Operational Definition of the Temperature of a Quantum State

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Temperature is usually defined for physical systems at thermal equilibrium. Nevertheless one may wonder if it would be possible to attribute a meaningful notion of temperature to an arbitrary quantum state, beyond simply the thermal (Gibbs) state. In this Letter, we propose such a notion of temperature considering an operational task, inspired by the zeroth law of thermodynamics. Specifically, we define two effective temperatures for quantifying the ability of a quantum system to cool down or heat up a thermal environment. In this way we can associate an operationally meaningful notion of temperature to any quantum density matrix. We provide general expressions for these effective temperatures, for both single- and many-copy systems, establishing connections to concepts previously discussed in the literature. Finally, we consider a more sophisticated scenario where the heat exchange between the system and the thermal environment is assisted by a quantum reference frame. This leads to an effect of "coherent quantum catalysis," where the use of a coherent catalyst allows for exploiting quantum energetic coherences in the system, now leading to much colder or hotter effective temperatures. We demonstrate our findings using a two-level atom coupled to a single mode of the electromagnetic field.

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Introduction.—Temperature is a well-defined property of macroscopic systems in thermal equilibrium [1]. When considering equilibrium systems of finite size, subtleties on the notion of temperature can arise due to the breakdown of the equivalence of statistical ensembles [2–8] and the non-negligible effect of interactions between constituents [9–13]. Moving on to nonequilibrium (quantum) systems, assigning an effective temperature can be useful in certain physical contexts [14–17]. Given some quantum state ρ evolving under Hamiltonian H, the most common approach is to assign an effective temperature T^* given by the temperature of an equilibrium (Gibbs) state with the same average energy, that is

$$\mathrm{Tr}[H\rho] = \mathrm{Tr}[H\gamma(T^*, H)] \tag{1}$$

where $\gamma(T, H) \equiv e^{-\beta H}/Z$, $Z = \mathrm{Tr}e^{-\beta H}$ is the partition function, and $\beta = 1/k_B T$ ($k_B \equiv 1$). The relevance of the identification [Eq. (1)] naturally arises in the dynamics of isolated quantum many-body systems: seminal results suggest that ρ will become in practice indistinguishable [18] from $\gamma(T^*, H)$ after a transient thermalization time [24–30]. Beyond isolated systems, different notions of effective temperatures have been discussed for characterizing nonequilibrium states [31,32], and also in the context of quantum thermal machines [33–39].

Here we propose an alternative and operational approach for defining temperature for quantum systems. We consider a system with Hamiltonian H in a quantum state ρ, and place it in contact with another (reference) system initially at thermal equilibrium. We then assign two temperatures for the system, T_c and T_h, which correspond to the lowest and the highest temperatures at which the reference system can be cooled down or heated up. That is, T_c and T_h characterize the potential of ρ to heat up or cool down a reference state in thermal equilibrium (see Fig. 1). This approach establishes a natural direction of heat flow

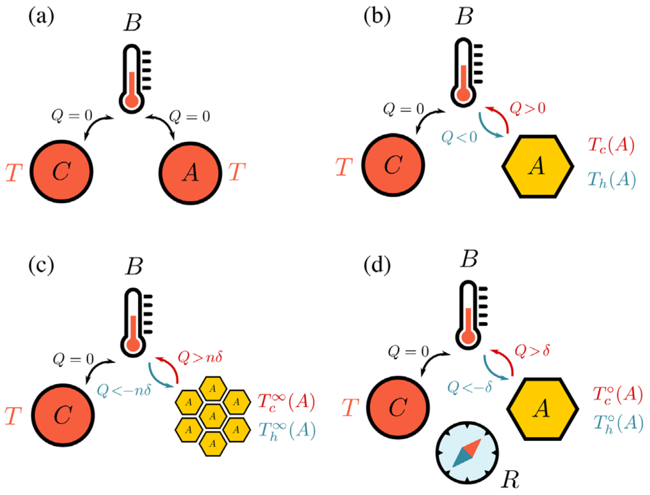

FIG. 1. Setups used to define effective temperatures for non-equilibrium quantum systems. (a) Equilibrium setting addressed by the zeroth law. (b) Setup used to assign effective cold $T_c(A)$ and hot $T_h(A)$ temperatures with system A. (c) The case when effective temperatures are assigned to multiple copies of A. In panel (d), we extend the setting by adding a reference frame (catalyst), i.e., a system that aids the process without providing heat itself. For details see the main text.

between ρ and a thermal environment at temperature T: Heat will always flow toward the environment when $T \leq T_c$ and, likewise, the environment will always release heat when $T \geq T_h$. Instead, for $T_c \leq T \leq T_h$, the direction of heat flow depends on the particular process. As expected, $T_c \leq T^* \leq T_h$, with equality when the system itself is in thermal equilibrium with temperature T^*.

We apply this approach to three different situations. First, we find explicit expressions for the effective temperatures of quantum systems, which are related to the concept of virtual temperatures [33–36,40–42]. Second, we show that for macroscopic quantum systems, the two effective temperatures are closely related to T^*. Third, we extend the framework by introducing a reference frame, or a quantum catalyst [43–50]. This gives access to strictly colder and hotter effective temperatures by exploiting energy coherences present in the system.

Operational definition of temperature.—A system S will be described by a tuple (H_S, ρ_S), where H_S stands for the system's Hamiltonian and ρ_S its density matrix. We say that a system is in thermal equilibrium at temperature T if its state can be written as $\rho_S = \gamma(T, H_S)$.

The zeroth law of thermodynamics states that when system A is in a thermal equilibrium with another system B that is in a thermal equilibrium with C, then A must be in a thermal equilibrium with C [see Fig. 1(a)] [1,51]. Importantly, the zeroth law associates temperature with systems in thermal equilibrium. Here we will use a similar approach to define *effective temperatures* for nonequilibrium systems. We will consider three systems, A, B, and C, where C is a macroscopic heat bath at temperature T, system $B = (H_B, \gamma(T, H_B))$ is a thermometer probe, and $A = (H_A, \rho_A)$ is the quantum system whose effective temperatures we want to quantify. For that, we consider the following steps: (i) we couple B to C until B reaches thermal equilibrium at temperature T, (ii) we decouple them, and (iii) we couple B to A to infer the effective temperature of A by measuring B.

Let us now describe in detail step (iii). First, we demand that energy is preserved within the joint system AB, i.e., the evolution is described by a unitary process U satisfying $[U, H_A + H_B] = 0$. This ensures that only the energy of A is used to heat up or cool down the thermometer. Second, we assume perfect control over the joint system, meaning we allow for arbitrary processes U. The dynamics is then characterized by the full set of energy-preserving unitaries [40,52]. Notice that we make no assumptions about the strength of interaction (weak or strong), its complexity (local or collective), or duration (short or long) with respect to the natural timescales. Third, we assume the initial state of AB factorizes, i.e., $\rho_{AB} = \rho_A \otimes \gamma_B(T, H_B)$, ensuring that B has a well-defined temperature, and its energy changes may be interpreted as heat.

The joint state of the system and the thermometer after the interaction is given by $\sigma_{AB} = U[\rho_A \otimes \gamma_B(T, H_B)]U^\dagger$. The heat transferred to the thermometer is therefore

$$Q(T, H_B, U) := \mathrm{Tr}\{H_B[\sigma_B - \gamma_B(T, H_B)]\}, \tag{2}$$

with $\sigma_B := \mathrm{Tr}_A \sigma_{AB}$. It is well known that heat can only flow in one direction when A is a Gibbs state at some temperature $T(A)$, i.e., $\rho_A = \gamma_A[T(A), H_A]$. More specifically,

$$\begin{aligned} Q(T, H_B, U) &\geq 0 \quad \text{for all } T \leq T(A), \\ Q(T, H_B, U) &\leq 0 \quad \text{for all } T \geq T(A), \end{aligned} \tag{3}$$

which holds for all possible H_B and U [53,54]. In other words, the direction of heat is well defined between Gibbs states: Heat can only flow from hot to cold, regardless of the particular thermometer B or process U. Instead, for nonthermal states the direction of heat flow is not always unique, as illustrated by its reversal in the presence of correlations [53–56]. That is, the sign of $Q(T, H_B, U)$ in general depends on H_B and the process U.

The crucial insight of our Letter is that there are temperatures for which heat has a well-defined direction even for nonequilibrium states (i.e., it is independent of H_B and U and depends only on A). Given some $A = (H_A, \rho_A)$, we will show that there exist temperatures $T_c(A)$ and $T_h(A)$ that satisfy

$$\begin{aligned} Q(T, H_B, U) &\geq 0 \quad \text{for all } T \leq T_c(A), \\ Q(T, H_B, U) &\leq 0 \quad \text{for all } T \geq T_h(A), \end{aligned} \tag{4}$$

for all possible H_B and U, in analogy with the equilibrium case [Eq. (3)]. As a consequence, A is effectively hotter or colder than any equilibrium state below or above $T_c(A)$ and $T_h(A)$, respectively. Conversely, A has the *potential* to cool down equilibrium states with temperature $T \geq T_c(A)$ and heat up states with $T \leq T_h(A)$. Hence, $T_c(A)$ and $T_h(A)$ bound the ability of A to heat up or cool down a thermal environment.

In order to find the effective cold $T_c(A)$ and hot $T_h(A)$ temperatures, we look for the minimal (maximal) temperature T for which $Q(T, H_B, U)$ is negative (positive) for *some* thermometer B and *some* energy-preserving interaction U, i.e.,

$$\begin{aligned} T_c(A) := \min_{H_B, U} \quad & T \\ \text{such that} \quad & Q(T, H_B, U) < 0, \\ & [U, H_A + H_B] = 0. \end{aligned} \tag{5}$$

Similarly, we define $T_h(A)$ by replacing max with min above and reversing the inequality.

Effective temperatures of single-copy quantum systems.—The protocol discussed above is effectively described using a channel acting on the system A:

$$\mathcal{E}_T(\cdot) = \mathrm{Tr}_B\{U[\cdot \otimes \gamma_B(T, H_B)]U^\dagger\}. \tag{6}$$

This class of channels is known as *thermal operations* [40,44,57–60]. We use this correspondence to prove our first main result. More specifically, for *any* quantum system $A = (H_A, \rho_A)$ with $H_A = \sum_i \epsilon_i |\epsilon_i\rangle\langle\epsilon_i|$ and $p_i \coloneqq \langle\epsilon_i|\rho_A|\epsilon_i\rangle$, we show that the effective temperatures are given by

$$T_c(A) = \min_{i\neq j} T_{ij}, \qquad T_h(A) = \max_{i\neq j} T_{ij}, \tag{7}$$

where $T_{ij} \coloneqq (\epsilon_j - \epsilon_i)/\log(p_i/p_j)$ are the virtual temperatures of the state [33–36,40–42]. As expected, for Gibbs states $T_c(A) = T_h(A)$, whereas for nonequilibrium states $T_c(A) \neq T_h(A)$. The proofs proceed similarly for both effective temperatures, so we only discuss $T_c(A)$. First, we show that for any system A there is an interaction and a thermometer B that can be cooled down when $T \geq \min_{i\neq j} T_{ij}$. The cooling protocol is simple: Consider the two-dimensional subspace $\{|\epsilon_k\rangle, |\epsilon_l\rangle\}$ corresponding to the lowest virtual temperature, i.e., $T_c(A) = T_{kl}$. We then introduce a two-level thermometer B with levels $\{|g\rangle, |e\rangle\}$ and energy gap $\epsilon_k - \epsilon_l$, thus in resonance with the selected subspace. By coupling such subspaces via an energy-conserving operation $U = e^{-iH_{\text{int}}t}$ acting for time $t = \pi/2$ with $H_{\text{int}} = |\epsilon_l\rangle\langle\epsilon_k|_A \otimes |g\rangle\langle e|_B + \text{H.c.}$, the energy of A will necessarily increase, and hence B will be cooled down, as desired. Second, we use the resource-theoretic approach to show that when $T \leq \min_{i\neq j} T_{ij}$, there exists no protocol that can cool down any thermometer B [61]. This proves that $T_c(A)$ is equal to $\min_{i\neq j} T_{ij}$. For details see Appendix A in the Supplemental Material [61].

The effective temperatures can be both positive and negative. This is a consequence of their operational character: A system with a negative effective temperature has its energy population inverted {note that the effective temperature [Eq. (1)] also becomes negative in this case}. Therefore, a quantum system with $T_h(A) < 0$ can heat up equilibrium systems at any real temperature T. Similarly, when $T_c(A) < 0$, the system cannot cool down any equilibrium system, even when its real temperature is arbitrarily large.

A quantum system A is out of equilibrium with respect to temperature T when it contains at least one virtual temperature different from T. Moreover, since virtual temperatures depend only on the occupations in the energy basis, i.e., on $p_i = \langle\epsilon_i|\rho_A|\epsilon_i\rangle$, superpositions of energy levels have the same ability to generate heat as corresponding probabilistic mixtures. This means that energy coherences are irrelevant from the perspective of cooling or heating the thermometer —which is intimately connected to the time-translation symmetry of the allowed operations [59,64–66] We now discuss two ways to overcome this restriction. First, we consider processing multiple copies of the system collectively [67–69] and show that the degeneracy of energy levels allows one to exploit coherence locked in the quantum system. Second, we extend the framework by introducing a reference frame (or a catalyst), i.e., a system that allows one to locally lift some of the restrictions imposed by the presence of conserved quantities.

Effective temperatures of macroscopic quantum systems.—Suppose that system A consists of multiple identical copies, i.e., $A \equiv A^n \coloneqq (H_A^{\otimes n}, \rho_A^{\otimes n})$ [see Fig. 1(c)]. As we will see, it is then convenient to extend the definition of effective temperatures [Eq. (5)] by introducing a parameter $\delta > 0$ capturing the minimal amount of heat transferred to (or measured by) the thermometer, i.e.,

$$\begin{aligned} T_c(A,\delta) \coloneqq \min_{H_B,U} \quad & T \\ \text{such that} \quad & Q(T, H_B, U) \leq -\delta, \\ & [U, H_A + H_B] = 0. \end{aligned} \tag{8}$$

The definition for $T_h(A,\delta)$ is obtained by replacing max with min, reversing the inequality, and changing the sign of δ. For consistency, we can verify that $\lim_{\delta\to 0_+} T_c(A,\delta) \equiv T_c(A)$. For macroscopic systems comprised of n particles, we require that δ is proportional to n, so that the transferred heat is also macroscopic. Therefore, we define the *asymptotic effective temperatures* as

$$T^{\infty}_{c/h}(A,\delta) \equiv \beta^{\infty}_{c/h}(A,\delta)^{-1} \coloneqq \lim_{n\to\infty} T_{c/h}(A^n, n\delta). \tag{9}$$

In Supplemental Material B [61] we show that $\beta^{\infty}_{c/h}(A,\delta)$ can be expressed as

$$\beta^{\infty}_c(A,\delta) = \frac{1}{\delta}\{S[\gamma_A(E+\delta)] - S(\rho_A)\}, \tag{10}$$

$$\beta^{\infty}_h(A,\delta) = \frac{1}{\delta}\{S(\rho_A) - S[\gamma_A(E-\delta)]\}, \tag{11}$$

where $\gamma_A(x)$ stands for a Gibbs state with Hamiltonian H_A and average energy x. Notice the change of notation for the Gibbs state introduced to simplify the formulas that follow. Furthermore, we introduced a parameter $E \coloneqq \text{tr}(\rho_A H_A)$, and $S(\rho) \coloneqq -\text{Tr}\rho\log\rho$ is the von Neuman entropy. It can be noted that, while $T_c(A)$ and $T_h(A)$ correspond to the minimal and maximal virtual temperatures of A, the temperatures $T_c(A,\delta)$ and $T_h(A,\delta)$ depend on the whole spectrum of ρ_A and hence all its virtual temperatures.

To develop some intuition about the effective temperatures we can look at the thermodynamic limit. Here it corresponds to the regime with $n \to \infty$ and $\delta \to 0$ with A prepared in a Gibbs state with average energy E, i.e., $\rho_A = \gamma_A(E)$. In this regime $\beta^{\infty}_{c/h}(A,\delta)$ both converge to the usual definition of (inverse) temperature, i.e.,

$$\lim_{\delta\to 0} \beta^{\infty}_c(A,\delta) = \lim_{\delta\to 0} \beta^{\infty}_h(A,\delta) = \frac{\partial S[\gamma_A(E)]}{\partial E}. \tag{12}$$

For any quantum state ρ_A we can further expand up to $\mathcal{O}(\delta^2)$,

$$\beta^{\infty}_{c/h}(A,\delta) \approx \pm\frac{\Delta S(\rho_A)}{\delta} + \beta^*(E) - \frac{\delta}{2\Delta^2 E(\gamma_A)}, \qquad (13)$$

where $\Delta S(\rho_A) \coloneqq S[\gamma_A(E)] - S(\rho_A)$ and $\Delta^2 E(\gamma_A) \coloneqq \mathrm{tr}[H_A^2 \gamma_A(E)] - [H_A \gamma_A(E)]^2$. Expression (13) naturally connects $\beta^{\infty}_{c/h}(A,\delta)$ with the effective temperature β^* defined in Eq. (1). For generic states $\beta_{c/h}(A,\delta)$ differ, i.e., quantum systems can be both hot and cold, even in the asymptotic limit. Note that $\beta_{c/h}(A,\delta)$ diverge in the limit $\delta \to 0$, indicating that an asymptotically large source of nonequilibrium can cool down or heat up reference systems at any temperature by a sublinear amount in n. To illustrate how the range of effective temperatures changes by considering multiple copies of A, in Appendix C of the Supplemental Material, we discuss a simple toy example [61].

The effective temperatures [Eq. (10)] directly depend on $S(\rho_A)$, which means that quantum (energy) coherences are relevant in this collective scenario, in contrast to the single-copy case. One way to understand this is that by considering more copies of the system, one increases the size of degenerate energy eigenspaces. This enables more flexibility in transferring population, or equivalently, generating and accepting heat using energy-conserving interactions. In what follows we discuss an alternative approach to achieve the same goal.

Catalysis and the role of quantum coherence.—We now explore the possibility of exploiting energy coherences via the concept of catalysis [43–48,66,70–79]. In this case an auxiliary system (the catalyst) provides a phase reference for the main system. Crucially, after the interaction, the catalyst must be returned to its initial state. This ensures that it provides no energy and can be later reused. This mechanism allows one to take advantage of energy coherences at the level of a single copy of the system. Let us consider a simple example to illustrate the strength of this approach.

Consider the evolution of a two-level atom coupled to a single mode of electromagnetic field in an optical cavity (see Fig. 2). For that, let A denote the cavity with bosonic creation and annihilation operators $a^\dagger$ and a. Furthermore, let R be the two-level system with raising and lowering operators $\sigma_+ = |e\rangle\langle g|$ and $\sigma_- = |g\rangle\langle e|$. The interaction is modeled using the Jaynes-Cummings Hamiltonian [80], which in the rotating wave approximation reads as

$$H_{AR} = \omega_A a^\dagger a + \omega_R |e\rangle\langle e| + H_{\mathrm{int}}, \qquad (14)$$

where $H_{\mathrm{int}} \coloneqq g(\sigma_+ a + \sigma_- a^\dagger)$, ω_A is the angular frequency of the mode, and ω_R is the atomic transition frequency. To keep this example relatively simple we truncate the number of Fock states of A to three levels [81]. Moreover, we assume that the atom is driven on resonance, i.e., $\omega_A = \omega_R$. This ensures that the unitary evolution $U(t) = e^{-iH_{AR}t}$ generated by H_{AR} satisfies $[U(t), H_{AR}] = 0$ for all times t. Our goal is to quantify the effective temperatures of the cavity, $T_{c/h}(A)$.

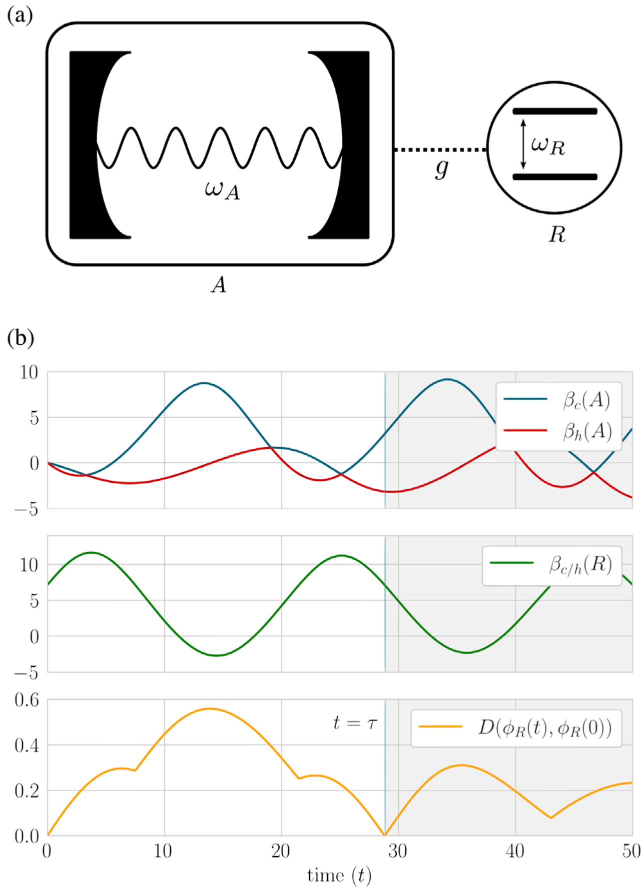

FIG. 2. The illustrative example described in the main text. (a) Sketch of the scenario: a two-level system R interacting resonantly with a single-mode optical cavity A. (b) Time evolution of the effective temperatures of both systems. The top figure shows effective temperatures of A as a function of time t. The middle panel shows the evolution of the effective temperatures of R. The bottom panel shows the distance between the states of the atom at some time t and $t = 0$ as quantified by the trace distance $D(\rho,\sigma) \coloneqq \mathrm{Tr}[\sqrt{(\rho-\sigma)^\dagger(\rho-\sigma)}]/2$. Notice that at time $t = \tau$ the system R returns to its initial state; therefore it acts as a catalyst. The parameters chosen are $\omega_R = \omega_A = 1$, $g = 0.1$, and $\tau = 28.5$.

Assume that the field A and atom R start in states $|\psi\rangle_A = (|0\rangle + |1\rangle + |2\rangle)/3$, $\phi_R = X(\tau)$, where τ is a free parameter and $X(\tau)$ is the state of the atom obtained by solving the operator equation

$$X(\tau) = \mathrm{Tr}_A\{U(\tau)[|\psi\rangle\langle\psi|_A \otimes X(\tau)]U(\tau)^\dagger\}. \qquad (15)$$

In other words, the state of the atom is chosen so that time $t = \tau$ returns to its initial state. We now compare two different cases: noninteracting ($g = 0$) and interacting ($g > 0$).

When $g = 0$ both systems evolve independently. The effective temperatures $T_{c/h}(A)$ can be computed from Eq. (7) and, in our particular case, they read as $T_c(A) = T_h(A) = 0$. As expected, in the absence of interaction, the presence of the atom does not influence the effective temperatures of the electromagnetic field.

When $g > 0$, the coupling between the field A and the atom R changes their energy occupations with time, and therefore also changes their effective temperatures. After time $t = \tau$ the atom returns to its initial state, $\phi_R(\tau) = \phi_R(0)$; however the field may end up in a different state [see Fig. 2(b)]. As a consequence, its spectrum of virtual temperatures can change, as shown in Fig. 2(b). This is a generic effect, i.e., for any value of τ we can find the corresponding state of the atom which returns to its initial state by solving Eq. (15). Interestingly, after time τ the photonic mode A has lost quantum coherence, indicating a tradeoff between coherence of A and its ability to generate a flow of heat, as captured by the effective temperatures. This indicates a genuinely quantum mechanism that exploits energy coherence to generate the desired flow of heat.

We now ask how general this behavior is, i.e., what are the effective temperatures when using general catalysts? For that, we shall now consider arbitrary (energy-conserving) interactions and arbitrary states of the catalyst. In Supplemental Material E [61], we show that, via a catalytic system, one can reach the same effective temperatures as in the macroscopic case of Eq. (9). This naturally connects the two approaches considered. Importantly, in this case, system A is microscopic, i.e., δ quantifies the total transferred heat (rather than heat per particle). Moreover, no catalyst R that remains unchanged can lead to lower cold and higher hot effective temperatures.

Discussion.—We proposed an operational definition of temperature for nonequilibrium quantum systems. We defined two effective temperatures that quantify the ability of a quantum state to generate a flow of heat when coupled to a thermal environment (thermometer). We showed that these effective temperatures are given by the maximal and minimal virtual temperatures of the system and connected them with the effective temperature T^* in the asymptotic limit. We then extended this setting by allowing for the use of coherent reference frames, and found that energy coherences can influence effective temperatures.

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