Fluctuation Theorem for Many-Body Pure Quantum States

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We prove the second law of thermodynamics and the nonequilibrium fluctuation theorem for pure quantum states. The entire system obeys reversible unitary dynamics, where the initial state of the heat bath is not the canonical distribution but is a single energy eigenstate that satisfies the eigenstate-thermalization hypothesis. Our result is mathematically rigorous and based on the Lieb-Robinson bound, which gives the upper bound of the velocity of information propagation in many-body quantum systems. The entanglement entropy of a subsystem is shown connected to thermodynamic heat, highlighting the foundation of the information-thermodynamics link. We confirmed our theory by numerical simulation of hard-core bosons, and observed dynamical crossover from thermal fluctuations to bare quantum fluctuations. Our result reveals a universal scenario that the second law emerges from quantum mechanics, and can be experimentally tested by artificial isolated quantum systems such as ultracold atoms.

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Introduction.—Although the microscopic laws of physics do not prefer a particular direction of time, the macroscopic world exhibits inevitable irreversibility represented by the second law of thermodynamics. Modern research has revealed that even a pure quantum state, described by a single wave function, can relax to macroscopic thermal equilibrium by a reversible unitary evolution [1–11]. Thermalization of isolated quantum systems, which is relevant to the zeroth law of thermodynamics, is now a very active area of research in theory [1–6], numerics [10–16], and experiments [17–23]. In particular, the concepts of typicality [9,24–26] and the eigenstate thermalization hypothesis (ETH) [10–12,27–36] have played significant roles.

However, the second law of thermodynamics, which states that the thermodynamic entropy increases, or does not change, in isolated systems, has not been fully addressed in this context. We would emphasize that the informational entropy (i.e., the von Neumann entropy) of an isolated quantum system in a pure state never increases, but is always zero [37]. In this sense, a fundamental gap between the microscopic and macroscopic worlds has not yet been bridged: How does the second law emerge from pure quantum states?

In a rather different context, a general theory of the second law and its connection to information has recently been developed even out of equilibrium [38–45]. This has revealed that information contents and thermodynamic quantities can be treated on an equal footing, as originally illustrated by Szilard and Landauer in the context of Maxwell's demon [46,47]. This research direction invokes a crucial assumption that the heat bath is, at least in the initial time, in the canonical distribution [48]; this special initial condition breaks the time translation invariance and leads to the second law of thermodynamics. The same assumption has been employed in various modern studies on thermodynamics, such as the nonequilibrium fluctuation theorem [48–58] and the thermodynamic resource theory [59,60].

Based on these streams of researches, in this Letter we rigorously derive the second law of thermodynamics for isolated quantum systems in pure states. We consider a small system and a large heat bath, where the bath is initially in a single energy eigenstate. Such an eigenstate is a pure quantum state, and does not include any statistical mixture as is the case for the canonical distribution. The second law that we show here is formulated with the von Neumann entropy of the system, ensuring the information-thermodynamics link, which is a characteristic of our study in contrast to previous approaches [36,61,62]. Furthermore, we prove the integral fluctuation theorem [50,53,54,63], a universal relation in nonequilibrium statistical mechanics, which expresses the second law as an equality rather than an inequality.

To prove the main results (i.e., the second law and the fluctuation theorem), our key idea is combining the following two distinct fundamental concepts. One is the Lieb-Robinson bound [64,65], which characterizes the finite group velocity of information propagation in quantum many-body systems with local interaction. The other is the ETH, which states that even a single energy eigenstate can behave as thermal [10–12,27–36]. In this Letter, we newly prove a variant of the ETH [12,35], which is referred to as the weak ETH and states that most of the energy eigenstates satisfy the ETH, if an eigenstate is randomly sampled from the microcanonical energy shell. Our approach would be applicable to quite a broad class of modern researches of thermodynamics, from thermalization in ultracold atoms [20] to scrambling in black holes [66–69].

Setup.—We first formulate our setup with a heat bath in a pure state. Suppose that the entire system consists of system

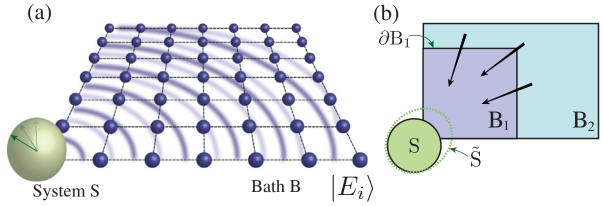

FIG. 1. Schematics of our setup. (a) The total system, where the initial state of B is an energy eigenstate $|E_i\rangle$. (b) Subregions used in our argument.

S and bath B. We assume that bath B is a quantum many-body system on a d-dimensional hypercubic lattice with N sites. The Hamiltonian is given by

$$\hat{H} = \hat{H}_S + \hat{H}_I + \hat{H}_B, \tag{1}$$

where $\hat{H}_S$ and $\hat{H}_B$ are, respectively, the Hamiltonians of system S and bath B, and $\hat{H}_I$ represents their interaction. We assume that $\hat{H}_B$ is translation invariant with local interaction, and system S is locally in contact with bath B [see Fig. 1(a)]. We also assume that the correlation functions in the canonical distribution with respect to $\hat{H}_B$ are exponentially decaying for any local observables, which implies that bath B is not on a critical point.

The initial state of the total system is given by

$$\hat{\rho}(0) = \hat{\rho}_S(0) \otimes |E_i\rangle\langle E_i|, \tag{2}$$

where $\hat{\rho}_S(0)$ is the initial density operator of system S, and $|E_i\rangle$ is the initial energy eigenstate of bath B. We sample $|E_i\rangle$ from the set of the energy eigenstates in the microcanonical energy shell in a uniformly random way, as will be described in detail later. We can then define temperature T of $|E_i\rangle$ as the temperature of the corresponding energy shell. We note that the initial correlation between S and B is assumed to be zero.

The total system then obeys a unitary time evolution by the Hamiltonian: $\hat{\rho}(t) = \hat{U}\hat{\rho}(0)\hat{U}^\dagger$ with $\hat{U} \coloneqq \exp(-i\hat{H}t/\hbar)$. Such a situation can experimentally be realized with ultracold atoms by quenching an external potential at time 0. Let $\hat{\rho}_S(t) \coloneqq \mathrm{tr}_B[\hat{\rho}(t)]$ and $\hat{\rho}_B(t) \coloneqq \mathrm{tr}_S[\hat{\rho}(t)]$ be the density operators of system S and bath B at time t, respectively. The change in the von Neumann entropy of S is given by $\Delta S_S \coloneqq S_S(t) - S_S(0)$ with $S_S(t) \coloneqq -\mathrm{tr}_S[\hat{\rho}_S(t)\ln\hat{\rho}_S(t)]$. We also define the heat emitted from bath B by $Q \coloneqq -\mathrm{tr}_B\{\hat{H}_B[\hat{\rho}_B(t) - \hat{\rho}_B(0)]\}$.

If the initial state of system S is pure [i.e., $\hat{\rho}_S(0) = |\psi\rangle\langle\psi|$], the total system is also pure, whose von Neumann entropy vanishes. In such a case, the final state $\hat{\rho}(t)$ remains in a pure state because of the unitarity, but is entangled. Correspondingly, the final state of S is mixed and has nonzero von Neumann entropy, which is regarded as the entanglement entropy.

Second law.—We now discuss our first main result. If $|E_i\rangle$ is a typical energy eigenstate that satisfies the ETH, the second law of thermodynamics is shown to hold within a small error,

$$\Delta S_S - \beta Q \geq -\varepsilon_{\mathrm{2nd}}, \tag{3}$$

where $\varepsilon_{\mathrm{2nd}}$ is a positive error term. We can rigorously prove that $\varepsilon_{\mathrm{2nd}}$ can be arbitrarily small if bath B is sufficiently large. The error in inequality (3) decreases at least polynomially in N, as will be discussed in more detail later. The left-hand side of inequality (3) is regarded as the average entropy production $\langle\sigma\rangle \coloneqq \Delta S_S - \beta Q$, where $\langle\cdots\rangle$ describes the ensemble average, and σ is the stochastic entropy production that will be introduced later. We note that if the initial state of bath B is not pure but in the canonical distribution $\hat{\rho}_B^{\mathrm{can}} \coloneqq e^{-\beta\hat{H}_B}/\mathrm{tr}[e^{-\beta\hat{H}_B}]$, inequality (3) exactly holds without any error [48].

The second law (3) implies that the information-thermodynamics link emerges in an isolated quantum systems in a pure state, if we look at the informational entropy of subsystem S, though that of the total system remains unchanged. In this sense, inequality (3) is regarded as a kind of Landauer principle. While the Landauer principle and its generalizations have been derived in various ways [38,70–75], we here showed that it can emerge in the presence of a pure quantum bath.

We will prove inequality (3) in the Supplemental Material in a mathematically rigorous way [76]. Here, we only discuss the essentials of the proof, where the key ingredients are the Lieb-Robinson bound [64,65] and the weak ETH [12,35].

Lieb-Robinson bound.—The Lieb-Robinson bound gives an upper bound of the velocity of information propagation, and is applicable to any system on a generic lattice with local interaction. To apply the Lieb-Robinson bound, we divide bath B into B_1 and B_2, such that B_1 is near system S and B_2 is far from S [see Fig. 1(b)]. Then, the Lieb-Robinson bound [64,65] sets the shortest time τ at which information about B_2 reaches S across B_1. We refer to τ as the Lieb-Robinson time.

The detailed formulation of the Lieb-Robinson bound is the following. Let $\tilde{S}$ be the union of S and the support of $\hat{H}_I$. Let $\hat{A}_{\tilde{S}}$ and $\hat{B}_{\partial B_1}$ be arbitrary operators with the supports $\tilde{S}$ and ∂B_1, respectively, where ∂B_1 is the boundary between B_1 and B_2. Let $\mathrm{dist}(\tilde{S}, \partial B_1)$ be the spatial distance between $\tilde{S}$ and ∂B_1 on the lattice, and let $|\tilde{S}|$ and $|\partial B_1|$ be the numbers of the sites in $\tilde{S}$ and ∂B_1 respectively. The Lieb-Robinson bound is formulated in terms of the operator norm $\|\cdot\|$ as

$$\frac{\|[\hat{A}_{\tilde{S}}(t), \hat{B}_{\partial B_1}]\|}{\|\hat{A}_{\tilde{S}}\|\|\hat{B}_{\partial B_1}\|} \leq C|\tilde{S}||\partial B_1|e^{-\mu\mathrm{dist}(\tilde{S},\partial B_1)}(e^{v|t|} - 1), \tag{4}$$

where $\hat{A}_{\tilde{S}}(t) \coloneqq \hat{U}^\dagger \hat{A}_{\tilde{S}} \hat{U}$ represents the time evolution in the Heisenberg picture, and C, v, μ are positive constants. In particular, v/μ represents the velocity of information propagation. The Lieb-Robinson time is then given by $\tau \coloneqq \mu \mathrm{dist}(\tilde{S}, \partial B_1)/v$.

Weak ETH.—We next consider the concept of the weak ETH. Let D be the dimension of the Hilbert space of the microcanonical energy shell of bath B, which is exponentially large with respect to N, and let $\{|E_i\rangle\}_{i=1}^D$ be an orthonormal set of the energy eigenstates of $\hat{H}_B$ in the energy shell. Suppose that we choose $|E_i\rangle$ from $\{|E_i\rangle\}_{i=1}^D$ in a uniformly random way. As proven in the Supplemental Material [76], if B_2 is sufficiently larger than B_1, we typically have that

$$\mathrm{tr}_B[\hat{O}_{B_1}|E_i\rangle\langle E_i|] \simeq \mathrm{tr}_B[\hat{O}_{B_1}\hat{\rho}_B^{\mathrm{can}}], \tag{5}$$

which implies that $|E_i\rangle$ is indistinguishable from $\hat{\rho}_B^{\mathrm{can}}$ if we only look at any operator $\hat{O}_{B_1}$ on B_1 with $\|\hat{O}_{B_1}\| = 1$. We refer to this theorem as the weak ETH, which is a variant of a theorem shown in Refs. [12,35]. We note that the equivalence of the canonical and the microcanonical ensembles for reduced density operators [85,86] plays an important role.

We note that the weak ETH is true even if bath B is an integrable system [31,34]. The reason why the weak ETH is called "weak" is that there is another concept called the "strong" ETH (or just ETH) that is believed to be true only for nonintegrable systems, where every energy eigenstate satisfies Eq. (5) without exception [31].

Outline of the proof of Eq. (3).—We are now in the position to discuss the outline of the proof of the second law (3). In the short-time regime $t \ll \tau$, system S cannot feel the existence of B_2, and the heat bath effectively reduces to B_1. From the weak ETH, if B_2 is sufficiently larger, the initial state $|E_i\rangle$ of bath B is typically indistinguishable from the canonical distribution, if we only look at any operator in B_1. Thus, the reduced density operators of system S at time $t \ll \tau$ are almost the same for the initial energy eigenstate and the initial canonical distribution. Therefore, the conventional proof of the second law with the canonical bath approximately applies to the present situation, leading to inequality (3).

Integral fluctuation theorem.—We next discuss the integral fluctuation theorem (IFT) for the case that bath B is initially in an energy eigenstate, which is our second main result. Let σ be the stochastic entropy production defined as follows. Suppose that one performs projection measurements of $\hat{\sigma}(t) \coloneqq -\ln\hat{\rho}_S(t) + \beta\hat{H}_B$ at the initial and the final times, where the first and the second terms on the right-hand side, respectively, represent the informational and the energetic terms, corresponding to the first and second terms on the left-hand side of inequality (3). Then, σ is given by the difference between the obtained outcomes of these measurements. The average of the stochastic entropy production is equivalent to the aforementioned average entropy production, $\langle\sigma\rangle = \Delta S_S - \beta Q$.

The conventional IFT states that, if the initial state of bath B is the canonical distribution,

$$\langle e^{-\sigma}\rangle = 1. \tag{6}$$

We note that the IFT holds even when system S is far from equilibrium. A crucial feature of the IFT is that it reproduces the second law $\langle\sigma\rangle \geq 0$ from the Jensen inequality $\langle e^{-\sigma}\rangle \geq e^{-\langle\sigma\rangle}$. Furthermore, the IFT can reproduce the fluctuation-dissipation theorem [54].

Our result is the IFT in the case that bath B is initially in a typical energy eigenstate [i.e., with initial condition (2)],

$$|\langle e^{-\sigma}\rangle - 1| \leq \varepsilon_{\mathrm{FT}}, \tag{7}$$

where $\varepsilon_{\mathrm{FT}}$ is a positive error term. We can rigorously prove that $\varepsilon_{\mathrm{FT}}$ can be arbitrarily small if bath B is sufficiently large. The error in Eq. (7) again scales at least polynomially in N. We note that the detailed fluctuation theorem [54] also holds with an initial typical eigenstate, from which we can prove the IFT as a corollary (see Supplemental Material for details [76]).

The central idea of the proof of the IFT (7) is almost the same as that of the second law, which is outlined above. On the other hand, we need to make an additional assumption to prove inequality (7) that

$$[\hat{H}_S + \hat{H}_B, \hat{H}_I] \simeq 0, \tag{8}$$

which means that the sum of the energies of S and B is conserved at the level of fluctuations, and does not necessarily mean that $\hat{H}_I$ itself is small. We note that assumption (8) is consistent with the concept of "thermal operation" in the thermodynamic resource theory [59,60], where the left-hand side of Eq. (8) is assumed to be exactly zero. If the left-hand side of Eq. (8) is nonzero but small, a small positive error term ε_I should be added to the right-hand side of inequality (7), which cannot be arbitrarily small even in the large-bath limit. However, we will numerically show later that this additional term is negligible in practice.

Estimation of the error terms.—We evaluate the error terms in inequalities (3) and (7) with respect to the size N of bath B. We set $|B_1| = \mathcal{O}(N^\alpha)$, with $0 < \alpha < 1/2$. The error from the weak ETH is bounded by $\mathcal{O}(N^{-(1-2\alpha)/4+\delta}) + \mathcal{O}(N^{-(1-2\alpha)/8+\delta/2}/\sqrt{\tilde{\varepsilon}})$, where $\delta > 0$ is an unimportant constant that can be arbitrarily small, and $\tilde{\varepsilon}$ is the fraction of atypical eigenstates in the weak ETH. The error from the Lieb-Robinson bound is bounded by $e^{-\mu\mathrm{dist}(\tilde{S},\partial B_1)}(e^{vt} - vt - 1)$, which is negligible compared with the error term from the weak ETH for sufficiently large N, but increases in time with $\mathcal{O}(t^2)$ up to $t \simeq 1/v$.

Numerical simulation.—We performed numerical simulation of hard-core bosons with nearest-neighbor repulsion by exact diagonalization. System S is on a single site and bath B is on a two-dimensional lattice (see the inset of Fig. 2). The annihilation (creation) operator of a boson at site i is written as $\hat{c}_i$ ($\hat{c}_i^\dagger$), which satisfies the commutation relations $[\hat{c}_i,\hat{c}_j]=[\hat{c}_i^\dagger,\hat{c}_j^\dagger]=[\hat{c}_i,\hat{c}_j^\dagger]=0$ for $i\neq j$, $\{\hat{c}_i,\hat{c}_i\}=\{\hat{c}_i^\dagger,\hat{c}_i^\dagger\}=0$, and $\{\hat{c}_i,\hat{c}_i^\dagger\}=1$. The occupation number is defined as $\hat{n}_i \coloneqq \hat{c}_i^\dagger\hat{c}_i$. Let $i=0$ be the index of the site of system S. The Hamiltonians in Eq. (1) are then given by

$$\hat{H}_S=\omega\hat{n}_0,\qquad \hat{H}_I=-\gamma'\sum_{\langle 0,j\rangle}(\hat{c}_0^\dagger\hat{c}_j+\hat{c}_j^\dagger\hat{c}_0),\tag{9}$$

$$\hat{H}_B=\omega\sum_i\hat{n}_i-\gamma\sum_{\langle i,j\rangle}(\hat{c}_i^\dagger\hat{c}_j+\hat{c}_j^\dagger\hat{c}_i)+g\sum_{\langle i,j\rangle}\hat{n}_i\hat{n}_j,\tag{10}$$

where $\omega>0$ is the on-site potential, $-\gamma$ is the hopping rate in bath B, $-\gamma'$ is the hopping rate between system S and bath B, and $g>0$ is the repulsion energy. The initial state of system S is given as $|\psi\rangle \coloneqq \hat{c}_0^\dagger|0\rangle$. We set the size of bath B by $16=4\times 4$, and the initial number of bosons in bath B by 4. To evaluate the Lieb-Robinson time, we set $\mathrm{dist}(\tilde{S},\partial B_1)=1$. We can then evaluate that $v\simeq\gamma$ and $\mu=1$ if $g\ll\gamma$; therefore, the Lieb-Robinson time is given by $\tau\simeq\gamma^{-1}$. We set the inverse temperature of the initial eigenstate as $\beta=0.1$.

Figure 2 shows the time dependence of $\langle\sigma\rangle$, which implies that the second law indeed holds. The average entropy production gradually increases up to $t\simeq\tau$, and then saturates with some oscillations around the time average. We note that the oscillation for $\gamma'=4\omega$ is the Rabi oscillation between system S and a part of B. Remarkably, we observed that the second law holds even in a much longer time regime $t\gg\tau$, though our theorem ensures the second law only up to $t\simeq\tau$. This implies that the second law is robust against bare quantum fluctuations of pure quantum states.

We next confirmed the IFT (7). As shown in Fig. 3, $\langle e^{-\sigma}\rangle$ is very close to unity up to $t\simeq\tau$, as predicted by our theorem. After $t\simeq\tau$, however, the deviation of $\langle e^{-\sigma}\rangle$ from unity becomes significant, which is consistent with our theorem. This deviation comes from the effect of bare quantum fluctuations of the initial state; if the initial state was the canonical distribution, such deviation would never be observed. As time increases, system S more and more feels the effect of bare quantum fluctuations, and the deviation becomes larger. This is regarded as a dynamical crossover from emergent thermal fluctuations to bare quantum fluctuations across the Lieb-Robinson time τ; the IFT holds only for the former. Such a crossover is not clearly observed in the second law (Fig. 2), because the second law only concerns the average of the stochastic entropy production, though its fluctuations play a significant role in the IFT. Our numerical result also clarifies that our theory indeed accounts for the validity of IFT in the short-time regime, because the numerically observed time scale of the breakdown of the IFT is consistent with our theory.

As shown in the inset of Fig. 3, the error term of the IFT is proportional to t^2 up to $t\simeq 1/v\simeq\tau$ in our numerical simulation. In fact, our error evaluation based on the Lieb-Robinson bound predicts that an error term increases in time with t^2 dependence as discussed before, if the additional error term ε_{I}, which could also increase in time, is zero [or, equivalently, the left-hand side of Eq. (8) is zero]. Therefore, our numerical result clarifies that the contribution from the left-hand side of Eq. (8) is negligible in our setup, though it is not exactly zero in our Hamiltonians (9) and (10).

Concluding remarks.—In this Letter, we have established the second law (3) and the IFT (7) for unitary dynamics in the presence of a heat bath that is initially in a typical energy eigenstate. Our result implies that thermal

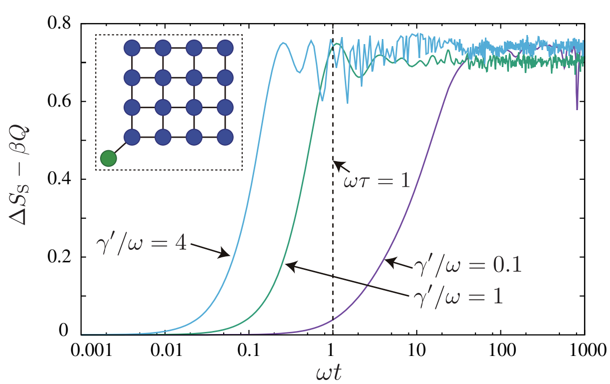

FIG. 2. Time dependence of average entropy production $\langle\sigma\rangle$ with parameters $\gamma'/\omega=0.1,1,4$, $\gamma/\omega=1$, and $g/\omega=0.1$. Inset: The lattice structure for the numerical calculation; system S (green) attached to bath B (cyan).

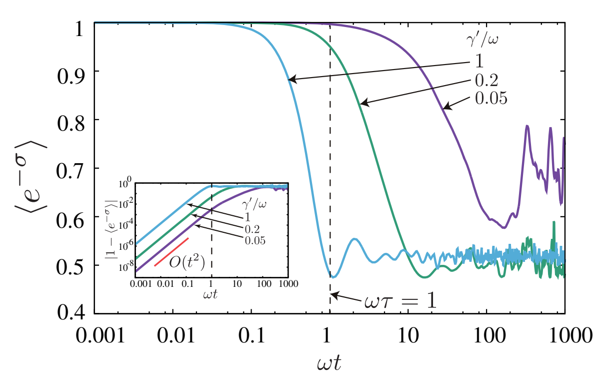

FIG. 3. Time dependence of $\langle e^{-\sigma}\rangle$ that numerically confirms the IFT. The structure of S and B is the same as that in the inset of Fig. 2. The parameters are given by $\gamma'/\omega=0.05,0.2,1$, $\gamma/\omega=1$, and $g/\omega=0.1$. Inset: Time dependence of the deviation of $\langle e^{-\sigma}\rangle$ from unity.

fluctuations can emerge from quantum fluctuations in a short-time regime, and the former crosses over to the latter in time. Our rigorous mathematical proof is based on the Lieb-Robinson bound (4) and the weak ETH (5). We also performed numerical simulation of two-dimensional hard-core bosons, and confirmed our theoretical results.

Our results can experimentally be tested with artificial isolated quantum systems, such as ultracold atoms on an optical lattice [87] and superconducting qubits [88]. Examining the relevance of our theory to nonartificial complex materials in noisy open environment is a future issue.

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