Thermodynamic Uncertainty Relation for Arbitrary Initial States

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The thermodynamic uncertainty relation (TUR) describes a trade-off relation between nonequilibrium currents and entropy production and serves as a fundamental principle of nonequilibrium thermodynamics. However, currently known TURs presuppose either specific initial states or an infinite-time average, which severely limits the range of applicability. Here we derive a finite-time TUR valid for arbitrary initial states from the Cramér-Rao inequality. We find that the variance of an accumulated current is bounded from below by the instantaneous current at the final time, which suggests that "the boundary is constrained by the bulk". We apply our results to feedback-controlled processes and successfully explain a recent experiment which reports a violation of a modified TUR with feedback control. We also derive a TUR that is linear in the total entropy production and valid for discrete-time Markov chains with nonsteady initial states. The obtained bound exponentially improves the existing bounds in a discrete-time regime.

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Introduction.—Over the last two decades, stochastic thermodynamics [1,2] has provided a general framework for understanding dissipation and thermal fluctuations far from equilibrium. Among the most important achievements are the fluctuation theorems [3–10], which refine various second-law inequalities into equalities. Recently, yet another rigorous result known as the thermodynamic uncertainty relation (TUR) was discovered [11], which dictates that the precision of a nonequilibrium time-integrated current observable J be bounded from below by the inverse of the total entropy production (EP) σ:

$$\mathcal{Q}_C \equiv \frac{\mathrm{Var}[J]}{\langle J\rangle^2}\sigma \geq 2, \tag{1}$$

where $\langle J\rangle$ and $\mathrm{Var}[J]$ are the average and the variance of J. The inequality (1) was originally discovered in biochemical networks [11] and proved by large deviation theory [12].

The original TUR (1) has a rather limited range of applicability [13], where the system is assumed to obey a Markovian continuous-time dynamics and should start from a nonequilibrium steady state (NESS) [14,15] or wait until the system relaxes to the NESS [12]. Without any one of these assumptions the bound could be violated [13,16–19]. A number of generalizations have been discussed, such as discrete-time Markov chains [16], periodically driven systems [17,18], measurement and feedback control [19,20], active matter systems [21–23], and quantum Markovian dynamics [24]. In particular, fluctuation theorems are found to directly lead to a bound involving an exponentiated EP, which is known as the generalized TUR (GTUR) [25–27]. Information-theoretic approaches such as the Martingale theory [28] and the Cramér-Rao inequality [29–32] have been utilized to derive the original TUR and its variants.

However, none of these generalizations are quite satisfactory because their bounds are either very loose such as the GTURs or involving terms with no clear physical meaning. Moreover, most of these bounds require an initialization to a NESS or other specific states. In this Letter, we fill the gaps by deriving universal bounds on fluctuation and dissipation valid for an arbitrary finite time and arbitrary initial states in continuous-time and discrete-time Markov processes via the Cramér-Rao inequality. For continuous-time processes, our bound is a highly nontrivial generalization of Eq. (1), where the ensemble-averaged time-integrated current $\langle J\rangle$ is replaced by the final-time instantaneous current multiplied by the time period, which implies that the boundary current is constrained by the bulk fluctuation and EP. Our formula reduces to the original TUR when the initial state is a NESS. We illustrate our result with minimal models and apply it to feedback-controlled processes. In particular, we explain a recent experiment which reports a violation in a modified TUR with feedback control [33]. For discrete-time processes, we find that the total EP modified by a certain sum of Kullback-Leibler divergences is rescaled by the minimal staying probability of the Markov chain. Our result exponentially improves the existing results in a discrete-time regime [16,34].

Setup.—We consider a general multichannel Markovian system S (see Fig. 1) described by the master equation

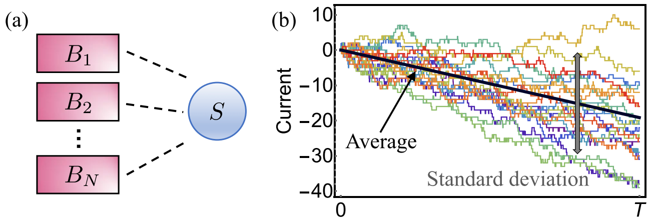

FIG. 1. (a) Schematic illustration of our setup. The system of interest S is coupled with several thermal reservoirs B_ν. The dynamics of the system is governed by a Markovian master equation (2). The state transition at each time is caused by the reservoirs. The current can be heat flow from the system to one of the reservoirs or a linear combination thereof. (b) Monte Carlo simulation of the time-integrated current in a two-heat-bath minimal model with a nonequilibrium steady state. Different colors correspond to different realizations. The black line indicates the average current $\langle J\rangle$. The length of the gray double arrow shows twice the standard deviation of the accumulated current.

$$\dot{\mathbf{P}}(t) = \mathcal{R}\mathbf{P}(t), \tag{2}$$

where $[\mathbf{P}(t)]_x \equiv P(x;t)$ is the system-state distribution at time t and $[\mathcal{R}]_{yx} \equiv r(x,y) = \sum_\nu r^\nu(x,y)$ is the time-independent transition rate matrix. Here $r^\nu(x,y)$ is the transition rate from x to y via channel ν; i.e., the transition is caused by the νth heat bath B_ν at inverse temperature β_ν. For a trajectory $\omega = (x_0, t_0 = 0; x_1, \nu_1, t_1; x_2, \nu_2, t_2; \ldots; x_n, \nu_n, t_n \le T \equiv t_{n+1})$, where a transition from x_{j-1} to x_j via channel ν_j occurs at t_j $(j = 1, 2, \ldots, n)$ during a finite time period T, the path probability density governed by Eq. (2) is given by

$$\mathcal{P}[\omega] = P(x_0)e^{-\sum_x \lambda(x)\tau_x[\omega] + \sum_{x\neq y,\nu} n^\nu_{xy}[\omega]\ln r^\nu(x,y)}, \tag{3}$$

where $P(x_0)$ is the initial distribution, $\lambda(x) = \sum_{y:y\neq x} r(x,y)$ is the escape rate for state x, $\tau_x[\omega] \equiv \sum_{j=0}^n \delta_{x_j x}(t_{j+1} - t_j)$ is the total time during which the system stays in state x, and $n^\nu_{xy}[\omega] \equiv \sum_{j=1}^n \delta_{x_{j-1}x}\delta_{x_j y}\delta_{\nu_j \nu}$ is the total number of transitions from x to y through channel ν. A general stochastic accumulated current is defined as

$$J[\omega] \equiv \sum_{x\neq y,\nu} n^\nu_{xy}[\omega] d^\nu(x,y), \tag{4}$$

where $d^\nu(x,y) = -d^\nu(y,x)$ is the antisymmetric increment associated with transition $x \to y$ via channel ν. For example, $d^\nu(x,y) = \delta_{x_0 x}\delta_{y_0 y}\delta_{\nu_0 \nu}$ gives the net number of transitions from x_0 to y_0 via channel ν_0, while $d^\nu(x,y) = (E_x - E_y)\delta_{\nu_0\nu}$ (E_x: energy of state x) gives the net heat flow into the ν_0th bath. Provided that the local detailed balance $r^\nu(x,y)e^{-\beta_\nu E_x} = r^\nu(y,x)e^{-\beta_\nu E_y}$ holds, the ensemble-averaged total EP for the dynamics is given by [35]

$$\sigma = \int_0^T dt \sum_{x\neq y,\nu} P(x;t) r^\nu(x,y) \ln\frac{P(x;t)r^\nu(x,y)}{P(y;t)r^\nu(y,x)}. \tag{5}$$

Main result.—We show that the fluctuation of an arbitrary accumulated current (4) is bounded by the total EP and the final instantaneous current:

$$\mathcal{Q}_T \equiv \frac{\mathrm{Var}[J]}{[Tj(T)]^2}\sigma \ge 2, \tag{6}$$

where $j(T) \equiv \sum_{x\neq y,\nu} P(x;T)r^\nu(x,y)d^\nu(x,y)$ is the ensemble-averaged final instantaneous current. Such an inequality can equivalently be written as

$$|j(T)| \le \sqrt{\frac{1}{2}\mathrm{Var}\left[\frac{J}{T}\right]\sigma}, \tag{7}$$

which implies that the boundary current is constrained by the bulk (time-averaged) current fluctuation and dissipation. In other words, if we want to achieve a large instantaneous current, which means driving the system far from equilibrium, we should either suffer large dissipation or sacrifice the quality (small fluctuation) of the time-integrated current. This statement refines the dissipation-precision trade-off of conventional TURs for NESSs [11,12,14,15].

Some remarks are in order here. First, the bound (6) holds for arbitrary initial states and there can be multiple transition channels. If there is only a single heat bath and the initial state is a NESS, the denominator is nothing but the accumulated current; thus the original TUR (1) is recovered. Second, every term in our bound allows a clear physical interpretation and is experimentally measurable [36–38]. Previous efforts at generalizing the TUR mainly focus on modifying the EP [17,18,31,32]; however, the modification lacks a clear physical meaning. Third, our result implies a sufficient (necessary) condition for the validity (violation) of the original TUR (1) for a nonsteady initial state—the final current $j(T)$ is larger (smaller) than the time-averaged one $\bar{j} \equiv \langle J\rangle/T$. This is primarily due to an increase (decrease) of the current, as we will illustrate in some minimal models. Finally, we emphasize that even the widely applicable GTUR generally breaks down for an arbitrary initial state since it requires that the initial and final states coincide [25].

Two minimal models.—Before going into the derivation of the main result, let us examine the main result (6) in some minimal models. We first consider the simplest example for an equilibrium steady state. As shown in Fig. 2(a), a two-level system with states 0 and 1 couples to a single heat reservoir at inverse temperature β. The energy gap between the two states is set to be $\Delta = 1$ and the state 0 is assumed to be lower in energy. We start from an arbitrary initial state $\mathbf{P}(0) = [p, 1-p]^\mathbb{T}$ ($\mathbb{T}$: transpose) and let the system relax to its equilibrium steady state. The current is chosen to be the

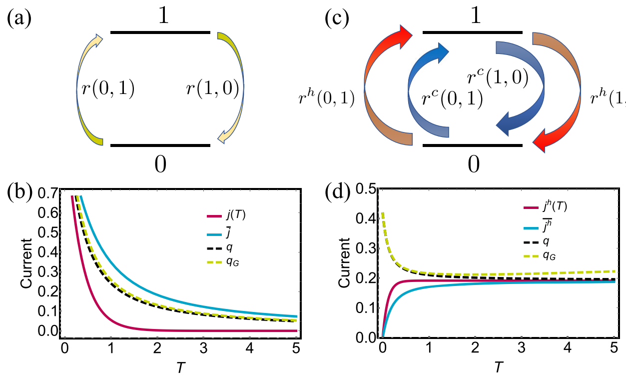

FIG. 2. (a) Two-level system coupled with a single heat bath. (b) Comparison between the final instantaneous current (red), the time-averaged current $\bar{j} \equiv \langle J \rangle / T$ (blue) and the current bounds from the conventional (black dashed, $q \equiv T^{-1}\sqrt{\mathrm{Var}[J]\sigma/2}$) and generalized [green dashed, $q_G \equiv T^{-1}\sqrt{\mathrm{Var}[J](e^{\sigma}-1)/2}$] TURs. Our inequality (7) is satisfied, whereas the original one (1) is not. The initial state is chosen to be $\mathbf{P}(0) = [0.3, 0.7]^{\mathbb{T}}$ and the transition rates are $r(0,1) = 1$ and $r(1,0) = 2$. (c) Two-level system coupled with cold and hot baths. Red arrows represent the transitions via coupling to the hot heat bath, and blue ones represent the cold bath. (d) Same quantities as in (b) for the model in (c), where both inequalities (6) and (1) are valid. The initial state is chosen so that the initial hot current vanishes. We set $\beta_h = 1$, $\beta_c = 1.5$, and $r^h(0,1) = r^c(0,1) = 1$ in our simulation.

net flow from 1 to 0. According to the local detailed balance condition, two transition rates $r(0,1)$ and $r(1,0)$ satisfy $r(0,1) = e^{-\beta} r(1,0)$. By utilizing full counting statistics [39–41], we can analytically calculate all the quantities in the bound (6) [42]. In Fig. 2(b), we find that only our bound holds, whereas the conventional TUR and the GTUR are violated. This is because the currents decrease exponentially with time, implying that the time-averaged current is larger than the current at the final time. Consequently, our $\mathcal{Q}_T$ value should be larger than the conventional $\mathcal{Q}_C$, and therefore the conventional TUR may fail.

We now consider a simplest model for an NESS which involves a two-level system with states 0 and 1 and the energy gap $\Delta = 1$ in contact with two heat baths at inverse temperatures β_h and β_c. Since the state transition can be induced by either of the baths, there is a total of four transition rates [see Fig. 2(c)] which satisfy two local detailed balance relations: $r^h(1,0) = e^{\beta_h} r^h(0,1)$ and $r^c(1,0) = e^{\beta_c} r^c(0,1)$. The current is chosen to be the heat flow from the hot bath, whose instantaneous value at time t reads $j^h(t) = P_0(t) r^h(0,1) - P_1(t) r^h(1,0)$. We start from a special initial state so that $j^h(0)$ vanishes. The current fluctuation is again calculated from full counting statistics [42]. In Fig. 2(d), we see that both $j^h(T)$ and $\overline{j^h}$ are bounded from above by q, while $j^h(T)$ is tighter. This is because the current monotonically increases so that the final current is larger than the time-averaged one. Accordingly, our $\mathcal{Q}_T$ should be smaller than $\mathcal{Q}_C$. Since

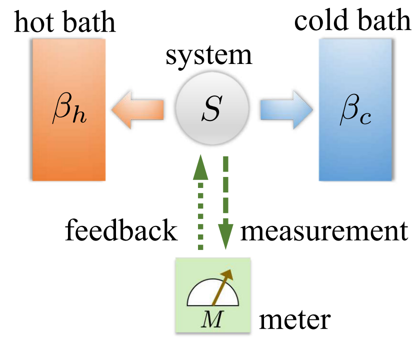

FIG. 3. System in contact with cold and hot baths subject to measurement and feedback. The system is probed by a meter M and subject to feedback control according to the measurement outcome. After the feedback, the system undergoes Markovian dynamics by interacting with two heat baths.

$\mathcal{Q}_T$ is bounded from below by 2, the larger quantity $\mathcal{Q}_C$ should be bounded from below by 2 as well.

Application to feedback-controlled processes.—Our TUR (6) can readily be extended to include the effect of measurement and feedback control in the context of information thermodynamics [43]. As a general setup, the system of interest S couples with multiple heat baths B_νs at inverse temperatures β^νs. In addition, as shown in Fig. 3, a meter M probes the state of the system and performs feedback control by changing the transition matrix to $\mathcal{R}_m$ according to the measurement outcome m [44]. We assume that the measurement and feedback are done instantaneously, after which the system will relax during a time interval τ through coupling to the baths. This assumption is justified if they are performed sufficiently fast compared with the stochastic transitions in the system [9,33,44]. At the end of the relaxation the meter will be reset to its default state, e.g., 0, and then the next cycle begins [45]. The system will eventually reach a stroboscopic steady state in the sense that the state of the system will be statistically the same after one period while it can change during each cycle. Within a single relaxation period, the total EP should be $\sigma = \mathcal{I}(0) - \mathcal{I}(\tau) + \sigma_S + \sigma_B$, where $\mathcal{I}(t) \equiv \sum_{s,m} P(s,m;t) \ln\{[P(s,m;t)]/[P_S(s;t)P_M(m)]\}$ is the mutual information between the system and the meter at time t with $P(s,m;t)$, $P_S(s;t)$ and $P_M(m)$ being the joint distribution of the system and the meter, the marginal distribution of the system and that of the meter; σ_S and σ_B are the entropy changes in the system and baths, respectively. Here we have used the fact that $P_M(m)$ is time independent and thus there is no entropy production in the meter. Defining the consumed mutual information $\Delta\mathcal{I} \equiv \mathcal{I}(0) - \mathcal{I}(\tau)$ and the physical entropy production $\sigma_P \equiv \sigma_S + \sigma_B$, we have

$$\mathcal{Q}_T = \frac{\mathrm{Var}[J]}{[\tau j(\tau)]^2}(\sigma_P + \Delta\mathcal{I}) \geq 2, \tag{8}$$

where J can be an arbitrary current determined from an antisymmetric increment $d_m^\nu(x,y)$ that generally depends on the measurement outcome. Note that if the system reaches a stroboscopic steady state, then $\sigma_P = \sigma_B$.

We can explain a recent experiment on feedback control [33] with the criteria described in the previous section. The authors in Ref. [33] constructed an information engine consisting of an optically trapped colloidal particle immersed in a heat reservoir at inverse temperature β, following a repeated protocol of measurement, feedback, and relaxation. In the ith cycle, the demon measures the position x_i of the particle. Due to noise, the outcome y_i could be different from x_i. The center of the potential λ_{i-1} is suddenly shifted to y_i and let the particle relax for a period τ before the next cycle begins according to the overdamped Langevin equation. The system will reach a stroboscopic steady state after many cycles. The stochastic current is the work βW performed on the particle by shifting the potential. Because there is only one heat bath, the dynamics after feedback control is simply a relaxation process toward equilibrium. The absolute value of the current always decreases with time. The conventional TUR can be violated for a certain range of parameters as reported in Ref. [33].

Generalization to discrete-time Markov chains.—We consider a general multichannel Markovian system S starting from an arbitrary initial state as in Fig. 1(a) which is now described by the following discrete-time evolution equation:

$$P(x,t_i) = \sum_{y,\nu} A^\nu(x|y) P(y,t_{i-1}), \tag{9}$$

where $P(x,t_i)$ is the probability of the system being in state x at time t_i and $A^\nu(x|y)$ is the transition probability from state y to state x through channel ν. The transition probabilities satisfy the normalization condition: $\sum_{x,\nu} A^\nu(x|y) = 1$. The total EP for n steps is given by [42,46,47]

$$\sigma = \sum_{i=1}^{n} \sum_{x,y,\nu} P(x,t_{i-1}) A^\nu(y|x) \ln \frac{P(x,t_{i-1}) A^\nu(y|x)}{P(y,t_i) A^\nu(x|y)}. \tag{10}$$

The TUR valid for this process (9) reads [42]

$$\mathcal{Q}_D \equiv \frac{\mathrm{Var}[J]}{[n j(t_{n-1})]^2} \frac{\tilde{\sigma}}{a} \geq 2, \tag{11}$$

where the tilde EP is defined as $\tilde{\sigma} \equiv \sigma + \sum_{i=1}^{n} D_{\mathrm{KL}}[\mathbf{P}(t_i)||\mathbf{P}(t_{i-1})]$ with D_{KL} being the Kullback-Leibler divergence, a is the minimal staying probability $a \equiv \min_x A(x|x)$, and $j(t_{n-1}) \equiv \sum_{x\neq y,\nu} P(x,t_{n-1}) A^\nu(y|x) d^\nu(y|x)$ is the current at the final step. We make two comments. First, the bound (11) can be reduced to the continuous-time bound (6) in the limit of $\Delta t \to 0$. Second, there exists a discrete-time TUR exponentiated in the total EP for NESS [16]. Our bound (11) exponentially improves the result because it is linear in the total EP.

Derivation of the main result.—We finally prove inequality (6). We can employ large deviation theory to derive our result (6) [42,48]. However, a more straightforward and elegant approach is based on the generalized Cramér-Rao inequality [49]:

$$\mathrm{Var}_\theta[\Theta] \geq \frac{\psi'(\theta)^2}{F(\theta)}, \tag{12}$$

where θ is a parameter, $F(\theta)$ is the Fisher information and $\Theta[\omega]$ is an unbiased estimator for a smooth function $\psi(\theta)$, i.e., $\langle \Theta \rangle_\theta = \psi(\theta)$. Here, the average is defined as $\langle g \rangle_\theta \equiv \int \mathcal{D}\omega g[\omega] \mathcal{P}_\theta[\omega]$ for a parametrized distribution $\mathcal{P}_\theta[\omega]$. Our goal is to relate each term in (12) to the thermodynamic quantities in Eq. (6) [30–32]. To this end, we first parametrize a typical path probability density in Eq. (3) as

$$\mathcal{P}_\theta[\omega] = P_\theta(x_0) e^{\sum_{j=1}^{n} \ln r_\theta^{\nu_j}(x_{j-1},x_j;t_j) - \sum_{j=0}^{n} \int_{t_j}^{t_{j+1}} dt \lambda_\theta(x_j;t)}, \tag{13}$$

which is determined from an auxiliary transition matrix $\mathcal{R}_\theta(t)$ with time-dependent entries $[\mathcal{R}_\theta(t)]_{yx} = r_\theta^\nu(x,y;t)$ and $[\mathcal{R}_\theta(t)]_{xx} = -\lambda_\theta(x;t) \equiv -\sum_{y:y\neq x,\nu} r_\theta^\nu(x,y;t)$. When we set θ to be a certain value, say 0, $r_\theta^\nu(x,y;t)$ should go back to the time-independent typical value $r^\nu(x,y)$. By definition, the Fisher information can be calculated from Eq. (13) as

$$F(\theta) = \int_0^T dt \sum_{x\neq y,\nu} P_\theta(x;t) r_\theta^\nu(x,y;t) \left(\frac{\partial}{\partial\theta} \ln r_\theta^\nu(x,y;t) \right)^2, \tag{14}$$

where the initial auxiliary state is assumed to be a typical one, i.e., $P_\theta(x_0) = P(x_0)$. By choosing $\Theta[\omega] = \sum_{j=1}^{n} d^{\nu_j}(x_{j-1},x_j)$ to be a general accumulated current, $\mathrm{Var}_\theta[\Theta]$ at $\theta = 0$ simply gives the desired current fluctuation. In this case, $\psi(\theta)$ is nothing but the ensemble-averaged current given by

$$\langle \Theta \rangle_\theta = \int_0^T dt \sum_{x\neq y,\nu} P_\theta(x;t) r_\theta^\nu(x,y;t) d^\nu(x,y), \tag{15}$$

where $P_\theta(x;t)$ is determined from the solution of the parametrized master equation with generator $\mathcal{R}_\theta(t)$.

Comparing the structure of our TUR (6) with the Cramér-Rao inequality (12), we relate the Fisher information $F(0)$ and $\psi'(0)$ to half of the total EP σ given in Eq. (5) and the final current $j(T)$, respectively. As a sufficient condition, we choose the parametrization $r_\theta^\nu(x,y;t) = r^\nu(x,y) e^{\theta\alpha_{xy}^\nu(t)}$, and assume that for each pair of (x,y) at any time t and any channel ν, the following conditions are satisfied:

$$K_{xy}^{\nu}(\alpha_{xy}^{\nu})^2 + K_{yx}^{\nu}(\alpha_{yx}^{\nu})^2 = \frac{1}{2}(K_{xy}^{\nu} - K_{yx}^{\nu})\ln\frac{K_{xy}^{\nu}}{K_{yx}^{\nu}}, \quad (16)$$

$$K_{xy}^{\nu}\alpha_{xy}^{\nu} - K_{yx}^{\nu}\alpha_{yx}^{\nu} = K_{xy}^{\nu} - K_{yx}^{\nu}, \quad (17)$$

where $K_{xy}^{\nu}(t) \equiv P(x;t)r^{\nu}(x,y)$ and its time dependence [as well as that in $\alpha_{xy}^{\nu}(t)$] is omitted for simplicity. The above two equations, whose solutions always exist [42], guarantee $F(0) = \frac{1}{2}\sigma$ and $\psi'(0) = Tj(T)$ for an arbitrary $d^{\nu}(x,y)$. The former simply follows from Eqs. (5) and (14). To show the latter, we note that, up to the leading (first) order in θ, the parametrized probability is given by [42]

$$\mathbf{P}_{\theta}(t) = \mathbf{P}(t) + \theta t\dot{\mathbf{P}}(t) + O(\theta^2), \quad (18)$$

leading to $\partial_{\theta}\mathbf{P}_{\theta}(t)|_{\theta=0} = t\dot{\mathbf{P}}(t)$. Combining this result with Eq. (17), we find that $\psi'(0) \equiv \partial_{\theta}\langle\Theta\rangle|_{\theta=0}$ is an integral of a total derivative $(d/dt)[tj(t)]$ with $j(t) \equiv \sum_{x\neq y,\nu} P(x;t)r^{\nu}(x,y)d^{\nu}(x,y)$ being the instantaneous current. Therefore, we obtain $\psi'(0) = tj(t)|_0^T = Tj(T)$. For the case with feedback control, we have only to add another index m representing the meter's state.

Summary and outlook.—We have established new TURs (6) and (11) for general continuous- and discrete-time multichannel Markovian systems starting from an arbitrary initial state. Our results includes the conventional TURs [11,12,14,15] as special cases and incorporate the effect of measurement and feedback control [see inequality (8)]. The continuous bound (6) can also be used to explain the recent experiment [33]. The discrete bound (11) exponentially improves the TURs in a discrete-time regime. While our results greatly extend the range of validity of the TURs, the time-homogeneous assumption of transition rates and probabilities needs to be made. How to relax this requirement is an important subject for future studies. It should also be of interest to investigate the effect of absolute irreversibility [50,51] on the TURs.

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