phi$ with the same domain and optimizing for a, we get $a' := \langle\phi^{\alpha-1}\circ m\rangle_B/\langle\phi^\alpha\rangle_F$. Replacing $\phi = a'\phi$ in (26) leads to

$$\frac{1}{\alpha(\alpha-1)}\frac{\langle\phi^{\alpha-1}\circ m\rangle_B^\alpha}{\langle\phi^\alpha\rangle_F^{\alpha-1}} \leqslant \frac{\langle e^{-\alpha\Sigma}\rangle_F}{\alpha(\alpha-1)}, \quad (27)$$

which, for $\alpha = -n < 0$ [such that $\alpha(\alpha-1) > 0$] and redefining $\phi \to \phi^{-1}$, results in

$$\frac{\langle|\phi|^n\rangle_F^{n+1}}{\langle|\phi|^{n+1}\circ m\rangle_B^n} \leqslant \langle e^{n\Sigma}\rangle_F, \quad (28)$$

where we introduced $|\phi|$ so that the result (28) applies to all observables for $n > 0$. Note that this application (28) is a relation between higher-order statistics of the absolute value of general observables $|\phi|$ (LHS) and the statistics of the entropy production Σ (RHS), in the same spirit of the TUR.

D. Hellinger's case

As a particular case of (27), consider $\alpha = 1/2$. In this case, $D_f(P|Q)$ is the squared Hellinger's distance. We have from (27)

$$\langle|\phi|^{1/2}\rangle_F\langle|\phi|^{-1/2}\circ m\rangle_B \geqslant \langle e^{-\Sigma/2}\rangle_F^2. \quad (29)$$

As (29) is valid for all ϕ, we redefine $|\phi|^{1/2} \to \exp(s\phi)$ for any $s \in \mathbb{R}$, resulting in

$$\langle e^{s\phi}\rangle_F\langle e^{-s\phi}\circ m\rangle_B \geqslant \langle e^{-\Sigma/2}\rangle_F^2, \quad (30)$$

We note that (30) is a lower bound for the product of two mgfs: $G_F(s) = \langle\exp(s\phi)\rangle_F$ and $G_B(-s) = \langle\exp(s\phi)\circ m\rangle_B = \langle\exp(-s\phi)\rangle_{B\circ m}$, valid for any observable ϕ, obtained from the TVR (3). Considering the case $F = B$, we also have from a previous result [38] for the moment generating function, $G(-1/2) := \langle\exp(-\Sigma/2)\rangle \geqslant \mathrm{sech}[g(\langle\Sigma\rangle/2)]$, which combined with (30) results in

$$\langle e^{s\phi}\rangle\langle e^{-s\phi}\circ m\rangle \geqslant \langle e^{-\Sigma/2}\rangle^2 \geqslant \mathrm{sech}^2\left(\frac{g(\langle\Sigma\rangle)}{2}\right) \geqslant e^{-\langle\Sigma\rangle}. \quad (31)$$

In summary, the first inequality in (31) is given by the TVR (3), but it could also be derived directly from Cauchy-Schwarz inequality, and the second is given by the bound for the moment generating function (mgf) of the entropy production (for the symmetric case, $F = B$). Note that the last one is straightforward from Jensen's inequality, $\langle e^{s\phi}\rangle\langle e^{-s\phi} \circ m\rangle = \langle e^{s\phi}\rangle\langle e^{-s\phi-\Sigma}\rangle \geqslant \exp(\langle s\phi - \Sigma - s\phi\rangle) = \exp(-\langle\Sigma\rangle)$.

V. CONCLUSIONS

We investigated a principle from information theory that suggests f divergences possess a variational representation, which implies they can be seen as the maximum of certain observable statistics. Following this, we characterized the f divergence using the statistics of entropy production, thereby establishing a broad connection between observables and entropy production.

Depending on the choice of f, different relations can be derived. As applications, we obtained a relation for bounded observables in terms of the total variation (17), a universal TUR (4), a high-order statistics relation (28), and a lower bound for the product of two mgfs (31).

The relation (3) utilizes the detailed fluctuation theorem in the form of (1), even when the random variable Σ is not the actual thermodynamic entropy production. For instance, in situations with quantum correlations [24], all the results in the paper remain valid, as long as we replace Σ with the appropriate term that contains the actual entropy production as well as other quantum information terms. For that reason, we expect this result to be useful in several situations beyond stochastic thermodynamics.

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