Geometrical Bounds of the Irreversibility in Markovian Systems

Tan Van Vu* and Yoshihiko Hasegawa†
Department of Information and Communication Engineering, Graduate School of Information Science and Technology, The University of Tokyo, Tokyo 113-8656, Japan

(Received 20 July 2020; revised 3 November 2020; accepted 3 December 2020; published 4 January 2021)

We derive geometrical bounds on the irreversibility in both quantum and classical Markovian open systems that satisfy the detailed balance condition. Using information geometry, we prove that irreversible entropy production is bounded from below by a modified Wasserstein distance between the initial and final states, thus strengthening the Clausius inequality in the reversible-Markov case. The modified metric can be regarded as a discrete-state generalization of the Wasserstein metric, which has been used to bound dissipation in continuous-state Langevin systems. Notably, the derived bounds can be interpreted as the quantum and classical speed limits, implying that the associated entropy production constrains the minimum time of transforming a system state. We illustrate the results on several systems and show that a tighter bound than the Carnot bound for the efficiency of quantum heat engines can be obtained.

DOI: 10.1103/PhysRevLett.126.010601

Introduction.—Irreversibility, which is quantified by entropy production, is a fundamental concept in classical and quantum thermodynamics [1–3]. Most macroscopic natural phenomena are irreversible, although their microscopic physical processes are generally time symmetric. According to the second law of thermodynamics, a system undergoing an irreversible process generates (on average) a positive entropy amount $\Delta S_{\mathrm{tot}} \geq 0$. This bound can be saturated only when operations are performed in the infinite-time quasistatic limit. However, as real processes must be completed in finite time, they are accompanied by a certain dissipation. Tightening the lower bound on entropy production not only deepens our understanding of how much heat must be dissipated but also provides insights into quantum technologies such as quantum computation [4] and quantum heat engines [5].

In recent years, many studies have characterized the dissipation of thermodynamic processes using information geometry [6–16], which is the application of techniques from differential geometry to the manifolds of probability distributions and density matrices [17]. Reference [18] showed that entropy production in a closed driven quantum system is bounded from below by the Bures length between the final state and the corresponding equilibrium state. Following a similar approach, Ref. [19] determined a geometrical upper bound for the equilibration processes of open quantum systems. As is well known, in classical systems near equilibrium, irreversible entropy production is related to the distance between thermodynamic states [20,21]. Meanwhile, a lower bound on dissipation in terms of the Wasserstein distance [22] has been defined for nonequilibrium Markovian systems described by Langevin equations [23–25]. Information geometry is useful for deriving other important relations, such as speed limits [26–29], quantum work fluctuation-dissipation relations [30], and the efficiency-power trade-off in microscopic heat engines [31].

In this Letter, we enlarge the family of these universal relations by investigating quantum and classical open systems that satisfy the detailed balance condition. These systems obey microscopically reversible Markovian dynamics [32] and can be modeled as coupled to an infinite thermal reservoir. Examples include equilibration processes, which have received considerable interest in nonequilibrium physics [33–36]. Specifically, we derive geometrical lower bounds on the entropy production in reversible Markovian systems described by master equations. The spaces of quantum states and discrete distributions are treated as Riemannian manifolds, on which the time evolution of a system state is described by a smooth curve. By defining a modified Wasserstein metric, we prove that the entropy production is bounded from below by the square of the geodesic distance between the initial and final states divided by the process time [cf. Eqs. (3) and (9)]. The derived bounds strengthen the Clausius inequality of the second law for reversible Markovian systems. They can also be regarded as generalizations of the bounds reported in Refs. [23,25] to the discrete-state quantum and classical systems. The equality of these bounds is attained only when the system dynamics follow the shortest paths. Our modified metric is a quantum generalization of the Wasserstein metric, which measures the distance between two distributions and is widely used in optimal transport problems [22]. Interestingly, the obtained inequalities can be interpreted as speed limits [37–44], which establish the trade-off relations between the speed and dissipation cost of a state transformation. We numerically illustrate the results on a quantum Otto engine and a classical two-level system.

Riemannian geometry.—First, we briefly describe some relevant concepts of Riemannian geometry. Let M be a smooth Riemannian manifold equipped with a metric g_p on the tangent space at each point $p \in M$. Note that there is an infinite number of such metrics, as long as the linearity, symmetry, and positive-definite conditions are met. Notably, there exists a family of monotone metrics that are contractive under physical maps [45–47], a representative of which is the Fisher information metric [48,49]. In the quantum case, M can be the space of density operators ρ, which are positive (i.e., $\rho \geq 0$) and have unit trace (i.e., $\mathrm{tr}\rho = 1$). Meanwhile, in classical discrete-state systems, M can be the collection of discrete distributions $\boldsymbol{p} = [p_1, \ldots, p_N]^\top$, where $p_n \geq 0$ and $\sum_{n=1}^N p_n = 1$. The length of a smooth curve $\{\gamma(t)\}_{0\leq t\leq\tau}$ on the manifold can be defined as $\ell(\gamma) \coloneqq \int_0^\tau \sqrt{g_\gamma(\dot\gamma,\dot\gamma)}dt$, where the dot denotes a time derivative. The geodesic distance between two points can be then defined as the minimum length over all smooth curves γ connecting those points. Throughout this Letter, we use the standard notation $\langle\cdot,\cdot\rangle$ of the scalar inner product, i.e., $\langle \boldsymbol{x}, \boldsymbol{y}\rangle = \boldsymbol{x}^\top \boldsymbol{y}$ for the classical case and $\langle X, Y\rangle = \mathrm{tr}\{X^\dagger Y\}$ for the quantum case.

Bounds in Markovian quantum systems.—We first consider an open quantum system that is weakly coupled to a heat bath at the inverse temperature β. The time evolution of the density operator $\rho(t)$ of this system is described by this Lindblad master equation [50,51]:

$$\dot\rho = \mathcal{L}(\rho) \coloneqq -i[H(t),\rho] + \mathcal{D}(\rho), \tag{1}$$

where $\mathcal{L}$ is the Lindblad operator, $H(t)$ is the Hamiltonian, and $\mathcal{D}(\rho)$ is the dissipator given by $\mathcal{D}(\rho) \coloneqq \sum_{\mu,\omega}\alpha_\mu(\omega)[2L_\mu(\omega)\rho L_\mu^\dagger(\omega) - \{L_\mu^\dagger(\omega)L_\mu(\omega),\rho\}]$. Here, $\{\cdot,\cdot\}$ is the anticommutator and $L_\mu(\omega)$ is a jump operator that satisfies $L_\mu^\dagger(\omega) = L_\mu(-\omega)$ and $[L_\mu(\omega), H] = \omega L_\mu(\omega)$. Note that jump operators and coupling coefficients can be time dependent, but we omit the time notation for simplicity. We also assume that the detailed balance condition $\alpha_\mu(\omega) = e^{\beta\omega}\alpha_\mu(-\omega)$ is satisfied and the system is ergodic [52] (i.e., $[L_\mu(\omega), X] = 0$ for all μ, ω if and only if X is proportional to the identity operator). These assumptions are sufficient conditions for the Gibbs state $\rho^{\mathrm{eq}}(t) \coloneqq e^{-\beta H(t)}/Z_\beta(t)$ to be the instantaneous stationary state of the Lindblad master equation, i.e., $\mathcal{L}[\rho^{\mathrm{eq}}(t)] = 0$ [53,54], where $Z_\beta(t)$ is the partition function.

The entropy growth of the open system during time period τ is $\Delta S_{\mathrm{tot}} = \int_0^\tau \sigma_{\mathrm{tot}}(t)dt$, where $\sigma_{\mathrm{tot}}(t) = \dot S + \beta\dot Q$ is the entropy production rate [55]. Here, $S = -\mathrm{tr}\{\dot\rho(t)\ln\rho(t)\}$ denotes the von Neumann entropy flux of the system and $\dot Q = -\mathrm{tr}\{H(t)\dot\rho(t)\}$ denotes the heat flux dissipated from the system to the bath. The entropy production rate can be rewritten as $\sigma_{\mathrm{tot}}(t) = -\langle \ln\rho(t) - \ln\rho^{\mathrm{eq}}(t), \dot\rho(t)\rangle = -(d/dt)S[\rho(t)||\rho^{\mathrm{eq}}(t)]$, where $S(\rho_1||\rho_2) \coloneqq \mathrm{tr}\{\rho_1(\ln\rho_1 - \ln\rho_2)\}$ is the relative entropy of ρ_1 with respect to ρ_2, and the time derivative does not act on $\rho^{\mathrm{eq}}(t)$. $\sigma_{\mathrm{tot}}(t)$ is non-negative because the relative entropy is monotonic under completely positive trace-preserving maps; thereby, one can obtain the Clausius inequality $\Delta S_{\mathrm{tot}} \geq 0$.

We now construct an operator $\mathcal{K}_\rho$, and alternatively express the Lindblad master equation [Eq. (1)] in the form $\dot\rho = \mathcal{K}_\rho(-\ln\rho + \ln\rho^{\mathrm{eq}})$ [56]. For an arbitrary density operator ρ, we define a tilted operator $[\rho]_\theta(X) \coloneqq e^{-\theta/2}\int_0^1 e^{s\theta}\rho^s X\rho^{1-s}ds$, where θ is a real number. Using this operator, $\mathcal{K}_\rho$ can be explicitly constructed as $\mathcal{K}_\rho(\psi) \coloneqq i\beta^{-1}[\psi,\rho] + \mathcal{O}_\rho(\psi)$. Here, $\mathcal{O}_\rho(\psi) \coloneqq \sum_{\mu,\omega} e^{-\beta\omega/2}\alpha_\mu(\omega)[L_\mu(\omega), [\rho]_{\beta\omega}([L_\mu^\dagger(\omega),\psi])]$ is a self-adjoint positive operator, which can be interpreted as a quantum analog of the Onsager matrix. For an arbitrary smooth curve $\{\gamma(t)\}_{0\leq t\leq\tau}$, there exists a unique vector field of traceless self-adjoint operators $\{\nu(t)\}_{0\leq t\leq\tau}$ such that $\dot\gamma(t) = \mathcal{K}_\gamma[\nu(t)]$ for all t. Exploiting this representation, one can define a metric g under which the gradient flow of the instantaneous relative entropy equals the flow associated with the system dynamics [58–61]. Specifically, we define the metric $g_\gamma(\dot\gamma,\dot\gamma) = \langle\nu, \mathcal{K}_\gamma(\nu)\rangle$, which is always non-negative because $\langle\nu,\mathcal{K}_\gamma(\nu)\rangle = \langle\nu,\mathcal{O}_\gamma(\nu)\rangle \geq 0$. Although the operator $\nu(t)$ is implicitly obtained from $\dot\gamma(t)$, it can be regarded as the generalized thermodynamic force, and $g_\gamma(\dot\gamma,\dot\gamma)$ is the quantum dissipation function [62]. This can be clarified as considering the path generated by the system dynamics, i.e., $\dot\rho = \mathcal{K}_\rho(\phi)$ and $g_\rho(\dot\rho,\dot\rho) = \sigma_{\mathrm{tot}}(t)$, where $\phi = -(\ln\rho - \ln\rho^{\mathrm{eq}}) + c$ is a traceless self-adjoint operator. In addition to the thermodynamic length $\ell(\gamma)$, the thermodynamic divergence of a path, defined as [20]

$$\ell_q(\gamma)^2 \coloneqq \tau\int_0^\tau g_\gamma(\dot\gamma,\dot\gamma)dt, \tag{2}$$

is a measure of the dissipation along the path. Note that by the Cauchy-Schwarz inequality, $\ell_q(\gamma) \geq \ell(\gamma)$. A modified Wasserstein distance between two states ρ_0 and ρ_τ can be defined as $\mathcal{W}_q(\rho_0,\rho_\tau) \coloneqq \inf_\gamma\{\ell_q(\gamma)\}$, where the infimum is taken over smooth curves with end points ρ_0 and ρ_τ. For relaxation processes, $\mathcal{W}_q$ is exactly the geodesic distance induced by the defined metric [63]. It has been shown that a clear-cut definition of the quantum Wasserstein distance, by the direct generalization of the classical one, is not achievable [65]. Our generalization here is based on the Benamou-Brenier flow formulation of the original L^2 Wasserstein [60,61,66]. Other generalized metrics based on quantum couplings [65,67,68] and the Kantorovich-Rubinstein duality [69] have also been proposed in the literature. From the definition of $\mathcal{W}_q$, the first main result is a geometrical lower bound of the entropy production:

$$\Delta S_{\mathrm{tot}} \geq \frac{\mathcal{W}_q[\rho(0),\rho(\tau)]^2}{\tau}. \tag{3}$$

The inequality Eq. (3) indicates that the irreversible entropy production is lower bounded by the distance between the

initial and final states. This bound is stronger than the conventional second law of thermodynamics; it can also be interpreted as a quantum speed limit, as it limits the time required to transform the system state. The limit is governed by dissipation and the geometrical distance between states. To generalize the result to the infinite-dimensional Hilbert space, the existence and the construction of the operator $\nu(t)$ in the definition of the metric must be clarified. Since the distance $\mathcal{W}_q$ is usually difficult to compute explicitly, we provide a lower bound of $\mathcal{W}_q$ in terms of the tracelike distance $d_T(\rho_0,\rho_\tau)=\sum_{n=1}^{N}|a_n-b_n|$, where $\{a_n\}$ and $\{b_n\}$ are increasing eigenvalues of ρ_0 and ρ_τ, respectively. Specifically, we prove that $\mathcal{W}_q(\rho_0,\rho_\tau)^2\geq d_T(\rho_0,\rho_\tau)^2/4\mathcal{A}_T$ [56], where $\mathcal{A}_T:=\tau^{-1}\int_0^\tau\sum_{\mu,\omega}\alpha_\mu(\omega)\|L_\mu(\omega)\|_\infty^2 dt$ characterizes the timescale of the quantum system and $\|X\|_\infty$ denotes the spectral norm of the operator X. Note that this lower bound on $\mathcal{W}_q$ is not invariant under the well-known unitary transformation of jump operators because the conditions of jump operators uniquely determine the parameterization of the dynamics. Consequently, the entropy production is also bounded from below by the tracelike distance between the initial and final states, given by

$$\Delta S_{\mathrm{tot}}\geq\frac{d_T[\rho(0),\rho(\tau)]^2}{4\tau\mathcal{A}_T}. \tag{4}$$

The Hamiltonian and jump operators of a system must be time independent in order to equilibrate with the environment and reach a steady state. Thus, during equilibration, the entropy production can be bounded by the distance $d_E(\rho_0,\rho_\tau)=|\mathrm{tr}\{H(\rho_0-\rho_\tau)\}|$ of the average energy change [56],

$$\Delta S_{\mathrm{tot}}\geq\frac{d_E[\rho(0),\rho(\tau)]^2}{\tau\mathcal{A}_E}, \tag{5}$$

where $\mathcal{A}_E:=\sum_{\mu,\omega}\alpha_\mu(\omega)\omega^2\|L_\mu(\omega)\|_\infty^2$. A tighter bound in terms of the square of the heat current to the reservoir [70] and another bound in terms of the change in entropy of the system can also be obtained [56]. However, these bounds are not tight in the zero-temperature limit compared to the bound reported in Ref. [71]. The inequalities Eq. (4) and Eq. (5) provide lower bounds not only on the entropy production but also on the equilibration time, which is an essential quantity in quantum-state preparation [72] and which aids our understanding of thermalization [33]. In applications, the equilibration time can be approximated without solving the Lindblad master equation, which may be time consuming in the weak coupling limit. The dissipation-current trade-off relation [73], which unveils the role of coherence between energy eigenstates in realizing a dissipationless heat current, can also be derived using our geometrical approach [56].

The system becomes classical when the initial density matrix has no coherence in the energy eigenbasis of the Hamiltonian. In what follows, we present the analysis for classical systems.

Bounds in Markovian classical systems.—Next, we consider a discrete-state system in contact with a heat bath at the inverse temperature β. During a time period τ, stochastic transitions between the states are induced by interactions with the heat bath. The dynamics obey a time-continuous Markov jump process and are described by this master equation:

$$\dot{p}_n(t)=\sum_{m(\neq n)}[R_{nm}(t)p_m(t)-R_{mn}(t)p_n(t)], \tag{6}$$

where $p_n(t)$ is the probability of finding the system in state n at time t and $R_{mn}(t)$ is the (possibly time dependent) transition rate from state n to state m ($1\leq n\neq m\leq N$). We assume an irreducible system in which the transition rates satisfy the detailed balance condition $R_{nm}(t)e^{-\beta\mathcal{E}_m(t)}=R_{mn}(t)e^{-\beta\mathcal{E}_n(t)}$ for all $m\neq n$, where $\mathcal{E}_n(t)$ is the instantaneous energy of state n at time t. Herein, we define the instantaneous equilibrium state $\boldsymbol{p}^{\mathrm{eq}}(t)$ as $p_n^{\mathrm{eq}}(t)\propto e^{-\beta\mathcal{E}_n(t)}$.

Within the stochastic thermodynamics framework [1], the irreversible entropy production ΔS_{tot} is quantified by the change in the system's Shannon entropy and the heat flow dissipated into the environment. Specifically, $\Delta S_{\mathrm{tot}}=\int_0^\tau\sigma_{\mathrm{tot}}(t)dt$, where $\sigma_{\mathrm{tot}}(t)=\sigma(t)+\sigma_M(t)$ is the total entropy production rate. The terms $\sigma(t)=\sum_{m,n}R_{mn}p_n\ln(p_n/p_m)$ and $\sigma_M(t)=\sum_{m,n}R_{mn}p_n\times\ln(R_{mn}/R_{nm})$ define the entropy production rates of the system and medium, respectively. Under the detailed balance condition, the entropy production rate can be explicitly calculated as $\sigma_{\mathrm{tot}}(t)=\langle\boldsymbol{f}(t),\dot{\boldsymbol{p}}(t)\rangle=-(d/dt)D[\boldsymbol{p}(t)||\boldsymbol{p}^{\mathrm{eq}}(t)]$, where $\boldsymbol{f}(t):=-\nabla_p D[\boldsymbol{p}(t)||\boldsymbol{p}^{\mathrm{eq}}(t)]$ is a vector of thermodynamic forces, and the time derivative does not act on $\boldsymbol{p}^{\mathrm{eq}}(t)$. Here, $D(\boldsymbol{p}||\boldsymbol{q})=\sum_n p_n\ln(p_n/q_n)$ is the relative entropy between the distributions $\boldsymbol{p}$ and $\boldsymbol{q}$, and $\nabla_p:=[\partial_{p_1},\ldots,\partial_{p_N}]^\top$ denotes the gradient with respect to $\boldsymbol{p}$. The second law of thermodynamics, $\Delta S_{\mathrm{tot}}\geq 0$, is affirmed from the positivity of the entropy production rate $\sigma_{\mathrm{tot}}(t)$.

The master equation [Eq. (6)] can be alternatively written as $\dot{\boldsymbol{p}}(t)=K_p(t)\boldsymbol{f}(t)$ [56], where $K_p(t)$ is a symmetric positive semidefinite matrix given by

$$K_p(t):=\sum_{n<m}R_{nm}(t)p_m^{\mathrm{eq}}(t)\Phi\left[\frac{p_n(t)}{p_n^{\mathrm{eq}}(t)},\frac{p_m(t)}{p_m^{\mathrm{eq}}(t)}\right]E_{nm}. \tag{7}$$

Here, $\Phi(x,y)=(x-y)/[\ln(x)-\ln(y)]$ is the logarithmic mean of $x,y>0$, and $E_{nm}=[e_{ij}]\in\mathbb{R}^{N\times N}$ is a matrix with $e_{nn}=e_{mm}=1$, $e_{nm}=e_{mn}=-1$, and zeros in all other elements. The symmetric matrix K_p is actually the Onsager matrix [62], which linearly relates the thermodynamic forces to the probability currents. For an arbitrary smooth curve $\{\boldsymbol{\gamma}(t)\}_{0\leq t\leq\tau}$, there exists a unique vector field $\{\boldsymbol{v}(t)\}_{0\leq t\leq\tau}$ such that $\dot{\boldsymbol{\gamma}}(t)=K_\gamma(t)\boldsymbol{v}(t)$ and $\langle\mathbf{1},\boldsymbol{v}(t)\rangle=0$, where $\mathbf{1}:=[1,\ldots,1]^\top$ is an all-ones vector. We can thus define the Riemannian metric $g_\gamma(\dot{\boldsymbol{\gamma}},\dot{\boldsymbol{\gamma}})=\langle\boldsymbol{v},K_\gamma\boldsymbol{v}\rangle$, which is

always non-negative. Using this metric, the thermodynamic divergence of a curve can be defined as

$$\ell_c(\boldsymbol{\gamma})^2 := \tau \int_0^\tau g_\gamma(\dot{\boldsymbol{\gamma}}, \dot{\boldsymbol{\gamma}}) dt. \tag{8}$$

The modified Wasserstein distance between two points $\boldsymbol{p}_0$ and $\boldsymbol{p}_\tau$ is then defined as $\mathcal{W}_c(\boldsymbol{p}_0, \boldsymbol{p}_\tau) := \inf_\gamma\{\ell_c(\boldsymbol{\gamma})\}$, where the infimum is taken over all smooth curves connecting $\boldsymbol{p}_0$ and $\boldsymbol{p}_\tau$ on the manifold. Notably, this distance is bounded from below by the total variation distance [56]. It is worth noting that the defined metric is not equivalent to the traditional discrete version of the classical Wasserstein metric. In practice, $\mathcal{W}_c$ can be numerically calculated by the geodesic equation [56], which computes the shortest path between two points. Defining $\boldsymbol{h}(t) := \boldsymbol{f}(t) - N^{-1}\langle \mathbf{1}, \boldsymbol{f}(t)\rangle \mathbf{1}$, one observes that $\dot{\boldsymbol{p}}(t) = K_p(t)\boldsymbol{h}(t)$ and $\langle \mathbf{1}, \boldsymbol{h}(t)\rangle = 0$. As $\sigma_{\mathrm{tot}}(t) = \langle \boldsymbol{h}(t), K_p(t)\boldsymbol{h}(t)\rangle$, $\tau\Delta S_{\mathrm{tot}}$ is exactly the thermodynamic divergence of the path described by the system dynamics. As the second main result, we obtain the following bound:

$$\Delta S_{\mathrm{tot}} \geq \frac{\mathcal{W}_c[\boldsymbol{p}(0), \boldsymbol{p}(\tau)]^2}{\tau}. \tag{9}$$

The inequality Eq. (9) provides a stronger bound than the Clausius inequality of the second law and is valid as long as the transition rates satisfy the detailed balance condition. Geometrically, Eq. (9) can be considered as a discrete-state generalization of the relation between dissipation and the Wasserstein distance, which has been studied in continuous-state Markovian dynamics governed by Langevin equations [23,25]. Concretely, Eq. (21) in Ref. [23] and Eq. (2) in Ref. [25] are referred to as the continuum analogs of Eq. (9). Our generalization newly and appropriately connects these thermodynamic and geometric quantities in the discrete case. Therefore, it is applicable to the many discrete physical phenomena in biological and quantum physics.

Examples.—First, we illustrate the bounds derived in Eqs. (4) and (5) on a quantum Otto heat engine [74–76], which consists of a two-level atom with the Hamiltonian $H(t) = \omega(t)\sigma_z/2$. This system is alternatively coupled to two heat baths at different inverse temperatures [one hot, one cold, $\beta_k = 1/T_k (k = h, c)$] and is cyclically operated through four steps, as demonstrated in Fig. 1(a). During adiabatic expansion (compression), the isolated system unitarily evolves during time τ_a, and its frequency changes from $\omega_h \to \omega_c$ ($\omega_c \to \omega_h$). The dynamics in each isochoric process $k = h, c$ are described by this Lindblad master equation [55]:

$$\begin{aligned}\dot{\rho} = &-i[H_k, \rho] + \alpha_k \bar{n}(\omega_k)(2\sigma_+\rho\sigma_- - \{\sigma_-\sigma_+, \rho\}) \\ &+ \alpha_k[\bar{n}(\omega_k) + 1](2\sigma_-\rho\sigma_+ - \{\sigma_+\sigma_-, \rho\}),\end{aligned} \tag{10}$$

where the frequency is fixed at ω_k, $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$, α_k is a positive damping rate, and $\bar{n}(\omega_k) = (e^{\beta_k\omega_k} - 1)^{-1}$ is the Planck distribution. The density operator ρ in this thermalization process is analytically solvable [77], and the total entropy production can be explicitly evaluated as $\Delta S^k_{\mathrm{tot}} = S[\rho(0)||\rho^{\mathrm{eq}}] - S[\rho(\tau_k)||\rho^{\mathrm{eq}}]$, where τ_k denotes the process time. Equations (4) and (5) constrain $\Delta S^k_{\mathrm{tot}}$ within the distances d_T and d_E, as numerically verified in Fig. 1(b). Note that unlike the classical case [36], $\Delta S^k_{\mathrm{tot}}$ in generic thermalization processes is not bounded by the relative entropy $S[\rho(0)||\rho(\tau_k)]$ [56].

The total entropy production in each cycle is the sum of those in the hot and cold isochoric processes, that is, $\Delta S_{\mathrm{tot}} = \Delta S^h_{\mathrm{tot}} + \Delta S^c_{\mathrm{tot}}$. Assuming a stationary-state system, let Q_h and Q_c denote the heat taken from the hot bath and the heat transferred to the cold bath, respectively. From the inequality $\Delta S_{\mathrm{tot}} = \beta_h Q_h - \beta_c Q_c \geq 0$ imposed by the second law, one can prove that the engine efficiency cannot exceed the Carnot efficiency $\eta := 1 - Q_c/Q_h \leq 1 - \beta_h/\beta_c =: \eta_C$. From the derived bounds, we can tighten the bound on the efficiency of the quantum Otto engine. Applying Eqs. (4) and (5) to isochoric processes, one readily obtains $\beta_h Q_h - \beta_c Q_c \geq \mathfrak{g}$, where $\mathfrak{g} := \max\{d_T(\rho_1,\rho_4)^2/4\tau_h\mathcal{A}^h_T, d_E(\rho_1,\rho_4)^2/\tau_h\mathcal{A}^h_E\} + \max\{d_T(\rho_2,\rho_3)^2/4\tau_c\mathcal{A}^c_T, d_E(\rho_2,\rho_3)^2/\tau_c\mathcal{A}^c_E\}$. Here, ρ_i denotes the density operator at the beginning of process $i\,(1 \leq i \leq 4)$, $\mathcal{A}^k_T := \alpha_k[2\bar{n}(\omega_k) + 1]$, and $\mathcal{A}^k_E := \omega_k^2\alpha_k[2\bar{n}(\omega_k) + 1]$ for each $k = h, c$. Consequently, the efficiency can be bounded from above as $\eta \leq \eta_C - \mathfrak{g}/\beta_c Q_h =: \eta_G$. This bound is

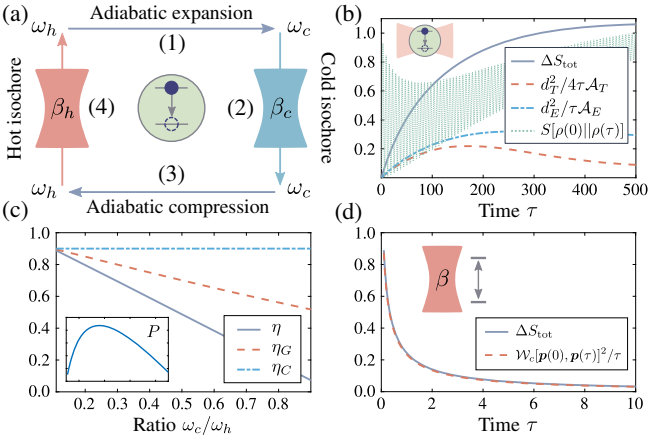

FIG. 1. Numerical verification. (a) Quantum Otto engine: a two-level atom undergoes two isochoric and two adiabatic processes. (b) Thermalization process of the two-level atom. Plotted are ΔS_{tot} (solid line), $d_T^2/4\tau\mathcal{A}_T$ (dashed line), $d_E^2/\tau\mathcal{A}_E$ (dash-dotted line), and $S[\rho(0)||\rho(\tau)]$ (dotted line). Parameters are $\beta_k = 1$, $\omega_k = 1$, $\alpha_k = 10^{-3}$, and $\rho(0) = (\mathbb{I}_2 + 0.1\sigma_x - 0.5\sigma_y + 0.8\sigma_z)/2$. (c) Engine efficiency η (solid line), Carnot efficiency η_C (dash-dotted line), and the derived efficiency bound η_G (dashed line), as functions of the cold-to-hot ratio of operating frequency. The inset plots the power output P of the engine over the same frequency-ratio range. Parameters are $\beta_c = 1$, $\beta_h = 0.1$, $\alpha_h = \alpha_c = 10^{-3}$, and $\tau_a = \tau_c = \tau_h = 1$. (d) Classical two-level system. Plotted are ΔS_{tot} (solid line) and $\mathcal{W}_c[\boldsymbol{p}(0), \boldsymbol{p}(\tau)]^2/\tau$ (dashed line). Parameters are fixed as $a = 0.7$, $b = 0.4$.

numerically verified in Fig. 1(c), which plots the efficiency against the ω_c/ω_h ratio.

Next, we numerically verify the bound derived in Eq. (9) in a time-driven two-level classical system. The instantaneous energies of states 1 and 2 are $\mathcal{E}_1(t) = \beta^{-1}\ln\{[1 - a + b(t+1)/\tau]/(a - bt/\tau)\}$ and $\mathcal{E}_2(t) = 0$, respectively, where $0 < b < a < 1$ are constants. Their respective transition rates are $R_{12}(t) = 1, R_{21}(t) = e^{\beta\mathcal{E}_1(t)}$. The probability distribution and entropy production can be analytically calculated. The entropy production and modified Wasserstein distance are plotted as functions of time τ in Fig. 1(d). The entropy production at all times was tightly bounded from below by the distance $\mathcal{W}_c$. This result numerically verifies Eq. (9). As another example, the thermalization process of a three-level system is presented in Ref. [56].

Conclusions.—In this Letter, we derived the geometrical bounds of irreversibility in both quantum and classical open systems, thus strengthening the Clausius inequality of the second law of thermodynamics. Furthermore, the study results elucidate that, beyond the linear response regime, the entropy production can be geometrically characterized. This finding sheds light on the problem of minimizing dissipation in discrete-state systems by methods of optimal control [23]. Interpreting the bounds as speed limits shows that the state-transformation speed is constrained by dissipation in quantum systems. By investigating the information-geometric structure underlying the system dynamics, we lay the foundations for obtaining useful thermodynamic relations. Exploring analogous bounds in generic systems, which violate the detailed balance condition, and for higher cumulants of dissipation [78,79] would be promising research directions.

We thank Shin-ichi Sasa, Keiji Saito, Sosuke Ito, and Andreas Dechant for fruitful discussions. We are also grateful to Keiji Saito for the careful reading of the manuscript and for the valuable comments. This work was supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT) KAKENHI Grant No. JP19K12153.

*Corresponding author.
tan@biom.t.u-tokyo.ac.jp
†Corresponding author.
hasegawa@biom.t.u-tokyo.ac.jp

[1] U. Seifert, Stochastic thermodynamics, fluctuation theorems and molecular machines, Rep. Prog. Phys. **75**, 126001 (2012).
[2] S. Vinjanampathy and J. Anders, Quantum thermodynamics, Contemp. Phys. **57**, 545 (2016).
[3] S. Deffner and S. Campbell, *Quantum Thermodynamics* (Morgan & Claypool Publishers, San Rafael, CA, 2019).
[4] F. Verstraete, M. M. Wolf, and J. I. Cirac, Quantum computation and quantum-state engineering driven by dissipation, Nat. Phys. **5**, 633 (2009).
[5] R. Kosloff and A. Levy, Quantum heat engines and refrigerators: Continuous devices, Annu. Rev. Phys. Chem. **65**, 365 (2014).
[6] P. Salamon and R. S. Berry, Thermodynamic Length and Dissipated Availability, Phys. Rev. Lett. **51**, 1127 (1983).
[7] G. Ruppeiner, Riemannian geometry in thermodynamic fluctuation theory, Rev. Mod. Phys. **67**, 605 (1995).
[8] E. H. Feng and G. E. Crooks, Length of Time's Arrow, Phys. Rev. Lett. **101**, 090602 (2008).
[9] B. B. Machta, Dissipation Bound for Thermodynamic Control, Phys. Rev. Lett. **115**, 260603 (2015).
[10] 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).
[11] S. Ito, Stochastic Thermodynamic Interpretation of Information Geometry, Phys. Rev. Lett. **121**, 030605 (2018).
[12] S. B. Nicholson, A. del Campo, and J. R. Green, Nonequilibrium uncertainty principle from information geometry, Phys. Rev. E **98**, 032106 (2018).
[13] S. J. Large, R. Chetrite, and D. A. Sivak, Stochastic control in microscopic nonequilibrium systems, Europhys. Lett. **124**, 20001 (2018).
[14] M. Scandi and M. Perarnau-Llobet, Thermodynamic length in open quantum systems, Quantum **3**, 197 (2019).
[15] C. Cafaro and P. M. Alsing, Information geometry aspects of minimum entropy production paths from quantum mechanical evolutions, Phys. Rev. E **101**, 022110 (2020).
[16] S. J. Bryant and B. B. Machta, Energy dissipation bounds for autonomous thermodynamic cycles, Proc. Natl. Acad. Sci. U.S.A. **117**, 3478 (2020).
[17] S.-i. Amari and H. Nagaoka, *Methods of Information Geometry* (Oxford University Press, New York, 2000), Vol. 191.
[18] S. Deffner and E. Lutz, Generalized Clausius Inequality for Nonequilibrium Quantum Processes, Phys. Rev. Lett. **105**, 170402 (2010).
[19] L. Mancino, V. Cavina, A. De Pasquale, M. Sbroscia, R. I. Booth, E. Roccia, I. Gianani, V. Giovannetti, and M. Barbieri, Geometrical Bounds on Irreversibility in Open Quantum Systems, Phys. Rev. Lett. **121**, 160602 (2018).
[20] G. E. Crooks, Measuring Thermodynamic Length, Phys. Rev. Lett. **99**, 100602 (2007).
[21] D. A. Sivak and G. E. Crooks, Thermodynamic Metrics and Optimal Paths, Phys. Rev. Lett. **108**, 190602 (2012).
[22] C. Villani, *Optimal Transport: Old and New* (Springer, Berlin, Heidelberg, 2008).
[23] E. Aurell, C. Mejía-Monasterio, and P. Muratore-Ginanneschi, Optimal Protocols and Optimal Transport in Stochastic Thermodynamics, Phys. Rev. Lett. **106**, 250601 (2011).
[24] E. Aurell, K. Gawędzki, C. Mejía-Monasterio, R. Mohayaee, and P. Muratore-Ginanneschi, Refined second law of thermodynamics for fast random processes, J. Stat. Phys. **147**, 487 (2012).
[25] A. Dechant and Y. Sakurai, Thermodynamic interpretation of Wasserstein distance, arXiv:1912.08405.
[26] D. P. Pires, M. Cianciaruso, L. C. Céleri, G. Adesso, and D. O. Soares-Pinto, Generalized Geometric Quantum Speed Limits, Phys. Rev. X **6**, 021031 (2016).

[27] S. Deffner, Geometric quantum speed limits: A case for Wigner phase space, New J. Phys. **19**, 103018 (2017).

[28] S. Ito and A. Dechant, Stochastic Time Evolution, Information Geometry, and the Cramér-Rao Bound, Phys. Rev. X **10**, 021056 (2020).

[29] K. Funo, N. Shiraishi, and K. Saito, Speed limit for open quantum systems, New J. Phys. **21**, 013006 (2019).

[30] H. J. D. Miller, M. Scandi, J. Anders, and M. Perarnau-Llobet, Work Fluctuations in Slow Processes: Quantum Signatures and Optimal Control, Phys. Rev. Lett. **123**, 230603 (2019).

[31] K. Brandner and K. Saito, Thermodynamic Geometry of Microscopic Heat Engines, Phys. Rev. Lett. **124**, 040602 (2020).

[32] G. E. Crooks, Nonequilibrium measurements of free energy differences for microscopically reversible Markovian systems, J. Stat. Phys. **90**, 1481 (1998).

[33] J. Goold, M. Huber, A. Riera, L. del Rio, and P. Skrzypczyk, The role of quantum information in thermodynamics—A topical review, J. Phys. A **49**, 143001 (2016).

[34] J. M. Deutsch, Eigenstate thermalization hypothesis, Rep. Prog. Phys. **81**, 082001 (2018).

[35] K. Ptaszyński and M. Esposito, Entropy Production in Open Systems: The Predominant Role of Intraenvironment Correlations, Phys. Rev. Lett. **123**, 200603 (2019).

[36] N. Shiraishi and K. Saito, Information-Theoretical Bound of the Irreversibility in Thermal Relaxation Processes, Phys. Rev. Lett. **123**, 110603 (2019).

[37] L. Mandelstam and I. Tamm, The uncertainty relation between energy and time in non-relativistic quantum mechanics, J. Phys. USSR **9**, 249 (1945).

[38] N. Margolus and L. B. Levitin, The maximum speed of dynamical evolution, Physica (Amsterdam) **120D**, 188 (1998).

[39] A. del Campo, I. L. Egusquiza, M. B. Plenio, and S. F. Huelga, Quantum Speed Limits in Open System Dynamics, Phys. Rev. Lett. **110**, 050403 (2013).

[40] M. M. Taddei, B. M. Escher, L. Davidovich, and R. L. de Matos Filho, Quantum Speed Limit for Physical Processes, Phys. Rev. Lett. **110**, 050402 (2013).

[41] S. Deffner and S. Campbell, Quantum speed limits: From Heisenberg's uncertainty principle to optimal quantum control, J. Phys. A **50**, 453001 (2017).

[42] M. Okuyama and M. Ohzeki, Quantum Speed Limit is Not Quantum, Phys. Rev. Lett. **120**, 070402 (2018).

[43] N. Shiraishi, K. Funo, and K. Saito, Speed Limit for Classical Stochastic Processes, Phys. Rev. Lett. **121**, 070601 (2018).

[44] B. Shanahan, A. Chenu, N. Margolus, and A. del Campo, Quantum Speed Limits Across the Quantum-to-Classical Transition, Phys. Rev. Lett. **120**, 070401 (2018).

[45] E. A. Morozova and N. N. Chentsov, Markov invariant geometry on manifolds of states, J. Sov. Math. **56**, 2648 (1991).

[46] D. Petz, Monotone metrics on matrix spaces, Linear Algebra Appl. **244**, 81 (1996).

[47] F. Hiai and D. Petz, Riemannian metrics on positive definite matrices related to means, Linear Algebra Appl. **430**, 3105 (2009).

[48] W. K. Wootters, Statistical distance and Hilbert space, Phys. Rev. D **23**, 357 (1981).

[49] S. L. Braunstein and C. M. Caves, Statistical Distance and the Geometry of Quantum States, Phys. Rev. Lett. **72**, 3439 (1994).

[50] G. Lindblad, On the generators of quantum dynamical semigroups, Commun. Math. Phys. **48**, 119 (1976).

[51] V. Gorini, A. Kossakowski, and E. C. G. Sudarshan, Completely positive dynamical semigroups of N-level systems, J. Math. Phys. (N.Y.) **17**, 821 (1976).

[52] D. A. Lidar, Lecture notes on the theory of open quantum systems, arXiv:1902.00967.

[53] R. Alicki and K. Lendi, *Quantum Dynamical Semigroups and Applications* (Springer, Berlin, 1987).

[54] P. Strasberg, G. Schaller, T. Brandes, and M. Esposito, Quantum and Information Thermodynamics: A Unifying Framework Based on Repeated Interactions, Phys. Rev. X **7**, 021003 (2017).

[55] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, New York, 2002).

[56] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.126.010601 for details of calculations, which includes Ref. [57].

[57] C. Maes, Frenesy: Time-symmetric dynamical activity in nonequilibria, Phys. Rep. **850**, 1 (2020).

[58] R. Jordan, D. Kinderlehrer, and F. Otto, The variational formulation of the Fokker-Planck equation, SIAM J. Math. Anal. **29**, 1 (1998).

[59] J. Maas, Gradient flows of the entropy for finite Markov chains, J. Funct. Anal. **261**, 2250 (2011).

[60] E. A. Carlen and J. Maas, Gradient flow and entropy inequalities for quantum Markov semigroups with detailed balance, J. Funct. Anal. **273**, 1810 (2017).

[61] C. Rouzé and N. Datta, Concentration of quantum states from quantum functional and transportation cost inequalities, J. Math. Phys. (N.Y.) **60**, 012202 (2019).

[62] L. Onsager, Reciprocal relations in irreversible processes. II, Phys. Rev. **38**, 2265 (1931).

[63] Since $\mathscr{C}_q(\gamma) \geq \mathscr{C}(\gamma)$, we have $\mathcal{W}_q(\rho_0, \rho_\tau) \geq \inf_\gamma\{\mathscr{C}(\gamma)\}$ in the general case. However, for relaxation processes (i.e., the operator $\mathcal{K}_\gamma$ is time independent), it can be shown that $\mathcal{W}_q(\rho_0, \rho_\tau) = \inf_\gamma\{\mathscr{C}(\gamma)\}$, where the equality is attained with a constant-speed path [64].

[64] J. Dolbeault, B. Nazaret, and G. Savaré, A new class of transport distances between measures, Calc. Var. Partial Dif. **34**, 193 (2008).

[65] J. Agredo and F. Fagnola, On quantum versions of the classical Wasserstein distance, Stochastics **89**, 910 (2017).

[66] J.-D. Benamou and Y. Brenier, A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem, Numer. Math. **84**, 375 (2000).

[67] F. Golse, C. Mouhot, and T. Paul, On the mean field and classical limits of quantum mechanics, Commun. Math. Phys. **343**, 165 (2016).

[68] G. D. Palma and D. Trevisan, Quantum optimal transport with quantum channels, arXiv:1911.00803.

[69] Y. Chen, T. T. Georgiou, L. Ning, and A. Tannenbaum, Matricial Wasserstein-1 distance, IEEE Control Syst. Lett. **1**, 14 (2017).

[70] N. Shiraishi, K. Saito, and H. Tasaki, Universal Trade-Off Relation between Power and Efficiency for Heat Engines, Phys. Rev. Lett. **117**, 190601 (2016).
[71] A. M. Timpanaro, J. P. Santos, and G. T. Landi, Landauer's Principle at Zero Temperature, Phys. Rev. Lett. **124**, 240601 (2020).
[72] A. J. Short and T. C. Farrelly, Quantum equilibration in finite time, New J. Phys. **14**, 013063 (2012).
[73] H. Tajima and K. Funo, Superconducting-like heat current: Effective cancellation of current-dissipation trade off by quantum coherence, arXiv:2004.13412.
[74] O. Abah, J. Roßnagel, G. Jacob, S. Deffner, F. Schmidt-Kaler, K. Singer, and E. Lutz, Single-Ion Heat Engine at Maximum Power, Phys. Rev. Lett. **109**, 203006 (2012).
[75] R. Kosloff and Y. Rezek, The quantum harmonic Otto cycle, Entropy **19**, 136 (2017).
[76] M. Kloc, P. Cejnar, and G. Schaller, Collective performance of a finite-time quantum Otto cycle, Phys. Rev. E **100**, 042126 (2019).
[77] M. Ramezani, F. Benatti, R. Floreanini, S. Marcantoni, M. Golshani, and A. T. Rezakhani, Quantum detailed balance conditions and fluctuation relations for thermalizing quantum dynamics, Phys. Rev. E **98**, 052104 (2018).
[78] M. Scandi, H. J. D. Miller, J. Anders, and M. Perarnau-Llobet, Quantum work statistics close to equilibrium, Phys. Rev. Research **2**, 023377 (2020).
[79] H. J. D. Miller, G. Guarnieri, M. T. Mitchison, and J. Goold, Quantum Fluctuations Hinder Finite-Time Information Erasure Near the Landauer Limit, Phys. Rev. Lett. **125**, 160602 (2020).