Quantum hydrodynamics from local thermal pure states

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We provide a pure state formulation for hydrodynamics of isolated quantum many-body systems. A pure state describing quantum systems in local thermal equilibrium is constructed, which we call a local thermal pure quantum (ℓTPQ) state. We show that the thermodynamic functional and the expectation values of local operators (including a real-time correlation function) calculated from the ℓTPQ state converge to those from a local Gibbs ensemble in the large fluid-cell limit. As a numerical demonstration, we investigate a one-dimensional spin chain and observe the hydrodynamic relaxation obeying Fourier's law. We further prove the second law of thermodynamics and the quantum fluctuation theorem, which are also validated numerically. The ℓTPQ formulation gives a useful theoretical basis to describe the emergent hydrodynamic behavior of quantum many-body systems furnished with a numerical efficiency applicable to both the nonrelativistic and relativistic regimes.

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I. INTRODUCTION

Nonequilibrium dynamics of isolated quantum many-body systems has been one of the central issues appearing at the crossroad of statistical physics and quantum physics. In particular, hydrodynamics [1–3] is an emergent macroscopic theory to investigate such dynamics under local equilibrium conditions. Recent experimental technologies have promoted further developments of hydrodynamic theory for isolated quantum systems, ranging from ultracold atoms [4–12] to quark-gluon plasma [13–22]. Furthermore, quantum or classical integrable systems, where conventional hydrodynamics is believed to break down, is now becoming a hot field on the basis of generalized hydrodynamics [23–27].

A recently developed microscopic derivation of hydrodynamics is based on an extended notion of the statistical ensembles, called the local Gibbs (LG) ensemble both in classical [28–30] and quantum systems [31–34]. An advantage of the local ensemble formulation lies in the fact that it does not require the quasiparticle description and thus is applicable to strongly coupled systems (see also another approach [35–38] based on the holographic principle and the pioneering works [39–45] along the line of the linear response theory). However, under unitary evolutions of isolated quantum systems, a pure state never falls into any mixed state such as the Gibbs ensemble. Thus it is still an open problem how macroscopic hydrodynamics emerges under unitary evolutions of pure states as observed in ultracold atoms [46–51].

In this paper, we provide a pure state-based derivation of the hydrodynamic equation for isolated quantum many-body systems. We introduce a special class of random pure quantum states describing systems in local thermal equilibrium, which we refer to as local thermal pure quantum (ℓTPQ) states. This is a generalization of thermal pure quantum (TPQ) states [52–59] randomly sampled from the Hilbert space to reproduce thermal equilibrium behaviors. We show that ℓTPQ states, having a numerical advantage in computing hydrodynamic expectation values [55,56,58,59], give the equivalent results with the conventional method based on the LG ensemble in the large fluid-cell limit.

We establish all the fundamental hydrodynamic behaviors from the ℓTPQ states equipped with a numerical efficiency. Specifically, we prove the Green-Kubo formula [60–62], the second law of thermodynamics, and the quantum fluctuation theorem [63–69], as well as the constitutive relation of hydrodynamics itself. We remark that our formulation is applicable to both the nonrelativistic and relativistic regimes, and therefore potentially covers a variety of phenomena from low to high energy scales. As a concrete demonstration, applying

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the ℓTPQ-state formulation to a one-dimensional quantum spin chain (see Refs. [70–76] and references therein for a review on recent theoretical approaches to thermal transport in low-dimensional systems), we numerically investigate the hydrodynamic relaxation starting from an ℓTPQ state, and confirm Fourier's law for thermal conduction.

The paper is organized as follows. In Sec. II, we construct the ℓTPQ state as a basis to describe the transport phenomena in quantum systems. In Sec. III, we present a derivation of hydrodynamics and quantum fluctuation theorem based on its equivalence to the ensemble formulation. In Sec. IV, we apply the ℓTPQ-state formulation to a nonintegrable spin chain and numerically confirm the hydrodynamic relaxation and the second law of thermodynamics. Section V is devoted to the summary and outlook. Appendixes A and B provide the proof of equivalence between the ℓTPQ and standard ensemble formulations, and a detail of the numerical evaluation of the Green-Kubo formula and quantum fluctuation theorem, respectively.

II. LOCAL THERMAL PURE QUANTUM (ℓTPQ) state

We first introduce the ℓTPQ state. Suppose that the nonintegrable system under consideration possesses a set of conserved currents $\hat{\mathcal{J}}_a^\mu(t)$ satisfying

$$\partial_\mu \hat{\mathcal{J}}_a^\mu(t) \equiv \partial_0 \hat{\mathcal{J}}_a^0(t) + \partial_i \hat{\mathcal{J}}_a^i(t) = 0, \tag{1}$$

where $\mu, \nu, \ldots$ denote space-time indices and $a, b, \ldots$ label conserved charges such as energy, momentum, and particle numbers. Throughout the paper, we use the Heisenberg picture, and Eq. (1) gives the equation of motion for conserved charge densities $\hat{c}_a(t) \equiv \hat{\mathcal{J}}_a^0(t)$.

Note that we assume that global symmetries of the nonintegrable system have been fully identified and Eq. (1) provides all independent conservation laws. We also note that summations over the repeated indices for Greek letters ($\mu, \nu, \ldots$) are assumed throughout the paper. The repeated indices for Latin letters is assumed to contain the spatial integral, e.g., $\lambda^a \hat{c}_a \equiv \int d^d x\, \lambda^a(\boldsymbol{x}) \hat{c}_a(\boldsymbol{x})$, where d denotes the spatial dimension. If we missed a subset of the conserved charges, we encounter the problem to derive the correct hydrodynamic equation (see the discussion in the end of Sec. III).

Then, we consider the system in local thermal equilibrium, which is described by local thermodynamic parameters λ^a conjugate to average charge densities $\langle \hat{c}_a \rangle$. We assume that each fluid cell contains many degrees of freedom so that thermodynamic parameters are smooth functions of spatial coordinates. Furthermore, we also consider a macroscopic time scale, where the hydrodynamic behavior is expected to emerge. In other words, we identify the current operators $\hat{\mathcal{J}}_a^\mu$ in Eq. (1) as space-time coarse-graining ones over a fluid-cell volume $V_{\rm cell}$ and time interval τ much larger than the microscopic scales. We will explicitly demonstrate this procedure for the spin chain in the subsequent section.

To describe the locally thermalized system, we introduce the ℓTPQ state at time t by

$$|\lambda_t; t\rangle \equiv \sum_\alpha z_\alpha e^{-\frac{1}{2}\hat{K}[\lambda_t;t]} |\alpha_t\rangle, \tag{2}$$

with $\hat{K}[\lambda_t; t] \equiv \lambda^a(t)\hat{c}_a(t)$, any orthonormal basis state vector $|\alpha_t\rangle$ at time t, and a complex random variable $z_\alpha \equiv (z'_\alpha + i z''_\alpha)/\sqrt{2}$ whose real/imaginary parts are taken from the normal distribution. Note that we distinguish two arguments in $\hat{K}[\lambda_t; t]$: one for thermodynamic parameters λ_t, whose suffix denotes its configuration $\lambda_t = \lambda(t)$ at time t, while the second argument t represents the time argument of charge densities as Heisenberg operators. When the system only contains the energy as the conserved charge, $\hat{K}$ reads $\hat{K}[\lambda_t; t] = \int d^d x\, \beta(t, \boldsymbol{x}) \hat{h}(t, \boldsymbol{x})$ with the local inverse temperature $\lambda_t = \beta(t, \boldsymbol{x})$ and energy density operator $\hat{h}(t, \boldsymbol{x})$, for instance. The normalization of the ℓTPQ state is defined by $Z_{\ell\rm TPQ}[\lambda_t] \equiv \langle \lambda_t; t | \lambda_t; t \rangle$, whose logarithm is identified as a thermodynamic functional. Using these, we define the entropy-functional operator at time t for the ℓTPQ state as

$$\hat{S}[\lambda_t; t] = \hat{K}[\lambda_t; t] + \ln Z_{\ell\rm TPQ}[\lambda_t], \tag{3}$$

and the average value over the ℓTPQ state as

$$\langle \hat{\mathcal{O}} \rangle_{\lambda_t}^{\ell\rm TPQ} \equiv \frac{1}{Z_{\ell\rm TPQ}[\lambda_t]} \langle \lambda_t; t | \hat{\mathcal{O}} | \lambda_t; t \rangle. \tag{4}$$

III. HYDRODYNAMICS AND THE QUANTUM FLUCTUATION THEOREM

Based on the ℓTPQ state, we derive hydrodynamics and the quantum fluctuation theorem. The hydrodynamic equation is regarded as the averaged Eq. (1) over a certain initial density operator $\hat{\rho}_0$. Here, we put a crucial assumption on the initial state: the system is in the ℓTPQ state at initial time t_0 parametrized by $\lambda_{t_0}^a$. Starting from this initial ℓTPQ state, we shall consider the subsequent time evolution of charge densities described by

$$\partial_\mu \langle \hat{\mathcal{J}}_a^\mu(t) \rangle = 0, \quad \text{with} \quad \langle \hat{\mathcal{J}}_a^\mu(t) \rangle \equiv \langle \hat{\mathcal{J}}_a^\mu(t) \rangle_{\lambda_{t_0}}^{\ell\rm TPQ}, \tag{5}$$

for $t \geqslant t_0$. To make Eq. (5) a closed set of equations, we need a constitutive relation, which expresses $\langle \hat{\mathcal{J}}_a^i(t) \rangle$ by the dynamical variable $\langle \hat{c}_a(t) \rangle = \langle \hat{\mathcal{J}}_a^0(t) \rangle$. Thus our problem is to find the constitutive relation.

The vital point here is that we have a solution to this problem if we replace the initial ℓTPQ-state average with the LG-ensemble average over the density operator [31–34]:

$$\hat{\rho}_{\rm LG}[\lambda_{t_0}; t_0] \equiv \frac{1}{Z_{\rm LG}[\lambda_{t_0}]} e^{-\hat{K}[\lambda_{t_0}; t_0]}, \tag{6}$$

where we defined the partition functional for the LG ensemble as $Z_{\rm LG}[\lambda_{t_0}] \equiv {\rm Tr}\, e^{-\hat{K}[\lambda_{t_0}; t_0]}$. We will express the LG average as $\langle \hat{\mathcal{O}} \rangle_{\lambda_t}^{\rm LG} \equiv {\rm Tr}(\hat{\rho}_{\rm LG}[\lambda_t; t] \hat{\mathcal{O}})$. Thus it is enough to show the equivalence between the ℓTPQ and LG averages for the purpose of deriving hydrodynamics from the ℓTPQ state.

Following the similar treatment of Refs. [55,56,58,59], we can indeed show such equivalence holds as convergence in probability $\xrightarrow{P}$ with respect to the random variable z_α (see Appendix A 1):

$$Z_{\ell\rm TPQ}[\lambda_t] \xrightarrow{P} Z_{\rm LG}[\lambda_t], \tag{7}$$

$$\langle \hat{\mathcal{O}} \rangle_{\lambda_t}^{\ell\rm TPQ} \xrightarrow{P} \langle \hat{\mathcal{O}} \rangle_{\lambda_t}^{\rm LG}, \tag{8}$$

where we took the large size limit of all fluid cells $V_{\rm cell} \to \infty$. Therefore, the LG-based derivation developed in Refs. [31–34] also provides a derivation of hydrodynamics from the ℓTPQ state in the large fluid-cell limit.

We summarize here some consequences of Eqs. (7) and (8). Within a first-order derivative expansion supplemented by the Markovian approximation for current-current correlators, the equivalence leads to the constitutive relation

$$\langle \hat{\mathcal{J}}_a^i(t)\rangle = \langle \hat{\mathcal{J}}_a^i(t)\rangle_{\lambda_t}^{\ell\rm TPQ} + L_{ab}^{ij}(t)\partial_j\lambda_t^b + O(\partial^2), \tag{9}$$

where transport coefficients L_{ab}^{ij} is given by the Green-Kubo formula with the TPQ state:

$$\begin{aligned} L_{ab}^{ij}(t) &= \beta_t \int_{-\infty}^{t} dt' \int d^dx' \int_0^1 d\tau \langle \widetilde{\delta}\hat{\mathcal{J}}_{a,\tau}^i(x)\widetilde{\delta}\hat{\mathcal{J}}_b^j(x')\rangle_{\lambda_t}^{\ell\rm TPQ} \\ &\simeq \frac{\beta_t}{4V}\int_{-\infty}^{\infty} dt' \langle\{\widetilde{\delta}\hat{\mathfrak{J}}_a^i(t), \widetilde{\delta}\hat{\mathfrak{J}}_b^j(t')\}\rangle_{\lambda_t}^{\rm TPQ}, \end{aligned} \tag{10}$$

where we defined $\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\rm TPQ}$ as a grand-canonical TPQ average parametrized by λ_t [55,56,58,59]. Here we defined a projected operator $\widetilde{\delta}\hat{\mathcal{O}} \equiv (1-\hat{\mathcal{P}})\delta\hat{\mathcal{O}}$ using the ℓTPQ version of Mori's projection [43,44]:

$$\hat{\mathcal{P}}\hat{\mathcal{O}}(t) \equiv \delta\hat{c}_a(t)\frac{\delta}{\delta c_a(t)}\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}, \tag{11}$$

together with $\delta\hat{\mathcal{O}}(t) \equiv \hat{\mathcal{O}}(t) - \langle\hat{\mathcal{O}}(t)\rangle_{\lambda_t}^{\ell\rm TPQ}$ and $\hat{\mathcal{O}}_\tau(t) \equiv e^{\hat{K}[\lambda_t;t]\tau}\hat{\mathcal{O}}(t)e^{-\hat{K}[\lambda_t;t]\tau}$. In the second line of Eq. (10), we neglected the higher-order derivative correction and defined total currents $\hat{\mathfrak{J}}_a^i(t) \equiv \int d^dx\, \hat{\mathcal{J}}_a^i(t,\boldsymbol{x})$ with the anticommutator $\{\hat{A},\hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$ and total volume $V \equiv \int d^dx$. Note that the constitutive relation (9) is expressed by the parameter $\lambda_t^a = \{\beta_t, \ldots\}$ at time t, which is defined by the matching condition $\langle\hat{c}_a(t)\rangle = \langle\hat{c}_a(t)\rangle_{\lambda_t}^{\ell\rm TPQ}$. Thanks to one-to-one correspondence between λ_t^a and $\langle\hat{c}_a(t)\rangle$ (apart from the first-order phase transition), Eq. (9) indeed expresses $\langle\hat{\mathcal{J}}_a^i(t)\rangle$ by $\langle\hat{c}_a(t)\rangle$. Then, once we evaluate $\langle\hat{\mathcal{J}}_a^i(t)\rangle_{\lambda_t}^{\ell\rm TPQ}$ following from the thermodynamic functional $\ln Z_{\ell\rm TPQ}[\lambda_t]$ (see, e.g., Refs. [31–34]) and the Green-Kubo formula (10), Eq. (9) closes the averaged conservation law (5), which completes an ℓTPQ-based derivation of the first-order hydrodynamics.

In addition to hydrodynamic equations, we can also show the quantum fluctuation theorem and the second law of thermodynamics for the ℓTPQ state within a small error. For that purpose, let us introduce the generating function of the total entropy production from initial time t_0 to arbitrary time $t\,(>t_0)$ with forward/backward evolution:

$$G_F^{\ell\rm TPQ}(z) = \langle\hat{\mathcal{U}}^\dagger(t)e^{iz\hat{S}[\lambda_t;t_0]}\hat{\mathcal{U}}(t)e^{-iz\hat{S}[\lambda_{t_0};t_0]}\rangle_{\lambda_{t_0}}^{\ell\rm TPQ}, \tag{12}$$

$$G_B^{\ell\rm TPQ}(z) = \langle\widetilde{\mathcal{U}}(t)e^{iz\hat{S}[\tilde{\lambda}_{t_0};t]}\widetilde{\mathcal{U}}^\dagger(t)e^{-iz\hat{S}[\tilde{\lambda}_t;t]}\rangle_{\tilde{\lambda}_t}^{\ell\rm TPQ}, \tag{13}$$

where $\hat{\mathcal{U}}(t)$ is the time evolution operator. By using a combined parity and time-reversal $\Theta \equiv \mathsf{PT}$, we also defined PT-transformed time evolution operator and parameter by $\widetilde{\mathcal{U}}(t) \equiv \Theta\hat{\mathcal{U}}(t)\Theta^{-1}$ and $\tilde{\lambda}_t \equiv \epsilon^a\lambda^a(t,-\boldsymbol{x})$ with ϵ^a being a PT eigenvalue of charge densities $\hat{c}_a$, respectively. We can then prove the second law of thermodynamics and quantum fluctuation theorem as (see Appendix A 2)

$$\langle\hat{S}[\lambda_t;t] - \hat{S}[\lambda_{t_0};t_0]\rangle \geqslant O(e^{-A_1V_{\rm cell}}), \tag{14}$$

$$\left|G_F^{\ell\rm TPQ}(z) - G_B^{\ell\rm TPQ}(-z+i)\right| = O(e^{-A_2V_{\rm cell}}), \tag{15}$$

where A_1 and A_2 denote certain numerical factors. Note that the violation of both the fluctuation theorem and the second law is exponentially small with respect to the volume of fluid cell $V_{\rm cell}$, which is the same as Eqs. (7) and (8).

Two remarks on our assumption are in order. First, it is crucial to identify the complete set of all conserved charges in the derivation (see also Ref. [77] for a recent discussion of the completeness of conserved charges). If we missed a subset of the conserved charges, two problems will arise. The Markovian approximation to derive Eq. (9) will break down (or equivalently Green-Kubo formula will diverge) due to a contribution from the missed hydrodynamic modes. Besides, the leading-order constitutive relation, given by the first term in Eq. (9), also fails to capture the correct hydrodynamic behavior. For instance, if we missed the momentum from a set of conserved charges, the linearized zeroth-order hydrodynamics following from our formulation cannot describe the sound mode that should be present.

Secondly, it is also important to perform coarse graining over appropriate spatial and temporal domains. Without the coarse-graining procedure, the charge densities—or conjugate local thermodynamic parameters—show violent behaviors in space-time evolution. This leads to the large derivatives of local thermodynamic parameters and breaks our derivative expansion employed in Eq. (9). Thus both the completeness of conserved charges and the appropriate coarse-graining procedure are crucial assumptions in the present derivation (and also in the derivation based on the LG ensemble [31–34]).

IV. APPLICATION TO SPIN CHAIN

In this section, we apply the developed ℓTPQ-state formalism to a one-dimensional nonintegrable spin chain. After presenting the model and smeared operator in Sec. IV A, we introduce a numerical way to implement the ℓTPQ simulation in Sec. IV B and show the result of our numerical simulation in Sec. IV C.

A. Model and setup

We now apply the developed formalism to a one-dimensional nonintegrable lattice half-integer spin system, whose Hamiltonian reads

$$\begin{aligned} \hat{H} = \sum_{n=1}^{N}\big[&J_z\sigma_n^z\sigma_{n+1}^z + D\big(\sigma_n^z\sigma_{n+1}^x - \sigma_n^x\sigma_{n+1}^z\big) \\ &+ \Gamma\sigma_n^x + B\sigma_n^z\big], \end{aligned} \tag{16}$$

where we impose the periodic boundary condition as $\sigma_{N+1}^i = \sigma_1^i$ with $i = x,y,z$ and set the coupling constants $J_z = \Gamma = -B = D = 0.2$ in the following simulations. The energy is the only conserved quantity of this system, so that the Heisenberg

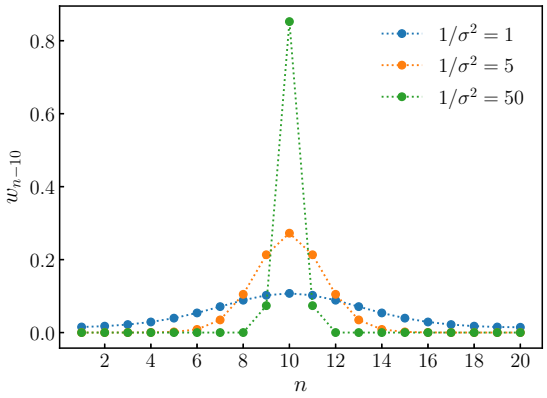

FIG. 1. Weight function Eq. (24).

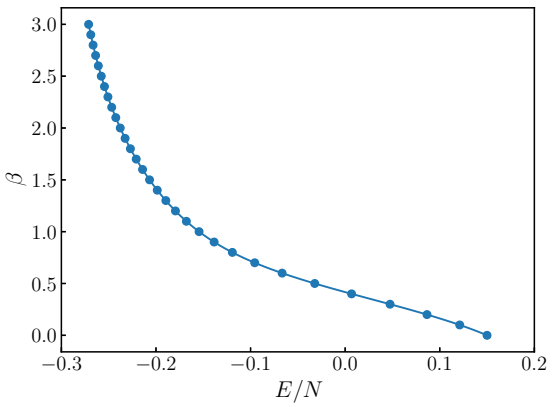

FIG. 2. Equation of state for the Hamiltonian Eq. (16) with the system size $N = 20$. The total energy is calculated at $\beta = 0.0, 0.1, \ldots, 3.0$ and they are represented by circles. The solid line is the interpolation of them.

equation of motion for the energy density operator $\hat{h}(t, n)$ becomes the conservation law:

$$\partial_t \hat{h}(t, n) + \nabla_x \hat{J}_E(t, n) = 0. \tag{17}$$

Here, we defined the energy density operator $\hat{h}(n)$ and energy current operator $\hat{J}_E(n - 1/2)$ as

$$\begin{aligned} \hat{h}(n) \equiv\ & J_z \sigma_n^z \sigma_{n+1}^z + D\left(\sigma_n^z \sigma_{n+1}^x - \sigma_n^x \sigma_{n+1}^z\right) \\ & + \Gamma \sigma_n^x + B \sigma_n^z, \end{aligned} \tag{18}$$

$$\begin{aligned} \hat{J}_E(n - 1/2) \equiv\ & -2D^2\left(\sigma_{n-1}^x \sigma_n^y \sigma_{n+1}^z - \sigma_{n-1}^z \sigma_n^y \sigma_{n+1}^x\right) \\ & + 4DJ_z \sigma_{n-1}^z \sigma_n^y \sigma_{n+1}^z - 2\Gamma J_z \sigma_{n-1}^z \sigma_n^y \\ & + 2D\Gamma \sigma_{n-1}^x \sigma_n^y + 2DB \sigma_{n-1}^z \sigma_n^y, \end{aligned} \tag{19}$$

and the discrete version of the spatial divergence as

$$\nabla_x \langle \hat{J}_E(t, n) \rangle \equiv \langle \hat{J}_E(t, n + 1/2) \rangle - \langle \hat{J}_E(t, n - 1/2) \rangle. \tag{20}$$

To investigate the hydrodynamic behavior, we define smearing of a local operator $\hat{\mathcal{O}}(t, n)$ in both spatial and temporal directions as

$$\bar{\mathcal{O}}(t, n) \equiv \frac{1}{\tau} \int_t^{t+\tau} dt' \sum_{m=1}^{N} w_{n-m} \hat{\mathcal{O}}(t', m), \tag{21}$$

with an appropriate weight function w_{n-m}, which is a positive and has a peak at $n = m$, and coarse-graining scale along the temporal direction τ (see also Ref. [78] for the necessity of space-time averaging of currents). We also require w_n to satisfy the periodic condition $w_{n-N} = w_n$ to have a well-defined smeared energy conservation law. In fact, thanks to the periodic condition, the continuity equation holds also for the smeared operator as

$$\partial_\tau \bar{h}(t, n) + \nabla_x \bar{J}_E(t, n) = 0, \tag{22}$$

where we defined the time derivative in the hydrodynamic scale as

$$\partial_\tau \bar{h}(t, n) \equiv \frac{\bar{h}(t + \tau, n) - \bar{h}(t, n)}{\tau}, \tag{23}$$

while the spatial gradient $\nabla_x \bar{J}_E(t, n)$ takes the same form as Eq. (20) for $\bar{J}_E$.

In our numerical simulations, we choose the weight function w_n as

$$w_n = \frac{1}{\sum_{m=1}^{N} e^{\frac{1}{\sigma^2} \cos \frac{2\pi m}{N}}} e^{\frac{1}{\sigma^2} \cos \frac{2\pi n}{N}}, \tag{24}$$

where σ^2 is a positive parameter controlling the smearing length. In the thermodynamic limit with $N \to \infty$, the typical width of this function is given by $1 - I_1(1/\sigma^2)/I_0(1/\sigma^2)$, where $I_n(x)$ is the modified Bessel function of the first kind. For our purpose, the width of the weight function, regarded as the effective size of the fluid cell Λ, should be taken to satisfy $1 \ll \Lambda \ll N$. Typical shapes of the weight function are shown in Fig. 1. For instance, the number of spins in the fluid cell is about 5 when $1/\sigma^2 = 5$.

B. Numerical implementation

a. Preparation of the ℓTPQ state. Let us first review a way to implement a canonical TPQ state, which is defined by

$$|\beta\rangle \equiv \exp\left(-\frac{N\beta\hat{h}}{2}\right) \sum_\alpha z_\alpha |\alpha\rangle, \tag{25}$$

where $\hat{h} = \hat{H}/N$ is the Hamiltonian density and $|\alpha\rangle$ is a random vector in the Hilbert space. We then expand the canonical TPQ state by microcanonical TPQ states as

$$\begin{aligned} |\beta\rangle &= e^{-N\beta l/2} \sum_{k=0}^{\infty} R_k |\psi_k\rangle \\ \text{with } & \begin{cases} |\psi_k\rangle = \frac{|k\rangle}{\langle k|k\rangle}, \\ |k\rangle \equiv (l - \hat{h})^k \sum_\alpha z_\alpha |\alpha\rangle, \\ R_k(\beta) = \frac{(N\beta/2)^k \langle k|k\rangle}{k!}, \end{cases} \end{aligned} \tag{26}$$

where l is a certain number larger than the maximum eigenvalue of $\hat{h}$. One can show that R_k has a sharp peak at a certain $k = k^*$, whose magnitude is controlled by the inverse temperature [55,56,58,59]. Thanks to this property, we can truncate the expansion at a certain order $k = k_{\max}$ with

$$\frac{R_{k_{\max}}}{\max_k R_k} > 10^{-u}, \tag{27}$$

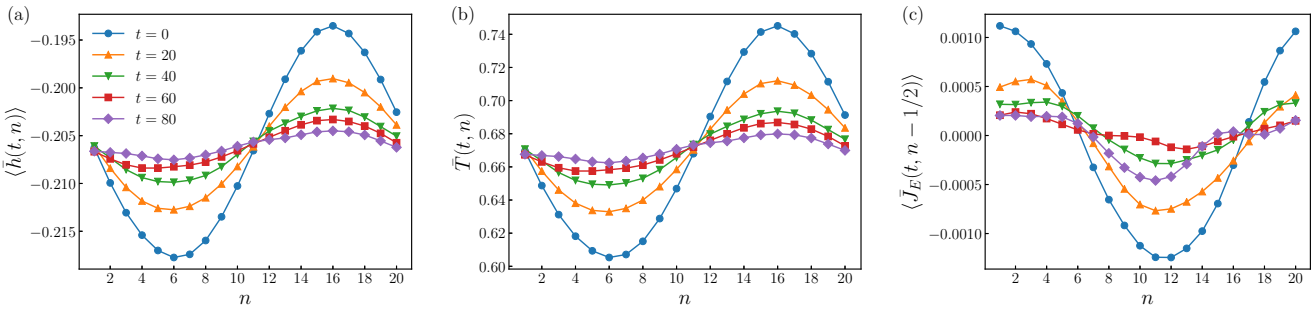

FIG. 3. Time evolutions of (a) local energy density, (b) local temperature, and (c) energy current of the model (16) with parameters $(J_z, D, \Gamma, B) = (0.2, 0.2, 0.2, -0.2)$.

for a given tolerance parameter u. In our simulations, we take $u = 20$ and confirm that the expectation values of observables are well converged.

One can generalize the above procedure in a straightforward manner to the implementation of ℓTPQ states. For that purpose, we first define the ℓTPQ state

$$|\{\beta(n)\}\rangle \equiv \exp\left(-\frac{\sum_{n=1}^{N}\beta(n)\hat{h}(n)}{2}\right)\sum_{\alpha} z_\alpha|\alpha\rangle, \tag{28}$$

where $\hat{h}(n)$ is the local Hamiltonian density. Expanding the exponential operator, we find

$$\begin{aligned}
&|\{\beta(n)\}\rangle \\
&= e^{-\frac{1}{2}\sum_n \beta(n) l_n} \exp\left(\frac{\sum_{n=1}^{N}\beta(n)[l_n - \hat{h}(n)]}{2}\right)\sum_{\alpha} z_\alpha|\alpha\rangle \\
&= e^{-\frac{1}{2}\sum_n \beta(n) l_n} \sum_k \frac{\bar{\beta}^k N^k}{2^k k!}|k, \{\beta(n)\}\rangle,
\end{aligned} \tag{29}$$

where l_n is a certain number larger than the maximum eigenvalue of $\hat{h}(n)$ and $\bar{\beta} = \frac{1}{N}\sum_{n=1}^{N}\beta(n)$ is the average inverse temperature. We also introduced the state $|k, \{\beta(n)\}\rangle$

$$|k, \{\beta(n)\}\rangle \equiv \left(\frac{1}{N\bar{\beta}}\sum_{n=1}^{N}\beta(n)[l_n - \hat{h}(n)]\right)^k \sum_{\alpha} z_\alpha|\alpha\rangle, \tag{30}$$

which can be regarded as a generalization of the microcanonical TPQ state. Indeed, we can show $|k, \{\beta(n)\}\rangle$ coincides with the microcanonical TPQ state when $\beta(n) = \text{const}$ and $l_n = \text{const}$. However, we note that the position dependence of the local temperature, in general, does not allow us to express the ℓTPQ state by the microcanonical counterpart, as is the case for global thermal equilibrium [55,56,58,59].

In short, we express the ℓTPQ state as

$$\begin{aligned}
&|\{\beta(n)\}\rangle = e^{-\frac{1}{2}\sum_n \beta(n) l_n}\sum_{k=0}^{\infty} R_k[\{\beta(n)\}]|\psi_k, \{\beta(n)\}\rangle, \\
&\text{with} \begin{cases} |\psi_k, \{\beta(n)\}\rangle = \frac{|k,\{\beta(n)\}\rangle}{\langle k,\{\beta(n)\}|k,\{\beta(n)\}\rangle}, \\ R_k[\{\beta(n)\}] = \frac{(N\bar{\beta}/2)^k\langle k,\{\beta(n)\}|k,\{\beta(n)\}\rangle}{k!}. \end{cases}
\end{aligned} \tag{31}$$

As is the case with the canonical TPQ state, we confirmed that $R_k[\{\beta(n)\}]$ also has a sharp peak at a certain $k = k^*$ so that we can truncate the summation over k in Eq. (31). Equations (30) and (31) define a way to prepare the ℓTPQ state starting from an arbitrary random vector $|\alpha\rangle$ in the Hilbert space.

b. The energy-temperature relation. To compare the numerical result with the hydrodynamic description, we need to introduce the local temperature according to the matching condition $\langle \bar{h}(t,n)\rangle = \langle \bar{h}(t,n)\rangle_{\beta_t}$. Within the derivative expansion, this condition is equivalent to use the thermodynamic relation to determine the local temperature from the given energy density.

One can use the equation of state as such a thermodynamic relation, which enables us to relate the energy density and local temperature. Using the canonical TPQ states, the total energy of the system is calculated as

$$E \equiv \frac{\langle\beta|\hat{H}|\beta\rangle}{\langle\beta|\beta\rangle}. \tag{32}$$

This relation gives the one-to-one correspondence between the energy and the inverse temperature as long as first order phase transitions do not occur. We calculate the total energy for several inverse temperatures $\beta = 0.0, 0.1, \ldots, 3.0$ for the system size $N = 20$. The results are shown in Fig. 2. Using this relation, we define the local inverse temperature $\beta_t(n)$ from the calculated expectation value of the energy density operator $\langle \bar{h}(t,n)\rangle$.

C. Result of ℓTPQ simulation

In accordance with our formal derivation, one can expect the long-time/length behavior of the energy current is governed by the hydrodynamic equation. In the present setup, the constitutive relation within the leading-order derivative expansion leads to Fourier's law:

$$\langle \hat{J}_E(t, n-1/2)\rangle = -\kappa_{\text{Fourier}}(t,n)\nabla_x T(t, n-1/2), \tag{33}$$

where we defined $\nabla_x T(t, n-1/2) \equiv T(t,n) - T(t,n-1)$ with $T(t,n) \equiv 1/\beta(t,n)$. The proportional coefficient $\kappa_{\text{Fourier}}(t,n)$ is identified as the thermal conductivity. On the other hand, we can also compute the thermal conductivity from the Green-Kubo formula:

$$\kappa(t,n) = \frac{\beta(t,n)^2}{4N}\lim_{\tau\to\infty}\int_{-\tau}^{\tau} dt\,\langle\{\delta\hat{\mathfrak{J}}_E(t), \delta\hat{\mathfrak{J}}_E(t_0)\}\rangle^{\text{TPQ}}_{\beta(t,n)}, \tag{34}$$

with the total energy current $\hat{\mathfrak{J}}_E(t) \equiv \sum_{n=1}^{N}\hat{J}_E(t, n-1/2)$. Our derivation tells us that κ_{Fourier} should agree with κ in the large fluid-cell limit. Thus we can quantitatively evaluate the

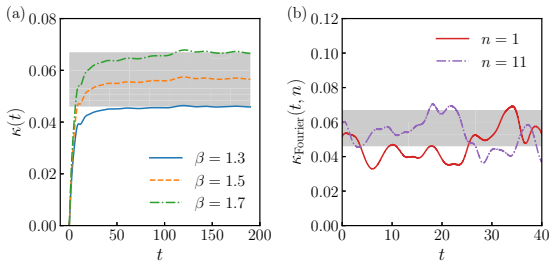

FIG. 4. Numerical results for (a) Green-Kubo formula (34) and (b) comparison of $\kappa_{\rm Fourier}(t,n)$ with the thermal conductivity evaluated from the Green-Kubo formula. The parameters are the same as in Fig. 3.

validity of the hydrodynamic description by comparing the values of $\kappa_{\rm Fourier}(t,n)$ and $\kappa(t,n)$, which are independently evaluated from Eqs. (33) and (34).

As we explained in the previous section, a numerical implementation of the ℓTPQ-based simulation is realized in a similar way with the canonical TPQ state [55,56,58,59]. We assume that the initial state is given by the ℓTPQ state defined in Eqs. (30) and (31) with an initial distribution of the local temperature $\beta(t_0,n)$, which we set as

$$\beta(t_0,n) = \bar{\beta} + \Delta\beta \sin\frac{2\pi(n-1)}{N} \quad (n = 1,\ldots,N), \quad (35)$$

with $\bar{\beta} = 1.5$ and $\Delta\beta = 0.2$. We numerically solve the Schrödinger equation by the fourth order Runge-Kutta method with a time slice $\Delta t = 0.01$, and calculated the local energy and the energy current. We also note that the smearing in Eq. (21) is also performed by choosing $1/\sigma^2 = 5$, which leads to the fluid-cell size to contain five spins or so), and $\tau = 10$.

Figure 3 shows the time evolution of the local energy density, local temperature, and energy current starting from an inhomogeneous temperature profile given in Eq. (35) (the local temperature is estimated from the local energy through the relation shown in Fig. 2 assuming that derivative corrections are negligible). We clearly see the diffusive relaxation of inhomogeneous temperature (or equivalently energy density). Furthermore, we can find a tendency of the energy current responding to the temperature gradient, which is compatible with Fourier's law (33). Note, however, that we cannot conclude that the system really obeys Eqs. (33) and (34) at this point because we have not shown the thermal conductivity, appearing in Eq. (33), indeed matches with that evaluated from the Green-Kubo formula (34).

To microscopically confirm the hydrodynamic relaxation, we evaluate the coefficient of Fourier's law Eq. (33) and compare it with the thermal conductivity $\kappa(t,n)$ independently evaluated from the Green-Kubo formula (34) (see Appendix B 1 in detail). If the system is really in the hydrodynamic regime, these quantities should coincide with each other.

The result is given in Fig. 4. Taking account of the temperature window, we compute the Green-Kubo formula for three values of temperatures (see shaded regions in Fig. 4). Figure 4(b) then indicates that the values of Fourier's law coefficient (33) stay comparable regions with those obtained from the Green-Kubo formula, though they fluctuate

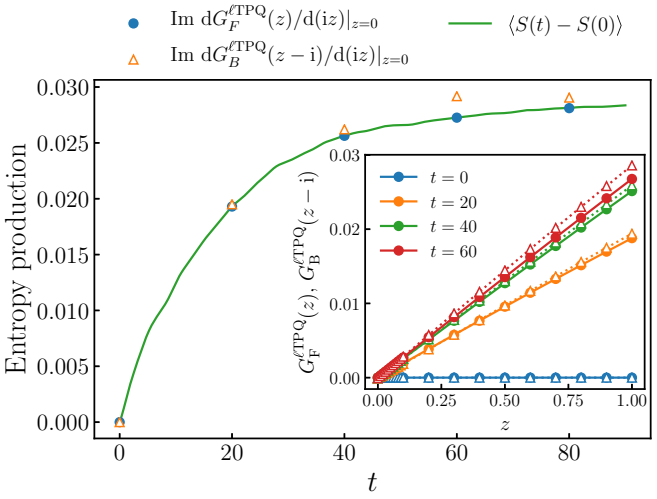

FIG. 5. Numerical result for the entropy production (14) [inset: the quantum fluctuation theorem (15)]. The parameters are the same as in Fig. 3.

depending on temporal and spatial positions. The agreement may be surprisingly good if we recall our fluid-cell contains just five spins or so, and the deviation is probably from the finite-volume effect. In short, we conclude that the hydrodynamic description is confirmed to be a good approximation on the basis of the Schrödinger equation.

We finally show the result on the second law of thermodynamics and the quantum fluctuation theorem (see Appendix B 2 in detail). Figure 5 demonstrates the time dependence of the entropy production (main figure) and the quantum fluctuation theorem (inset). The solid line in Fig. 5 for the entropy production is from a direct evaluation, and data are evaluated from the slopes of the generating functions $G_F^{\ell\rm TPQ}(z)$ and $G_B^{\ell\rm TPQ}(i-z)$, which are shown in the inset by solid and dotted lines, respectively. They take positive values in the entire time regions, which confirms the second law of thermodynamics. Moreover, one sees that $G_F^{\ell\rm TPQ}(z)$ indeed works as a generating function of the entropy production. However, due to uncertainty of the fluctuation theorem coming from the finiteness of the fluid cell as shown in Eq. (15), $G_B^{\ell\rm TPQ}(i-z)$ (and its slope) at a later time will deviate from $G_F^{\ell\rm TPQ}(z)$ (see also the inset of Fig. 5). Although we cannot analytically evaluate dependencies of the deviation on the time and z, this behavior looks similar to those obtained in Refs. [68,79].

V. CONCLUDING REMARKS

In this paper, we have formulated hydrodynamics based on a special class of random pure quantum states, which we call the ℓTPQ state. We have shown the equivalence of the ℓTPQ-state formalism to that of the LG ensemble in the large fluid-cell limit in Eqs. (7) and (8), from which we have derived the hydrodynamic equations (9) and (10), the second law of thermodynamics (14), and the quantum fluctuation theorem (15). Using the ℓTPQ state, we have performed the numerical simulation of a one-dimensional nonintegrable

spin chain model. From a careful analysis, we have numerically confirmed that the observed thermal diffusion allows the hydrodynamic description with Fourier's law and the Green-Kubo formula (Figs. 3 and 4). The validity of the second law of thermodynamics and quantum fluctuation theorem has also been confirmed (Fig. 5).

Let us comment on limitations of the ℓTPQ-state formulation both from the conceptual and practical viewpoints. First of all, the present formulation employs an ℓTPQ state mainly motivated by its numerical efficiency. However, an ℓTPQ state is a randomly sampled special state designed to reproduce local thermodynamics for isolated quantum systems. Therefore, an ℓTPQ state is not directly related to the eigenstate thermalization hypothesis (ETH) [80–89], as the latter concerns energy eigenstates that are responsible for quantum ergodicity of Hamiltonian dynamics. We thus believe that it is crucial to construct a pure state formulation based on the ETH in establishing a more solid foundation for hydrodynamics of isolated quantum systems, which is an important future issue.

Another limitation of the ℓTPQ-state formulation is set by the dimension of the Hilbert space of bosonic systems. Since we do not assume the relativistic or nonrelativistic nature of systems, the ℓTPQ formulation is, in principle, applicable to any quantum system including the quark-gluon plasma or relativistic/nonrelativistic Bose gas. Although a current computational resource does not allow us to perform the ℓTPQ simulation for such bosonic systems with huge degrees of freedom, it would be of immediate interest to perform the ℓTPQ simulation for fermionic systems.

There are also interesting prospects that can be clarified along the line of this paper. While we performed an ℓTPQ simulation for the system with the single conserved quantity, it is interesting to realize the simulation with multiple conserved charges. In particular, the existence of the momentum density in low-dimensional systems is interesting, because it is expected to drastically change conventional hydrodynamics due to a large hydrodynamic fluctuation [74]. Furthermore, it would be an interesting direction to extend our ℓTPQ framework so as to apply thermal transports for quantum integrable systems described by generalized hydrodynamics [23–27]. We left them as future works (some will be reported in the subsequent publication [90]).

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APPENDIX A: PROOFS OF EQUIVALENCE IN THE LARGE FLUID-CELL LIMIT

We here give proofs of equivalence between ℓTPQ formulation and the local Gibbs (LG) ensemble method, which includes a proof of the second law of thermodynamics and quantum fluctuation theorem in the ℓTPQ formulation.

1. Proof of Eqs. (7) and (8)

We give here a proof of Eqs. (7) and (8), which is similarly accomplished as is the case with the global thermal equilibrium [55,56,58,59]. For that purpose, we rely on Chebyshev's inequality:

$$\mathrm{Prob}_z[|\mathcal{O}-\langle\mathcal{O}\rangle_z|\geqslant\epsilon]\leqslant\frac{\langle(\mathcal{O}-\langle\mathcal{O}\rangle_z)^2\rangle_z}{\epsilon^2}=\frac{\langle\mathcal{O}^2\rangle_z-\langle\mathcal{O}\rangle_z^2}{\epsilon^2}. \tag{A1}$$

Let us first define the average over the random variable $z_\alpha=(z'_\alpha+iz''_\alpha)/\sqrt{2}$ by $\langle\mathcal{O}(z)\rangle_z$. Since both real and imaginary parts are independently sampled from the standard normal distribution, they satisfy, e.g.,

$$\langle z_\alpha\rangle_z=0,\quad \langle z^*_{\alpha_1}z_{\alpha_2}\rangle_z=\delta_{\alpha_1\alpha_2},\quad \langle|z_\alpha|^4\rangle_z=2,\quad \langle|z_{\alpha_1}|^2|z_{\alpha_2}|^2\rangle_z=1,\quad \langle z^*_{\alpha_1}z^*_{\alpha_2}z_{\alpha_3}z_{\alpha_4}\rangle_z=0, \tag{A2}$$

where $\delta_{\alpha_1\alpha_2}$ denotes the Kronecker delta and the last two equations hold for $\alpha_1\neq\alpha_2$. With the help of Eqs. (A2), we can show the following key identity for a state $|\psi_0\rangle\equiv\sum_\alpha z_\alpha|\alpha\rangle$:

$$\langle(\langle\psi_0|\hat{A}|\psi_0\rangle-\langle\langle\psi_0|\hat{A}|\psi_0\rangle\rangle_z)(\langle\psi_0|\hat{B}|\psi_0\rangle-\langle\langle\psi_0|\hat{B}|\psi_0\rangle\rangle_z)\rangle_z=\mathrm{Tr}(\hat{A}\hat{B}), \tag{A3}$$

where $\hat{A}$ and $\hat{B}$ denote arbitrary operators.

a. Proof of Eq. (7). In order to show the convergence of the partition functional (7), we use Chebyshev's inequality (A1) for $\mathcal{O}=Z_{\ell\mathrm{TPQ}}[\lambda_t]/Z_{\mathrm{LG}}[\lambda_t]=\langle\lambda_t;t|\lambda_t;t\rangle/\langle\langle\lambda_t;t|\lambda_t;t\rangle\rangle_z$. Recalling the definition of the partition functional for the ℓTPQ state and LG ensemble $Z_{\mathrm{LG}}[\lambda_t]\equiv\mathrm{Tr}\ e^{-\hat{K}[\lambda_t;t]}$, we find the identity (A3) with $\hat{A}=\hat{B}=e^{-\hat{K}[\lambda_t;t]}$ provides the right-hand side of Chebyshev's inequality thanks to

$$\begin{aligned}\langle\psi_0|e^{-\hat{K}[\lambda_t;t]}|\psi_0\rangle&=\langle\lambda_t;t|\lambda_t;t\rangle=Z_{\ell\mathrm{TPQ}}[\lambda_t],\\ \langle\langle\psi_0|e^{-\hat{K}[\lambda_t;t]}|\psi_0\rangle\rangle_z&=\langle\langle\lambda_t;t|\lambda_t;t\rangle\rangle_z=Z_{\mathrm{LG}}[\lambda_t].\end{aligned} \tag{A4}$$

As a consequence, we obtain

$$\left\langle\left(\frac{\langle\lambda_t;t|\lambda_t;t\rangle}{\langle\langle\lambda_t;t|\lambda_t;t\rangle\rangle_z}-1\right)^2\right\rangle_z=\frac{Z_{\rm LG}[2\lambda_t]}{(Z_{\rm LG}[\lambda_t])^2}=\exp\left[-2\int_\Lambda d^dx\,\beta_t\big(p(\beta_t,\mu_t^a)-p\big(2\beta_t,\mu_t^a\big)+O(\partial^2)\big)\right],\tag{A5}$$

where, to show the second equality, we used the leading-order expression of the Massieu-Planck functional $\ln Z_{\rm LG}[\lambda_t]$ for a parity-preserving fluid obtained in Refs. [31–33]. Here $\beta_t=\beta(t,\boldsymbol{x})$ denotes the local inverse temperature conjugate to the energy density, $\mu_t^a=\mu^a(t,\boldsymbol{x})$ local chemical potentials for charge densities $\hat{J}_a^0$ attached to internal symmetries of the system labeled by indices a. We explicitly put the size of the fluid cell Λ. Substituting this result into Chebyshev's inequality, we obtain

$$\mathrm{Prob}_z\left[\left|\frac{Z_{\ell\rm TPQ}[\lambda_t]}{Z_{\rm LG}[\lambda_t]}-1\right|\geqslant\epsilon\right]\leqslant\frac{1}{\epsilon^2}\exp\left(-2\int_\Lambda d^dx\,\beta_t[\Delta p(\beta_t,\mu_t^a)+O(\partial^2)]\right),\tag{A6}$$

where we introduced $\Delta p(\beta_t,\mu_t^a)\equiv p(\beta_t,\mu_t^a)-p(2\beta_t,\mu_t^a)$.

The vital point here is that the pressure of a fluid cell $p(\beta_t,\mu_t^a)$ is the decreasing function with respect to β_t and satisfies $p(\beta_t,\mu_t^a)-p(2\beta_t,\mu_t^a)>0$. Therefore, taking the large size limit of the fluid cell $V_{\rm cell}\equiv\int_\Lambda d^dx$, we see that the probability of finding the difference between $Z_{\ell\rm TPQ}[\lambda_t]$ and $Z_{\rm LG}[\lambda_t]$ will be exponentially small. This completes the proof of Eq. (7). ■

b. Proof of Eq. (8). Let us move on to the proof for Eq. (8). The average values over ℓTPQ and LG distribution are given by

$$\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}=\frac{\langle\lambda_t;t|\hat{\mathcal{O}}|\lambda_t;t\rangle}{\langle\lambda_t;t|\lambda_t;t\rangle},\quad\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\rm LG}=\frac{\langle\langle\lambda_t;t|\hat{\mathcal{O}}|\lambda_t;t\rangle\rangle_z}{\langle\langle\lambda_t;t|\lambda_t;t\rangle\rangle_z}.\tag{A7}$$

Noting $\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\rm LG}\neq\langle\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}\rangle_z$, we divide the proof into two steps. First, we evaluate the difference between $\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}$ and $\langle\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}\rangle_z$ and, second, we evaluate the difference between $\langle\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}\rangle_z$ and $\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\rm LG}$.

As a first step, we use Chebyshev's inequality for $\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}=\langle\lambda;t|\hat{\mathcal{O}}|\lambda_t;t\rangle/\langle\lambda_t;t|\lambda_t;t\rangle$. In order to evaluate the right-hand side of that inequality, we expand it as

$$\begin{aligned}\left\langle\left(\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}-\left\langle\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}\right\rangle_z\right)^2\right\rangle_z&=\left\langle\left(\frac{\langle\lambda_t;t|\hat{\mathcal{O}}|\lambda_t;t\rangle}{\langle\lambda_t;t|\lambda_t;t\rangle}-\left\langle\frac{\langle\lambda_t;t|\hat{\mathcal{O}}|\lambda_t;t\rangle}{\langle\lambda_t;t|\lambda_t;t\rangle}\right\rangle_z\right)^2\right\rangle_z\\&=\frac{\langle(\delta f)^2\rangle_z}{(Z_{\rm LG}[\lambda_t])^2}-\frac{2\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\rm LG}\langle\delta f\delta g\rangle_z}{(Z_{\rm LG}[\lambda_t])^2}+\frac{\big(\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\rm LG}\big)^2\langle(\delta g)^2\rangle_z}{(Z_{\rm LG}[\lambda_t])^2}+O(\delta^3),\end{aligned}\tag{A8}$$

where we defined

$$\delta f=\langle\lambda_t;t|\hat{\mathcal{O}}|\lambda_t t;t\rangle-\langle\langle\lambda_t;t|\hat{\mathcal{O}}|\lambda_t;t\rangle\rangle_z,\quad\delta g=\langle\lambda_t;t|\lambda_t;t\rangle-\langle\langle\lambda_t;t|\lambda_t;t\rangle\rangle_z.\tag{A9}$$

Since we have already evaluated $\langle(\delta g)^2\rangle_z$ in Eq. (A5), we only need to evaluate the first two terms in Eq. (A8): $\langle(\delta f)^2\rangle_z$ and $\langle\delta f\delta g\rangle_z$.

Let us first evaluate $\langle(\delta f)^2\rangle_z$. By the use of the identity (A3) with $\hat{A}=\hat{B}=e^{-\frac{1}{2}\hat{K}[\lambda_t;t]}\hat{\mathcal{O}}\,e^{-\frac{1}{2}\hat{K}[\lambda_t;t]}$, we obtain

$$\langle(\delta f)^2\rangle_z=\mathrm{Tr}(e^{-\hat{K}[\lambda_t;t]}\hat{\mathcal{O}}\,e^{-\hat{K}[\lambda_t;t]}\hat{\mathcal{O}}).\tag{A10}$$

Since $\hat{K}[\lambda_t;t]$ is a Hermitian operator, taking trace with its eigenstate $|n\rangle$ results in

$$\langle(\delta f)^2\rangle_z=\sum_{n,m}e^{-K_n[\lambda_t;t]}e^{-K_m[\lambda_t;t]}\langle n|\hat{\mathcal{O}}|m\rangle\langle m|\hat{\mathcal{O}}|n\rangle\leqslant\sum_{n,m}e^{-K_n[\lambda_t;t]}e^{-K_m[\lambda_t;t]}\langle n|\hat{\mathcal{O}}|m\rangle\langle m|\hat{\mathcal{O}}|n\rangle,\tag{A11}$$

where $K_n[\lambda_t;t]$ denotes the eigenvalue of $\hat{K}[\lambda_t;t]$ and we used the completeness for the eigenstate of $\hat{K}[\lambda_t;t]$ to show the first equality. The inequality results from the inequality of arithmetic and geometric means: $\sqrt{ab}\leqslant(a+b)/2$. The right-hand side of this inequality can be further rewritten as

$$\sum_{n,m}e^{-K_n[\lambda_t;t]}e^{-K_m[\lambda_t;t]}\langle n|\hat{\mathcal{O}}|m\rangle\langle m|\hat{\mathcal{O}}|n\rangle=Z_{\rm LG}[2\lambda_t]\langle\hat{\mathcal{O}}^2\rangle_{2\lambda_t}^{\rm LG},\tag{A12}$$

and we now obtain the following inequality for $\langle(\delta f)^2\rangle_z$:

$$\langle(\delta f)^2\rangle_z\leqslant Z_{\rm LG}[2\lambda_t]\langle\hat{\mathcal{O}}^2\rangle_{2\lambda_t}^{\rm LG}.\tag{A13}$$

To evaluate $\langle\delta f\delta g\rangle_z$, we simply apply the identity (A3) with $\hat{A}=e^{-\frac{1}{2}\hat{K}[\lambda_t;t]}\hat{\mathcal{O}}\,e^{-\frac{1}{2}\hat{K}[\lambda_t;t]}$ and $\hat{B}=e^{-\hat{K}[\lambda_t;t]}$:

$$\langle\delta f\delta g\rangle_z=\mathrm{Tr}(e^{-2\hat{K}[\lambda_t;t]}\hat{\mathcal{O}})=Z_{\rm LG}[2\lambda_t]\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\rm LG}.\tag{A14}$$

Substituting Eqs. (A5), (A13), and (A14) into Eq. (A8), we eventually obtain an upper bound of the variance as

$$\begin{aligned}\left\langle\left(\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}-\left\langle\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\rm TPQ}\right\rangle_z\right)^2\right\rangle_z&\leqslant\frac{Z_{\rm LG}[2\lambda_t]}{(Z_{\rm LG}[\lambda_t])^2}\left[\langle\hat{\mathcal{O}}^2\rangle_{2\lambda_t}^{\rm LG}-2\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\rm LG}\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\rm LG}+\big(\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\rm LG}\big)^2\right]\\&=\frac{Z_{\rm LG}[2\lambda_t]}{(Z_{\rm LG}[\lambda_t])^2}\left[\left\langle\big(\hat{\mathcal{O}}-\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\rm LG}\big)^2\right\rangle_{2\lambda_t}^{\rm LG}+\big(\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\rm LG}-\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\rm LG}\big)^2\right],\end{aligned}\tag{A15}$$

which results in the following inequality:

$$\mathrm{Prob}_z\Big[\big|\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\mathrm{TPQ}}-\big\langle\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\mathrm{TPQ}}\big\rangle_z\big|\geqslant\epsilon\Big]\leqslant\frac{e^{-2\int_\Lambda d^dx\,\beta_t\Delta p(\beta_t,\mu_t^a)}}{\epsilon^2}\Big[\big\langle\big(\hat{\mathcal{O}}-\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\mathrm{LG}}\big)^2\big\rangle_{2\lambda_t}^{\mathrm{LG}}+\big(\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\mathrm{LG}}-\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\mathrm{LG}}\big)^2\Big]. \tag{A16}$$

As a consequence, for any operator $\hat{\mathcal{O}}$ whose two variations $\langle(\hat{\mathcal{O}}-\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\mathrm{LG}})^2\rangle_{2\lambda_t}^{\mathrm{LG}}$ and $(\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\mathrm{LG}}-\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\mathrm{LG}})^2$ do not show an exponentially large behavior with respect to the volume of fluid cells V_{cell}, the inequality brings about the following result on convergence:

$$\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\mathrm{TPQ}}\xrightarrow{P}\big\langle\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\mathrm{TPQ}}\big\rangle_z, \tag{A17}$$

which gives the first step of the proof.

Thanks to Eqs. (A5) and (A14), the second step is mostly finished if we evaluate the average difference by expanding it as follows:

$$\begin{aligned}\big|\big\langle\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\mathrm{TPQ}}\big\rangle_z-\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\mathrm{LG}}\big|&=\frac{1}{(Z_{\mathrm{LG}}[\lambda_t])^2}\big|-\langle\delta f\delta g f\rangle_z+\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\mathrm{LG}}\langle(\delta g)^2\rangle_z\big|=\frac{Z_{\mathrm{LG}}[2\lambda_t]}{(Z_{\mathrm{LG}}[\lambda_t])^2}\big|\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\mathrm{LG}}-\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\mathrm{LG}}\big|\\&=e^{-2\int_\Lambda d^dx\,\beta_t\Delta p(\beta_t,\mu_t^a)}\big|\langle\hat{\mathcal{O}}\rangle_{2\lambda_t}^{\mathrm{LG}}-\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\mathrm{LG}}\big|.\end{aligned} \tag{A18}$$

We thus conclude that for any operator $\hat{\mathcal{O}}$ not showing the exponentially large fluctuation, the difference between $\langle\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\ell\mathrm{TPQ}}\rangle_z$ and $\langle\hat{\mathcal{O}}\rangle_{\lambda_t}^{\mathrm{LG}}$ is exponentially small. This completes the proof of Eq. (8). ■

2. Proof of Eqs. (14) and (15)

Although the second law of thermodynamics follows from the quantum fluctuation theorem (15), we provide independent proofs of them.

a. Proof of Eq. (14). The second law of thermodynamics can be easily shown by rewriting the entropy production as follows:

$$\begin{aligned}\langle\hat{\Sigma}[t,t_0;\lambda]\rangle&\equiv\langle\hat{S}[\lambda_t;t]\rangle_{\lambda_{t_0}}^{\ell\mathrm{TPQ}}-\langle\hat{S}[\lambda_{t_0};t_0]\rangle_{\lambda_{t_0}}^{\ell\mathrm{TPQ}}\\&=\underbrace{\langle\hat{S}[\lambda_t;t]\rangle_{\lambda_{t_0}}^{\ell\mathrm{TPQ}}-\langle\hat{S}[\lambda_t;t]\rangle_{\lambda_{t_0}}^{\mathrm{LG}}}_{(a)}\underbrace{-\big(\langle\hat{S}[\lambda_{t_0};t_0]\rangle_{\lambda_{t_0}}^{\ell\mathrm{TPQ}}-\langle\hat{S}[\lambda_{t_0};t_0]\rangle_{\lambda_{t_0}}^{\mathrm{LG}}\big)}_{(b)}+\underbrace{\langle\hat{S}[\lambda_t;t]\rangle_{\lambda_{t_0}}^{\mathrm{LG}}-\langle\hat{S}[\lambda_{t_0};t_0]\rangle_{\lambda_{t_0}}^{\mathrm{LG}}}_{(c)}.\end{aligned} \tag{A19}$$

Using the equivalence between the ℓTPQ state and LG ensemble, we can estimate the first and second terms to be exponentially small: $(a)=O(e^{-B_1V_{\mathrm{cell}}})$ and $(b)=O(e^{-B_2V_{\mathrm{cell}}})$ with some constants B_1 and B_2. Furthermore, the last term is shown to be positive: $(c)\geqslant 0$ (see Refs. [31,33,34]). This results in Eq. (14). ■

b. Proof of Eq. (15). To prove the quantum fluctuation theorem (15) for the ℓTPQ state, we first recall the LG ensemble [33]. For that purpose, let us introduce the generating function for the entropy production under the forward/backward evolution by

$$G_F^{\mathrm{LG}}(z)\equiv\mathrm{Tr}(\hat{\rho}_{\mathrm{LG}}[\lambda_{t_0};t_0]\hat{\mathcal{U}}^\dagger(t)e^{iz\hat{S}_{\mathrm{LG}}[\lambda_t;t_0]}\hat{\mathcal{U}}(t)e^{-iz\hat{S}_{\mathrm{LG}}[\lambda_{t_0};t_0]}), \tag{A20}$$

$$G_B^{\mathrm{LG}}(z)\equiv\mathrm{Tr}(\hat{\rho}_{\mathrm{LG}}[\tilde{\lambda}_t;t]\widetilde{\mathcal{U}}(t)e^{iz\hat{S}_{\mathrm{LG}}[\tilde{\lambda}_{t_0};t]}\widetilde{\mathcal{U}}^\dagger(t)e^{-iz\hat{S}_{\mathrm{LG}}[\tilde{\lambda}_t;t]}), \tag{A21}$$

where $\hat{\mathcal{U}}(t)$ is a time evolution operator. By using a combined parity and time reversal $\Theta\equiv\mathsf{PT}$, we also defined PT-transformed time evolution operator and parameter by $\widetilde{\mathcal{U}}(t)\equiv\Theta\hat{\mathcal{U}}(t)\Theta^{-1}$ and $\tilde{\lambda}_t\equiv\epsilon^a\lambda^a(t,-\boldsymbol{x})$ with ϵ^a being a PT eigenvalue of charge densities $\hat{c}_a$, respectively. Here, we introduced the LG distribution for the density operator $\hat{\rho}_{\mathrm{LG}}[\lambda_t;t]$ and the entropy functional operator $\hat{S}_{\mathrm{LG}}[\lambda_t;t]$ by

$$\hat{\rho}_{\mathrm{LG}}[\lambda_t;t]\equiv e^{-\hat{S}_{\mathrm{LG}}[\lambda_t;t]},\quad \hat{S}_{\mathrm{LG}}[\lambda_t;t]\equiv\hat{K}[\lambda_t;t]+\ln Z_{\mathrm{LG}}[\lambda_t]. \tag{A22}$$

The generating functions in Eqs. (A20) and (A21) are shown to satisfy the quantum fluctuation theorem [33]:

$$G_F^{\mathrm{LG}}(z)=G_B^{\mathrm{LG}}(-z+i). \tag{A23}$$

In order to show the quantum fluctuation theorem for the ℓTPQ state, we then introduce the reference generating function by

$$\overline{G}_F(z)\equiv\mathrm{Tr}(\hat{\rho}_{\mathrm{LG}}[\lambda_{t_0};t_0]e^{iz\hat{S}[\lambda_t;t]}e^{-iz\hat{S}[\lambda_{t_0},t_0]}). \tag{A24}$$

By the use of this reference generating function with the triangle inequality, we can evaluate the difference between $G_F^{\ell\mathrm{TPQ}}(z)$ and $G_F^{\mathrm{LG}}(z)$ as follows:

$$\begin{aligned}\big|G_F^{\ell\mathrm{TPQ}}(z)-G_F^{\mathrm{LG}}(z)\big|&=\big|G_F^{\ell\mathrm{TPQ}}(z)-\overline{G}_F(z)-G_F^{\mathrm{LG}}(z)+\overline{G}_F(z)\big|\\&\leqslant\underbrace{\big|G_F^{\ell\mathrm{TPQ}}(z)-\overline{G}_F(z)\big|}_{(A)}+\underbrace{\big|G_F^{\mathrm{LG}}(z)+\overline{G}_F(z)\big|}_{(B)}.\end{aligned} \tag{A25}$$

Defining $\Delta\Psi[\lambda_t, \lambda_{t_0}] \equiv \ln Z[\lambda_t] - \ln Z[\lambda_{t_0}]$ for both ℓTPQ and LG states, and using the error estimation for the partition functional, we can estimate the second term in the second line as

$$\begin{aligned}(B) &= |\operatorname{Tr}(\hat{\rho}_{\mathrm{LG}}[\lambda_{t_0}; t_0] e^{iz\hat{K}[\lambda_t;t]} e^{-iz\hat{K}[\lambda_{t_0};t_0]})(e^{iz\Delta\Psi_{\mathrm{LG}}[\lambda_t,\lambda_{t_0}]} - e^{iz\Delta\Psi_{\ell\mathrm{TPQ}}[\lambda_t,\lambda_{t_0}]})| \\ &= |\operatorname{Tr}(\hat{\rho}_{\mathrm{LG}}[\lambda_{t_0}; t_0] e^{iz\hat{K}[\lambda_t;t]} e^{-iz\hat{K}[\lambda_{t_0};t_0]}) e^{iz\Delta\Psi_{\ell\mathrm{TPQ}}[\lambda_t,\lambda_{t_0}]}(\exp[O(e^{-C_1 V_{\mathrm{cell}}})] - 1)| \\ &= O(e^{-C_1 V_{\mathrm{cell}}}). \end{aligned} \tag{A26}$$

Since the first term in Eq. (A25) is given by the difference of the averaged operator over the ℓTPQ state and LG distribution, we can evaluate it as

$$(A) = \left[\langle e^{iz\hat{S}[\lambda_t;t]} e^{-iz\hat{S}[\lambda_{t_0};t_0]}\rangle^{\ell\mathrm{TPQ}}_{\lambda_{t_0}} - \langle e^{iz\hat{S}[\lambda_t;t]} e^{-iz\hat{S}[\lambda_{t_0};t_0]}\rangle^{\mathrm{LG}}_{\lambda_{t_0}}\right] = O(e^{-C_2 V_{\mathrm{cell}}}), \tag{A27}$$

where we assumed that the variation of the averaged operator does not show the exponentially large behavior. Substituting Eqs. (A26) and (A27) into Eq. (A25), we obtain

$$\left|G_F^{\ell\mathrm{TPQ}}(z) - G_F^{\mathrm{LG}}(z)\right| \leqslant O(e^{-C_3 V_{\mathrm{cell}}}), \tag{A28}$$

which states the equivalence of the generating function for the entropy production for the forward evolution. On the other hand, a similar analysis also works for $G_B^{\ell\mathrm{TPQ}}(z) - G_B^{\mathrm{LG}}(z)$ and thus we have

$$\left|G_B^{\ell\mathrm{TPQ}}(-z+i) - G_B^{\mathrm{LG}}(-z+i)\right| \leqslant O(e^{-C_4 V_{\mathrm{cell}}}). \tag{A29}$$

Therefore, combining Eq. (A23) with Eqs. (A28) and (A29) and noting that $C_a\,(a = 1, \cdots, 4)$ is a certain constant, we can evaluate

$$\begin{aligned}&\left|G_F^{\ell\mathrm{TPQ}}(z) - G_B^{\ell\mathrm{TPQ}}(-z+i)\right| \\ &= \left|G_F^{\ell\mathrm{TPQ}}(z) - G_F^{\mathrm{LG}}(z) - \left(G_B^{\ell\mathrm{TPQ}}(-z+i) - G_B^{\mathrm{LG}}(-z+i)\right) + G_F^{\mathrm{LG}}(z) - G_B^{\mathrm{LG}}(-z+i)\right| \\ &\leqslant \left|G_F^{\ell\mathrm{TPQ}}(z) - G_F^{\mathrm{LG}}(z)\right| + \left|G_B^{\ell\mathrm{TPQ}}(-z+i) - G_B^{\mathrm{LG}}(-z+i)\right| \\ &= O(e^{-A_2 V_{\mathrm{cell}}}), \end{aligned} \tag{A30}$$

where the inequality in the third line again follows from the triangle inequality. This gives the quantum fluctuation theorem for the ℓTPQ state. ■

APPENDIX B: DETAIL OF NUMERICAL IMPLEMENTATION

We here summarize a detail of our numerical evaluations of the Green-Kubo formula, the quantum fluctuation theorem, and the second law of thermodynamics.

1. Thermal conductivity from the Green-Kubo formula

On the basis of the Green-Kubo formula, the thermal conductivity is given by

$$\kappa(t,n) = \frac{\beta(t,n)^2}{4N}\int_{-\infty}^{\infty} dt\,\langle\{\hat{\mathrm{J}}_E(t), \hat{\mathrm{J}}_E(0)\}\rangle^{\mathrm{TPQ}}_{\beta_n} \simeq \frac{\beta^2}{4N}\int_{-\infty}^{\infty} dt\,\langle\{\hat{\mathrm{J}}_E(t), \hat{\mathrm{J}}_E(0)\}\rangle^{\mathrm{TPQ}}_{\beta}, \tag{B1}$$

where $\hat{\mathrm{J}}_E(t) = \sum_{n=1}^{N} \hat{J}_E(t, n-1/2)$ is the total energy current. In the second equality, we neglect the spatial and temporal dependence of temperature, which gives rise to the higher-order derivative correction. Conceptually, the Green-Kubo formula does not require a fully microscopic time resolution but only a hydrodynamic one. Therefore, we also replace the bare correlation function $\langle\{\hat{\mathrm{J}}_E(t), \hat{\mathrm{J}}_E(0)\}\rangle^{\mathrm{TPQ}}_{\beta}$ with the temporally smeared one, which leads to

$$G(t) \equiv \frac{1}{\tau^2}\int_t^{t+\tau} ds \int_0^{\tau} ds'\,\langle\{\hat{\mathrm{J}}_E(s), \hat{\mathrm{J}}_E(s')\}\rangle^{\mathrm{TPQ}}_{\beta}. \tag{B2}$$

An appropriate course-graining time scale τ is estimated from the damping time of the bare correlation function $\langle\{\hat{\mathrm{J}}_E(t), \hat{\mathrm{J}}_E(0)\}\rangle^{\mathrm{TPQ}}_{\beta}$, and we set $\tau = 10$ in our setup. The thermal conductivity is now given by

$$\kappa(t,n) \simeq \frac{\beta^2}{2}[C(\infty) - C(-\infty)], \quad \text{with} \quad C(t) = \frac{1}{2N}\int_0^t dt' G(t'). \tag{B3}$$

Since $C(t)$ is defined by the symmetric Green's function, we can show it is equal to $-C(-t)$ within a small error, which is actually confirmed numerically. Thus we reach the following simple linear response result in the ℓTPQ formulation:

$$\kappa(t,n) \simeq \beta^2 C(\infty) \equiv \kappa. \tag{B4}$$

The left panel of Fig. 6 demonstrates a typical behavior of the function $C(t)$, from which one can confirm that $C(t)$ converges when $t \gtrsim 100$. The value at infinitely late time $C(\infty)$ is estimated by the average of $C(t)$ from $t = 100$ to 200. The resulting

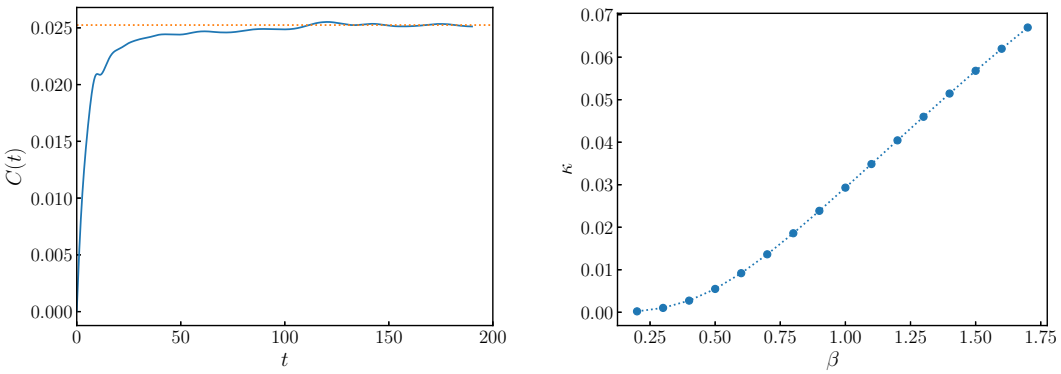

FIG. 6. (Left) Solid line represents $C(t)$ at $\beta = 1.5$. The dotted line shows the late time average of $C(t)$. (Right) The β dependence of the thermal conductivity.

thermal conductivity at each β is shown in the right panel of Fig. 6, which corresponds to the result shown in Fig. 4 in the main text.

2. Numerical evaluation of generating functions in fluctuation theorem

We present here a numerical method to compute the generating functions. When the Hamiltonian does not depend on time explicitly, we can rewrite the generating functions for the total entropy production (12) and (13) as follows:

$$G_F^{\ell\mathrm{TPQ}}(z;t) = \frac{e^{iz\ln(Z_{\ell\mathrm{TPQ}}[\{\beta(t,n)\}]/Z_{\ell\mathrm{TPQ}}[\{\beta(0,n)\}])}}{Z_{\ell\mathrm{TPQ}}[\{\beta(0,n)\}]}\langle\{\beta(0,n)\}\,|\,e^{iHt}e^{iz\hat{K}[\{\beta(t,n)\}]}e^{-iHt}e^{-iz\hat{K}[\{\beta(0,n)\}]}\,|\,\{\beta(0,n)\}\rangle,$$

$$G_B^{\ell\mathrm{TPQ}}(i-z;t) = \frac{e^{-iz^*\ln(Z_{\ell\mathrm{TPQ}}[\{\beta(t,n)\}]/Z_{\ell\mathrm{TPQ}}[\{\beta(0,n)\}])}}{Z_{\ell\mathrm{TPQ}}[\{\beta(0,n)\}]}$$
$$\times\langle\{\beta(t,n)\}\,|\,e^{-iHt}e^{-\hat{K}[\{\beta(0,n)\}]}e^{i\hat{K}[\{\beta(0,n)\}]z^*}e^{iHt}e^{-i\hat{K}[\{\beta(t,n)\}]z^*}e^{\hat{K}[\{\beta(t,n)\}]}\,|\,\{\beta(t,n)\}\rangle^*. \tag{B5}$$

Here $|\{\beta(t,n)\}\rangle$ is an ℓTPQ state, whose temperature profile is chosen to be that at time t. We compute these quantities based on the following steps.

(i) Make an ℓTPQ state $|\{\beta(0,n)\}\rangle$ whose temperature profile is set by the initial condition (35).
(ii) Compute $e^{-iHt}|\{\beta(0,n)\}\rangle$.
(iii) Compute spatially smeared and temporally averaged local energies $\{\langle\bar{h}(t,n)\rangle\}$.
(iv) Compute local temperatures $\{\beta(t,n)\}$ using the energy-temperature relation.
(v) Make an auxiliary ℓTPQ state $|\{\beta(t,n)\}\rangle$.

Exponential operators like $e^{iz\hat{K}[\{\beta(t,n)\}]}$ and $e^{-iz\hat{K}[\{\beta(0,n)\}]}$ are regarded as time-evolution operators. We compute these "time evolution" by the fourth order Runge-Kutta method.

The entropy production can be computed three independent ways. One way is to compute the expectation value of the entropy operator Eq. (3) directly. The others are to compute the gradient of $\mathrm{Im}\,G_F^{\ell\mathrm{TPQ}}(z)$ and $\mathrm{Im}\,G_B^{\ell\mathrm{TPQ}}(i-z)$ at $z=0$. Concretely, they are given by

$$\Sigma_F \equiv \mathrm{Im}\,\frac{dG_F^{\ell\mathrm{TPQ}}(z)}{d(iz)}\bigg|_{z=0}, \quad \Sigma_B \equiv \mathrm{Im}\,\frac{dG_B^{\ell\mathrm{TPQ}}(i-z)}{d(iz)}\bigg|_{z=0}. \tag{B6}$$

In Fig. 7, we demonstrate the estimation of the entropy production from $G_F^{\ell\mathrm{TPQ}}(z)$. At each time, we confirm that the generating function behaves as a linear function around the origin, which allows us to evaluate the entropy production according to Eq. (B6). In the figure, the solid line shows the fitting result using the data at $z = 0.00, 0.01, \ldots, 0.03$. The choice of the fitting range is insensitive to the result. The fitting of $G_B^{\ell\mathrm{TPQ}}(i-z)$ can be performed in the same manner.

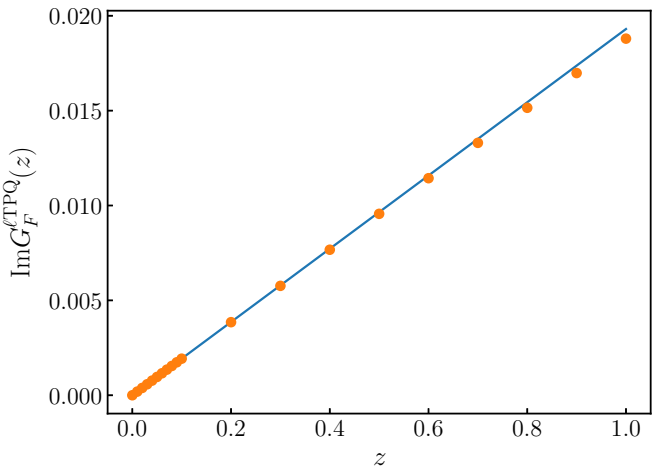

FIG. 7. Generating function $G_F^{\ell\mathrm{TPQ}}$ at $t = 20$. The solid line stands for the fitting function.

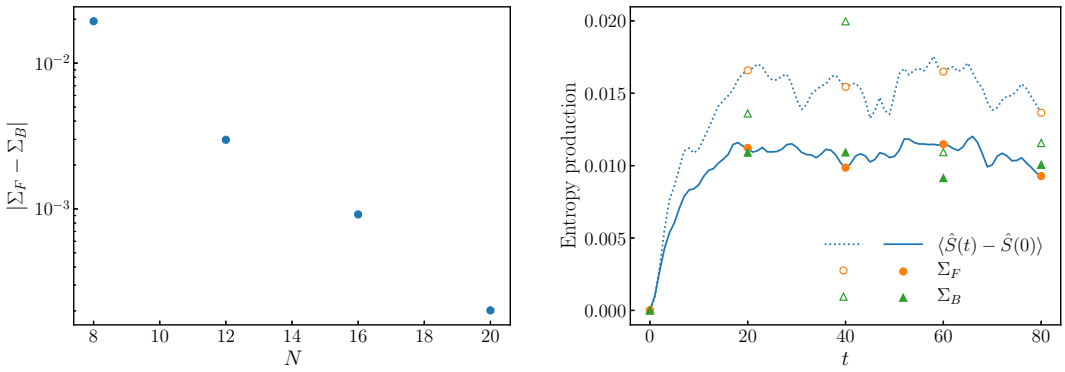

FIG. 8. (Left) Difference between Σ_F and Σ_B at $t = 20$. (Right) The entropy production for $N = 12$. The dotted line and the open symbols show the entropy production obtained for a single random vector. The solid line and the closed symbols show the average over five independent samples.

Unlike the standard quantum fluctuation theorem, Σ_F agrees with Σ_B only in the large fluid-cell limit. We numerically confirm that the difference between Σ_F and Σ_B scales as e^{-N}, where N is the system size. In the left panel of Fig. 8 we show the scaling behavior at $t = 20$.

We also check that the difference tends to vanish by taking the random vector average, which is consistent with our proof of equivalence. We compute the entropy production for five random vectors and take the random vector average. In the right panel of Fig. 8, the solid line and the closed symbols denote the averaged ones, while the dotted line and open symbols do the ℓTPQ result for the entropy production, namely, computed by a single random vector. Here, numerical simulations are performed for $N = 12$. This result is consistent with the fact that Σ_F coincides with Σ_B for the standard mixed state (or canonical ensemble) formulation.

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