Experimental study of the thermodynamic uncertainty relation

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A cost-precision trade-off relationship, the so-called thermodynamic uncertainty relation (TUR), has been recently discovered in stochastic thermodynamics. It bounds certain thermodynamic observables in terms of the associated entropy production. In this work, we experimentally study the TUR in a two-qubit system using an NMR setup. Each qubit is prepared in an equilibrium state, but at different temperatures. The qubits are then coupled, allowing energy exchange (in the form of heat). Using the quantum state tomography technique we obtain the moments of heat exchange within a certain time interval and analyze the relative uncertainty of the energy exchange process. We find that generalized versions of the TUR, which are based on the fluctuation relation, are obeyed. However, the specialized TUR, a tighter bound that is valid under specific dynamics, is violated in certain regimes of operation, in excellent agreement with analytical results. Altogether, this experiment-theory study provides a deep understanding of heat exchange in quantum systems, revealing favorable noise-dissipation regimes of operation.

Introduction. Obtaining universal bounds of experimentally accessible physical observables has been a fundamental topic in physics. Such bounds include the Heisenberg uncertainty relation of quantum mechanics, which sets a limit on the efficiency of heat engines and Landauer erasure principle stemming from the second law of thermodynamics. Likewise, recent studies have shown that for systems that are out-of-equilibrium, there exist trade-off relations between the relative uncertainty of integrated currents (heat, charge) and the associated entropy production8–10. These results are now collectively referred to as Thermodynamic uncertainty relations (TUR). The specialized version of the TUR (S-TUR) reads,

\[ \frac{\langle Q^2 \rangle_c}{\langle Q \rangle^2} \geq \frac{2}{\langle \Sigma \rangle}, \]

where \( Q \) represents any integrated current, such as heat or charge, and it is a stochastic variable. \( \langle Q \rangle_c \) and \( \langle Q^2 \rangle_c \) are the average integrated current and its noise, respectively, and \( \langle \Sigma \rangle \) is the net average entropy production in the heat exchange process, characterizing irreversibility, or how far the system is driven away from equilibrium. The S-TUR was first conjectured for continuous time, discrete state Markov process in steady state.1 It was later proved with the large deviation technique.2–6 Since then, this relation has been generalized to discrete time, discrete state Markov process, finite time statistics,6,7,15,16, Langevin dynamics,8,15,25,27,30, periodically driven systems,19,23, multidiimensional system,15, molecular motors,9, biochemical oscillations,10, interacting oscillators,11, run-and-tumble process,12, measurement and feedback control,18,21, broken time reversal symmetry systems,18,20,22,29,31, first passage times,13,14 and quantum transport problems.32–36,39, Tighter bounds have also been reported for some stochastic currents.8

More recently, following the fundamental nonequilibrium fluctuation relation,38, a generalized version of the TUR (G-TUR1) was derived, where the RHS of Eq. (1) was modified to \( \langle Q^2 \rangle_c \geq \frac{2}{\langle \Sigma \rangle} \exp(-\Delta T) \), which is a looser bound compared to Eq. (1). In fact, a more tighter version of the generalized bound had been obtained following a slightly different approach by Timpanaro et al.37 as \( \langle Q^2 \rangle_c \geq f(\langle \Sigma \rangle) \), where \( f(x) = \cosh^2(g(x/2)) \) and \( g(x) \) is the inverse function of \( x \tan(x) \). We refer to this bound as the G-TUR2. Interestingly, in the small dissipation limit, \( \langle \Sigma \rangle \to 0 \), both these generalized bounds reduce to the S-TUR of Eq. (1).

Despite intense theoretical efforts dedicated to derive and analyze the TUR, an experimental study of this trade-off relation is still missing. In this work, we experimentally study the TUR of quantum heat exchange between two initially thermalized qubits in a NMR setup, in the transient regime. Moments of heat exchange are obtained by performing quantum state tomography (QST) for the qubits. As expected, G-TURs are valid throughout. This agreement, while fundamentally important, does not offer practical input for the design of quantum heat machines. In contrast, by identifying violations of the S-TUR, observed in certain parameters and in excellent agreement with analytical results, we can pinpoint favorable regimes of operation.

Cumulants of heat exchange. Consider two systems with their Hamiltonians \( H_1 \) and \( H_2 \) that are initially \( (t < 0) \) decoupled and separately prepared at their respective thermal equilibrium state. The initial composite density matrix is thus given as a product state, \( \rho(0) = \rho_1 \otimes \rho_2 \), with \( \rho_i = \exp(-\beta_i H_i)/Z_i \), \( i = 1, 2 \) the Gibbs thermal state with inverse temperature \( \beta_i = 1/k_B T_i \) \( (k_B \) is the Boltzmann constant) and \( Z_i = \text{Tr}[e^{-\beta_i H_i}] \) the corresponding equilibrium partition function. The coupling between the systems is suddenly switched on at \( t = 0 \) for a duration \( \tau \) (total Hamiltonian \( H \)), which allows energy exchange between the two systems. Due to the randomness of the initial thermal state and the inherent proba-
biliistic nature of quantum mechanics, the exchanged energy is not a deterministic quantity, but rather quantified with a probability distribution function (PDF). In the quantum regime, this PDF is constructed by following a two-point projective measurement scheme. The first projective measurement of the energy of the two systems is performed before they are coupled. A second projective measurement is done at the end of the energy exchange process (after the systems are separated). This procedure respects the fundamental Jarzynski and Wójcik exchange fluctuation symmetry. For the bipartite setup considered here, the joint PDF corresponding to energy change $(\Delta E_i, i = 1, 2)$ between the systems, during a coupling interval $\tau$ is denoted by $p_\tau(\Delta E_1, \Delta E_2)$. It can be shown that

$$\left\langle (e^{-\beta_1 \Delta E_1 - \beta_2 \Delta E_2})^z \right\rangle_\tau = \int d(\Delta E_1) d(\Delta E_2) p_\tau(\Delta E_1, \Delta E_2) e^{-z \beta_1 \Delta E_1 - z \beta_2 \Delta E_2} = \text{Tr} \left[ \rho(0)^z \rho(\tau)^{1-z} \right],$$

with $\rho(0)$ the combined density matrix of the two systems at the moment they are coupled, and $\rho(\tau)$ their density matrix at the end of their coupled evolution. We now consider the case $\Delta E_1 \approx -\Delta E_2$, which is justified when the two systems are only weakly coupled. Alternatively, this approximation becomes an exact equality if there is no energy cost involved in turning on and off the interaction between the two systems. Interpreting the energy change for individual systems as heat, $\Delta E_1 = -\Delta E_2 = Q$, we directly get from Eq. (2) an expression for the moments of heat exchange

$$\langle Q^n \rangle = \frac{1}{(\Delta \beta)^n} \text{Tr} \left[ \rho(\tau) T_n (\ln \rho(\tau) - \ln \rho(0))^n \right],$$

where $n = 1, 2, \cdots$ corresponds to the order of the heat exchange moment and $\Delta \beta = \beta_1 - \beta_2$. $T_n$ is the time-ordering operator; it places operators at the latest time to the left. This powerful expression offers a unique way to gather moments of heat exchange, simply by performing quantum state tomography based on NMR experiments. Alternatively, cumulants of heat exchange can be obtained by implementing an ancilla-based interferometric technique. This method gives a direct access to the characteristic function (CF) of heat, defined using the two-point measurement protocol,

$$\chi_\tau(u) = \int dQ e^{iuQ} p_\tau(Q),$$

$$= \text{Tr} \left[ U^\dagger(\tau, 0)(e^{iuH_1} \otimes 1_2)U(\tau, 0)(e^{-iuH_1} \otimes 1_2)\rho(0) \right].$$

Here $u$ is the variable conjugate to $Q$, $U(t, 0) = e^{-iHt}/\hbar$ is the unitary propagator with the total Hamiltonian $H$. In the language of the CF, the exchange fluctuation symmetry translates to $\chi_\tau(u) = \chi_\tau(-u + i\Delta \beta)$. The first two cumulants, useful for the analysis of the TUR, are

$$\text{Theoretical analysis.}$$

We now describe a specific case, the so-called XY-model consisting two qubits with the Hamiltonian

$$H_{XY} = \frac{\hbar \nu_0}{2} \sigma_1^z \otimes 1_2 + 1_1 \otimes \frac{\hbar \nu_0}{2} \sigma_2^z$$

$$+ \frac{\hbar J}{2}(\sigma_1^x \otimes \sigma_2^y - \sigma_1^y \otimes \sigma_2^x).$$

Here, $H_1 = \hbar \nu_0 \sigma_1^z \otimes 1_2$, $H_2 = 1_1 \otimes \hbar \nu_0 \sigma_2^z$ with $\nu_0$ the frequency of the qubits, $\sigma_i, i = x, y, z$ are the standard Pauli matrices. The last term, denoted by $H_{12}$, represents the interaction between the qubits, with $J$ the coupling parameter. An important feature of this model is that $\{H_{12}, H_1 + H_2\} = 0$. This commutation implies that the change of energy for one qubit is exactly compensated by the other qubit, as there is no energy cost involved in turning on or off the interaction between the qubits. For such an ‘energy-preserving’ Hamiltonian $\Delta E_1 = -\Delta E_2 = Q$ is exact and the average entropy production simply reduces to $\langle \Sigma \rangle = (\beta_1 - \beta_2) \langle Q \rangle$.

Cumulants of heat exchange can either be computed from the composite density matrix or directly from the CF $\chi_\tau(u)$ of heat, following Eq. (4). We take the latter approach for the XY-model; algebraic manipulations of the Pauli matrices yield

$$\chi_\tau(u) = \left[ 1 + \sin^2(2\pi J\tau) \left\{ f_1(\nu_0)(1 - f_2(\nu_0))(e^{-i\hbar\nu_0} - 1) + f_2(\nu_0)(1 - f_1(\nu_0))(e^{i\hbar\nu_0} - 1) \right\} \right],$$

where $f_i(\nu_0) = (e^{\beta_i \hbar \nu_0} + 1)^{-1}, i = 1, 2$. For compactness, below we identify these functions as $f_{1,2}$. It is easy to verify that the above CF satisfies the exchange fluctuation symmetry for arbitrary values of $J$, $\tau$, $\beta_1$, $\beta_2$, and $\nu_0$. Expressions for the average heat current and the associated noise are derived by taking successive derivatives of $\ln \chi_\tau(u)$ with respect to $iu$. We write down the first three cumulants, useful for the analysis of the TUR,
\[ \langle Q \rangle_{\tau} = \hbar v \mathcal{T}_r(J) \left[ f_2 - f_1 \right] , \]
\[ \langle Q^2 \rangle_{\tau}^{\xi} = (\hbar v_0)^2 \left[ \mathcal{T}_r(J) \left( f_1 (1 - f_2) + f_2 (1 - f_1) \right) - \mathcal{T}_r^2(J) (f_2 - f_1)^2 \right] , \]
\[ \langle Q^3 \rangle_{\tau}^{\xi} = (\hbar v_0)^3 \mathcal{T}_r(J) (f_1 - f_2) \left[ 1 - 3 \mathcal{T}_r(J) (f_1 (1 - f_2) + (1 - f_1) f_2) + 2 \mathcal{T}_r^2(J) (f_1 - f_2)^2 \right] . \]  

Here, \( \mathcal{T}_r(J) = \sin^2 \left( 2 \pi J \tau \right) . \)

**Perturbative expansion of the S-TUR.** For arbitrary coupling time \( \tau \), the cumulants can be expanded close to equilibrium in terms of the thermal affinity \( \Delta \beta = \beta_1 - \beta_2 \), around a fixed inverse temperature \( \beta \). Specifically,

\[ \langle Q \rangle_{\tau} = \mathcal{G}_1(\tau) \Delta \beta + \mathcal{G}_2(\tau) \left( \frac{(\Delta \beta)^2}{2!} \right) + \cdots \]
\[ \langle Q^2 \rangle_{\tau}^{\xi} = S_0(\tau) + S_1(\tau) \Delta \beta + S_2(\tau) \left( \frac{(\Delta \beta)^2}{2!} \right) + \cdots \]
\[ \langle Q^3 \rangle_{\tau}^{\xi} = R_1(\tau) \Delta \beta + \cdots \]  

Here \( \mathcal{G}_1(\tau) \) is the time-dependent linear transport coefficient and \( S_0(\tau) \) is the equilibrium noise. \( \mathcal{G}_2(\tau), \mathcal{G}_3(\tau), \ldots \) (\( S_1(\tau), S_2(\tau), \ldots \)) are higher order nonequilibrium transport (noise) coefficients. As a consequence of the exact fluctuation symmetry, the following relations hold: \( S_0(\tau) = 2 \mathcal{G}_1(\tau) \), \( S_1(\tau) = \mathcal{G}_2(\tau) \), \( 3 S_2(\tau) - 2 \mathcal{G}_3(\tau) = R_1(\tau) \), and so on. This leads to

\[ \langle Q^2 \rangle_{\tau}^{\xi} = \mathcal{G}_1(\tau) \Delta \beta + \cdots \]  

Interestingly, the contribution of the linear term \( \Delta \beta \) disappears; the presence of this term could trivially violate the S-TUR by swapping the initial temperatures of the qubits. While the linear coefficient for the average heat exchange, \( \mathcal{G}_1(\tau) \), is always positive, \( R_1(\tau) \) does not take a definite sign; when \( R_1(\tau) < 0 \), the S-TUR is violated. For the XY-model we get \( \langle f(\omega) \rangle_{\tau}^{\xi} \) is evaluated at \( \beta \),

\[ \mathcal{G}_1(\tau) = (\hbar v_0)^2 \mathcal{T}_r(J) f(1 - f) \geq 0 , \]
\[ R_1(\tau) = (\hbar v_0)^4 \mathcal{T}_r(J) f(1 - f) \left[ 1 - 6 \mathcal{T}_r(J) f(1 - f) \right] \]  

To order \( (\Delta \beta)^2 \), Eq. (8) simplifies to

\[ \Delta \beta \langle Q^2 \rangle_{\tau}^{\xi} = 2 + (\Delta \beta \hbar v_0)^2 \left[ 1 - 6 \mathcal{T}_r(J) f(1 - f) \right] . \]  

The S-TUR is violated when \( R_1(\tau) < 0 \), that is \( \mathcal{T}_r(J) f(1 - f) > 1/6 \). However, since \( 0 \leq f(1 - f) \leq 1/4 \), the S-TUR is violated once \( \mathcal{T}_r(J) > 2/3 \). Interestingly, already in the quadratic order of \( \Delta \beta \) the TUR can drop below the value of 2 if \( \mathcal{T}_r(J) \) crosses a critical value. We assess the perturbative formula (10) in Ref. 46. However, in the weak coupling limit i.e., \( J \tau \ll 1, \mathcal{T}_r^2(J) \ll \mathcal{T}_r(J) \), and \( R_1(\tau) \) is always positive. Moreover, it can be shown that in this limit the S-TUR bound is always above 2, even far from equilibrium 57.

**Experimental setup and Results.** To study heat exchange between two qubits we use liquid-state NMR spectroscopy of the \(^{19}\text{F}\) and \(^{31}\text{P}\) nuclei in the molecule Sodium fluorophosphate dissolved in D$_2$O. Experiments are performed in 500MHz Bruker NMR spectrometer at ambient temperature. As shown in Fig. 1(a), \(^{19}\text{F}\) and \(^{31}\text{P}\) are identified as the two qubits, 1 and 2, exchanging heat under the desired coupling Hamiltonian, \( \mathcal{H}_{XY} \) in Eq. (4). The pulses are applied on qubits 1 and 2 in a time ordered manner from left to right. The black and white narrow solid bars represent \( \pi \) and \( \pi/2 \) pulses, respectively, with the phases mentioned above them. 1/2\( J_{12} \) represents the free evolution delay. The white box represents the \( \theta \) (in rads) angle pulse about y-axis.

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**FIG. 1.** (a) Molecular structure of the two-qubit NMR spin system, Sodium fluorophosphate. The NMR active spin-1/2, \(^{19}\text{F}\) and \(^{31}\text{P}\) nuclei in the molecule, labeled as qubit 1 and qubit 2 respectively, are coupled by the Hamiltonian (11) with the coupling strength \( J_{12} = 868 \text{ Hz} \). (b) Pulse sequence to realize heat exchange coupling Hamiltonian, \( \mathcal{H}_{XY} \) in Eq. (4).
exchange heat is realized from the internal Hamiltonian $H_{\text{int}}$ with the RF pulses displayed in Fig. 1(b). The net effect of the pulse sequence is that the two spins evolve under the coupling Hamiltonian $H_{XY}$ for a duration $\tau$ that is specified by the $\theta$ angle rotation about y-axis, as shown. For the duration of $1/2J_{12}$, the system evolves under the Hamiltonian $H_{\text{int}}$.

To start with, the two qubits are initialized in a pseudo-equilibrium state $\rho_{1} \otimes \rho_{2}$, where $\rho_{i} = \exp \left[ -\beta_{i} H_{i} \right] / Z_{i}$ is a Gibbs thermal state with inverse pseudo spin temperatures $\beta_{i}$ and $Z_{i}$ the partition function. For simplicity, we set $\beta_{2} = 0$ in all our measurements. Qubit 1 is prepared at a higher inverse temperature $\beta_{1}$ by initializing it in a pseudopure state (PPS) of $|0\rangle \langle 0|$, followed by applying pulses between 0 and $\pi/2$, and a pulse field gradient (PFG). The purpose of the PFG is to destroy coherences produced by 0 to $\pi/2$ angle pulses. The qubits—prepared at two different pseudoequilibrium states—are made to exchange heat under the coupling Hamiltonian $H_{XY}$ for different time interval $\tau$ and different $\beta_{1}$. Following the coupling period, we perform QST of the final state (in addition to the QST of the initial pseudoequilibrium state)\(^{46}\), and from Eq. (3) achieve the cumulants of heat exchange.

In Figs. 2 and 3 we present two cases, displaying agreement and violation, respectively, of the S-TUR. First, in Fig. 2 we set $J_\tau = 1/8$. According to the theoretical analysis, the S-TUR is valid when the skewness is positive, or $T_{\tau}(J) = 1/2 < 2/3$. Indeed, we find in Fig. 2(a) that both $R_{1}(\tau)$ and $\Delta_{\beta} \langle Q^{2} \rangle_{c} - 2$ are positive for all $\Delta_{\beta}$. In Fig. 2(b), we compare the different bounds on the relative uncertainty $\langle Q^{3} \rangle_{c} / \langle Q^{2} \rangle_{c}$, using experimental data as well as theoretically, and show that the S-TUR provides the tightest bound. Next, in Fig. 3(a) we display results for $J_\tau = 1/4$, for which according to our theory violations of the S-TUR are expected to occur already in the quadratic order of $\Delta_{\beta}$, as $T_{\tau}(J) = 1 > 2/3$. Indeed, we clearly see a violation for $0 < \beta_{1} \omega_{0} < 3.2$. Furthermore, the third cumulant, $\langle Q^{3} \rangle_{c}$, is negative in this region, which corroborates with Eq. (10). The theoretically predicted lowest value for the S-TUR for this model is $\Delta_{\beta} \langle Q^{2} \rangle_{c} / \langle Q^{2} \rangle_{r} \approx 1.86$, and we experimentally reach a value very close to this number. The violation of the S-TUR can also be seen in Fig. 3(b): The S-TUR bound $2/\langle \Sigma \rangle$ appears above the ratio $\langle Q^{3} \rangle_{c} / \langle Q^{2} \rangle_{c}$, and it is greater than the other, looser bounds. Measurements again closely match the theoretical curves.

A complete analysis of the TUR as a function of the
heat exchange duration $\tau$ and for a fixed $J = 1$ Hz, is presented in Fig. 4. We display the first three cumulants and note that the relative uncertainty is reduced (violation of S-TUR) within a certain region of parameters: The minimum value of the S-TUR precisely appears when the fluctuation of the heat exchange are reduced, below the value of the first cumulant. As expected, the skewness is found to be negative in this region.

Summary. We experimentally examined the TUR for heat exchange by realizing the XY-model, performing quantum state tomography and extracting the heat exchange cumulants. We found that the S-TUR provides a tight bound up to a certain threshold value for the qubit-qubit coupling parameter $\sin^2(2\pi J \tau)$, beyond which the bound is invalidated. As predicted theoretically, the validity of the S-TUR crucially depends on the sign of the third cumulant. Generalized versions of the TUR are satisfied throughout, as expected, since these (loose) bounds are derived from the universal fluctuation relations. Nevertheless, the S-TUR contains more information: The condition to invalidate it pinpoints to regimes of favorable performance for heat machines, operating with high constancy and little dissipation.

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In the weak coupling limit the second cumulant (6) can be organized as (using $x \coth(x) \geq 1$)

$$\langle Q^2 \rangle_r = (\hbar \omega_0)^2 T_r(J)(f_1(1-f_2)+f_2(1-f_1))$$

$$= (\hbar \omega_0)^2 \coth\left(\frac{\Delta \Delta \nu}{2}\right) T_r(J)(f_2 - f_1)$$

$$\geq \frac{2}{\Delta \beta} \hbar \omega_0 T_r(J)(f_2 - f_1) = \frac{2}{\Delta \beta} \langle Q \rangle_r,$$

proving that the S-TUR is satisfied even far from equilibrium.
S1. RELATION BETWEEN ENERGY EXCHANGE AND RÉNYI DIVERGENCES

We provide here details on the derivation of Eq. (2), which generalizes results of Ref. 45. We consider two systems with Hamiltonians $H_1$ and $H_2$, initially decoupled and prepared at their respective thermal equilibrium state. The initial composite density matrix is a product state, $\rho(0) = \rho_1 \otimes \rho_2$ with $\rho_i = \exp[-\beta_i H_i]/Z_i$, $i = 1, 2$ a Gibbs thermal state with inverse temperature $\beta_i = 1/k_B T_i$; $k_B$ the Boltzmann constant. $Z_i = \text{Tr}[\exp(-\beta_i H_i)]$ is the corresponding equilibrium partition function. The systems are coupled at $t = 0$ for a period $\tau$, which allows energy exchange between the two systems. This exchange of energy is not a deterministic process, but it is described by a probability distribution function (PDF). In the quantum regime, the PDF of energy exchange is constructed from a two-point projective measurement protocol 41-43 performed at the beginning of the energy exchange process, and after decoupling. This procedure respects the Jarzynski and Wójcik exchange fluctuation symmetry. For bipartite setups, we construct the joint PDF corresponding to energy change $(\Delta E_i, i = 1, 2)$ for both the systems, given as

$$p_\tau(\Delta E_1, \Delta E_2) = \sum_{m,n} \left( \prod_{i=1}^{2} \delta(\Delta E_i - (\epsilon^i_m - \epsilon^i_n)) \right) p^0_{m|n} p^0_{n|m}.$$ \hspace{1cm} (S1)

Here, $p^0_{m|n} = \prod_{i=1}^{2} e^{-\beta_i \epsilon^i_n}/Z_i$ is the probability to find the decoupled systems in the eigenstate $|n\rangle = |n_1, n_2\rangle$ with energy eigenvalues $\epsilon^i_n$, $H_i|n_i\rangle = \epsilon^i_n|n_i\rangle$, after the first projective measurement. The second projective measurement at $t = \tau$ collapses the system to the eigenstate $|m\rangle = |m_1, m_2\rangle$, $H_i|m_i\rangle = \epsilon^i_m|m_i\rangle$. The corresponding transition probability is $p^\tau_{m|n} = \langle m|U(\tau, 0)|n\rangle|^2$, where $U(t, 0) = e^{-itH/\hbar}$ is the unitary propagator with the total-composite Hamiltonian $H$. The principle of microreversibility of quantum dynamics for autonomous systems demands $p^\tau_{m|n} = p^\tau_{n|m}$. Following this relation and given the uncorrelated initial thermal condition for the composite system, we receive the following universal symmetry for the joint PDF,

$$p_\tau(\Delta E_1, \Delta E_2) = e^{\beta_1 \Delta E_1 + \beta_2 \Delta E_2} p_\tau(-\Delta E_1, -\Delta E_2).$$ \hspace{1cm} (S2)

This symmetry motivates us to define a characteristic function-like quantity, which leads to the following crucial relation

$$\langle (e^{-\beta_1 \Delta E_1 - \beta_2 \Delta E_2})^z \rangle = \int d(\Delta E_1)d(\Delta E_2)p_\tau(\Delta E_1, \Delta E_2)e^{-z \beta_1 \Delta E_1 - z \beta_2 \Delta E_2}$$

$$= \text{Tr}\left[\rho(0)^z \rho(\tau)^{1-z}\right].$$

$$= \exp\left\{ (z - 1)S_z [\rho(0)||\rho(\tau)] \right\}. \hspace{1cm} (S3)$$

Here $S_z [\rho(0)||\rho(\tau)] = \frac{1}{z - 1} \ln\left\{ \text{Tr}[\rho(0)^z \rho(\tau)^{1-z}] \right\}$ is the order-$z$ Renyi divergence, a metric for the relation between the states of a composite system at the initial $(t = 0)$ and the final $(t = \tau)$ times. As a special case, when $z = 1$ we receive the universal relation, $\langle e^{-\beta_1 \Delta E_1 - \beta_2 \Delta E_2} \rangle^\tau = 1$.

So far, the analysis is exact. However, it is relevant to consider the limit $\Delta E_1 \approx -\Delta E_2$, which is justified when the two systems are weakly coupled. Furthermore, $\Delta E_1 = -\Delta E_2$ if there is no energy cost involved in turning on and off the interaction between the systems. One can then interpret the energy change for an individual system as heat $(\Delta E_1 = -\Delta E_2 = Q)$. This modifies the symmetry relation in Eq. (S2) for the joint PDF to $p_\tau(Q) = \exp\left[ (\beta_1 - \beta_2)Q \right] p_\tau(-Q)$. Accordingly, Eq. (S3) leads to

$$\langle (e^{-\Delta \beta Q})^z \rangle = \exp\left\{ (z - 1)S_z [\rho(0)||\rho(\tau)] \right\}, \hspace{1cm} (S4)$$

which immediately generates expressions for the moments,

$$(Q^n)_z = \frac{1}{(\Delta \beta)^n} \text{Tr}\left[\rho(\tau)T_n \left( \ln \rho(\tau) - \ln \rho(0) \right)^n \right]. \hspace{1cm} (S5)$$

$T_n$ is the time-ordering operator, which orders operators at the latest time to the left and $\Delta \beta = \beta_1 - \beta_2$. 

The Supplemental Material is provided in multiple parts, each focusing on different aspects of the energy exchange and Rényi divergences. The content is structured to provide a comprehensive understanding of the theoretical framework and its applications in quantum systems.
The initial density matrix for the composite system is given by a direct product of the individual qubits, each prepared in an equilibrium state with a particular temperature. In the matrix form, we can then write,

$$\rho(0) = \begin{bmatrix}
    f_1 f_2 & 0 & 0 & 0 & 0 \\
    0 & f_1(1 - f_2) & 0 & 0 & 0 \\
    0 & 0 & f_2(1 - f_1) & 0 & 0 \\
    0 & 0 & 0 & (1 - f_1)(1 - f_2) & 0
\end{bmatrix}.$$ 

where $f_i(\nu_0) = 1/(\exp(\beta_i h \nu_0) + 1)$. The density matrix evolves under the interaction Hamiltonian according to the Liouville equation $\rho(\tau) = U(\tau, 0) \rho(0) U^\dagger(\tau, 0)$ where $U(t, 0) = e^{-iHt/\hbar}$ and for the XY model is given by,

$$U(\tau, 0) = \begin{bmatrix}
    e^{-2i\pi \nu \tau} & 0 & 0 & 0 & 0 \\
    0 & \cos(2\pi J \tau) & \sin(2\pi J \tau) & 0 & 0 \\
    0 & -\sin(2\pi J \tau) & \cos(2\pi J \tau) & 0 & 0 \\
    0 & 0 & 0 & e^{2i\pi \nu \tau} & 0
\end{bmatrix}.$$ 

The density matrix for the composite system at any arbitrary heat exchange duration time $\tau$ can be analytically found, and is given as

$$\rho(\tau) = \begin{bmatrix}
    f_1 f_2 & 0 & 0 & 0 & 0 \\
    0 & f_1(1 - f_2) \cos^2(2\pi J \tau) + f_2(1 - f_1) \sin^2(2\pi J \tau) & \frac{1}{2} \sin(4\pi J \tau)(f_2 - f_1) & 0 & 0 \\
    0 & \frac{1}{2} \sin(4\pi J \tau)(f_2 - f_1) & f_2(1 - f_1) \cos^2(2\pi J \tau) + f_1(1 - f_2) \sin^2(2\pi J \tau) & 0 & 0 \\
    0 & 0 & 0 & (1 - f_1)(1 - f_2) & 0
\end{bmatrix}.$$ 

One can similarly find the logarithm of this matrix,

$$\log \rho(\tau) = \begin{bmatrix}
    \log(f_1 f_2) & 0 & 0 & 0 & 0 \\
    0 & \log(f_1(1 - f_2)) + \Delta \beta \hbar \nu_0 \sin^2(2\pi J \tau) & \frac{1}{2} \Delta \beta \hbar \nu_0 \sin(4\pi J \tau) & 0 & 0 \\
    0 & \frac{1}{2} \Delta \beta \hbar \nu_0 \sin(4\pi J \tau) & \log(f_2(1 - f_1)) - \Delta \beta \hbar \nu_0 \sin^2(2\pi J \tau) & 0 & 0 \\
    0 & 0 & 0 & \log[(1 - f_1)(1 - f_2)] & 0
\end{bmatrix}.$$ 

We substitute these expressions for the composite density matrix into Eq. (S5) and receive all moments for heat exchange.

FIG. S1. Quantum state tomography for the real components of the density matrix elements for both initial and final states. Parameters are $J \tau = 1/4$, $\beta_2 = 0$, $\nu_0 = \pi/20$, $\beta_1 \omega_0 = 2.02$, corresponding to Fig. 3.
S3. QUANTUM STATE TOMOGRAPHY OF THE XY MODEL

In Fig. (S1) we provide both theoretical and the experimental quantum state tomography results for a particular realization. We display only the real components for both the initial and final density matrices of the composite system. The imaginary components for both these states are vanishingly small. In our tomography experiments the states are realized with fidelity higher than 97%. Both the initial and final states are obtained by performing 6 independent experiments and measurements.

S4. VALIDITY OF THE PERTURBATIVE EXPANSION

For the XY model, the ratio $\Delta \beta \frac{\langle Q^2 \rangle}{\langle Q \rangle}$ can be simulated exactly using the closed-form expressions for the cumulants, Eq. (6). Thoroughout the paper, these exact expressions were used to compare with measurements. Nevertheless, the $(\Delta \beta)^2$ perturbative analysis of the S-TUR, Eq. (10), is constructive as it serves to quickly identify S-TUR violations: The S-TUR is disobeyed if $T_{\gamma}(J) > 2/3$. In Fig. S2 we display the ratio $\Delta \beta \frac{\langle Q^2 \rangle}{\langle Q \rangle} - 2$ based on the exact expressions for the cumulants, and compare is to $C_2(\Delta \beta) \equiv \left[ \frac{1}{6} - T_{\gamma}(J)f(1-f) \right]$, which measures the deviation from the equilibrium value, as received in Eq. (10). We observe an excellent agreement up to $\beta_1 \omega_0 \approx 1$, and meaningful results up to $\beta_1 \omega_0 \approx 1.5$. For larger $\Delta \beta$, the quadratic expansion obviously fails to track the recovery of the S-TUR in Fig. S2 (b).

![Fig. S2](image_url)

FIG. S2. Analysis of the S-TUR based on exact expressions for the cumulants (full) and the $(\Delta \beta)^2$ expansion (dashed), see text for the definition of $C_2(\Delta \beta)$. (a) $J\tau = 1/8$ thus $T_{\gamma}(J) < 2/3$, corresponding to Fig. 2. (b) $J\tau = 1/4$ thus $T_{\gamma}(J) > 2/3$, corresponding to Fig. 3. Parameters are $\beta_2 = 0$ and $h\nu_0 = 1$. 