Out-of-equilibrium quantum thermodynamics in the Bloch sphere: Temperature and internal entropy production

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An explicit expression for the temperature of an open two-level quantum system is obtained as a function of local properties under the hypothesis of weak interaction with the environment. This temperature is defined for both equilibrium and out-of-equilibrium states and coincides with the environment temperature if the system reaches thermal equilibrium with a heat reservoir. Additionally, we show that within this theoretical framework the total entropy production can be partitioned into two contributions: one due to heat transfer and another, associated to internal irreversibilities, related to the loss of internal coherence by the qubit. The positiveness of the heat capacity is established, as well as its consistency with the well-known results at thermal equilibrium. We apply these concepts to two different systems and show that they behave in analogous ways as their classical counterparts.

I. INTRODUCTION

Despite the enormous success of classical thermodynamics during the first half century after its creation, some important thermodynamic properties only acquired their deepest physical interpretation when considering the microscopic degrees of freedom, that is, with the advent of statistical mechanics. Entropy, for example, is a typical case of the above: The famous Boltzmann equation $S = k_B \ln \Omega$ associates the classical entropy concept with the logarithm of the number of microscopic configurations that are compatible with the actual macroscopic state.

Something similar has occurred with the notion of temperature. Its intrinsic phenomenological character associated to our ability of distinguishing various degrees of cold and hot objects made it difficult to express temperature in terms of other well-established physical quantities. The first relevant step came via the kinetic theory, which established the proportionality between temperature and the average kinetic energy of the microscopic components of the system in a simple physical model. Once the relation between entropy and microscopic world was clear, the equation

$$\frac{1}{T} = \frac{\partial S}{\partial E} \qquad (1)$$

deduced in classical thermodynamics can be adopted as a mechanical definition of temperature, for cases for which we are able to write the number of microscopic configurations as a function of the energy. For a recent review of the temperature concept in statistical mechanics, see Ref. [1].

The statistical interpretation is important to shed light onto the thermodynamic theory based on classical mechanics. When considering quantum mechanics as the underlying theory, the probabilistic nature of the theory and the fact that open systems generally find themselves in mixed states, make the statistical approach not only convenient but also mandatory.

In this case, the statistical description of the possible results of the measurements performed on the system is made through the reduced density matrix ρ_s, which allows us to obtain the expected values of the local observables by means of the rule:

$$\langle A \rangle = \text{tr}[\rho_s A]. \qquad (2)$$

This inherently statistical behavior suggests that in the attempt of extending thermodynamics to the quantum regime, the natural candidates to occupy the role of thermodynamic properties are the expected values of certain operators or, in the general case, functions of them. Typical examples are the internal energy, usually defined as the expected value of the local Hamiltonian, H_s, in the weak-coupling regime (i.e., if the interaction energy can be neglected):

$$E = \langle H_s \rangle = \text{tr}[H_s \rho_s], \qquad (3)$$

and the von Neumann entropy, which can be defined as the expected value of the entropy operator $-\ln \rho_s$,

$$S_{vN} = -\text{tr}[\rho_s \ln_{\rho_s}]. \qquad (4)$$

Adopting this point of view, in this work we explore the possibility of introducing the concept of temperature for a qubit that undergoes an open dynamic. The question about the need, convenience, or even the mere possibility of defining the temperature of such a two-level system is not new [2]. More recently, several "temperatures" have been proposed and demonstrated to be useful in order to explain certain quantum thermodynamic processes [3–8]. Unlike these approaches, some of them very sophisticated, our approach here is very simple and consists in explicitly applying Eq. (1), but employing the von Neumann entropy S_{vN}, instead of the thermodynamic entropy S, an idea that, to the best of our knowledge, has not been implemented. Unlike S, which is only defined for equilibrium states, S_{vN} can be assigned to arbitrary states. As a consequence, the expression obtained for

the temperature is valid even far from equilibrium, generalizing the usual equilibrium temperature. A completely different perspective about the temperature problem in quantum mechanics is presented in Ref. [9], where the authors propose that the temperature must be considered as an operator instead of a realistic local variable. In the same direction, several temperature-energy uncertainty relations have been found in the context of statistical mechanics, and more recently in quantum mechanics [10].

This work is organized as follows. In Sec. II, we establish a thermodynamic theory for the qubit based on considering the expected values of the spin operators as the elementary thermodynamic properties. In Sec. III, we deduce the expression for the temperature of the system, the specific heat, and the entropy production and we discuss the results. An analysis of the behavior of the defined quantities for some simple two-level models is developed in Sec. IV. Finally, some remarks and conclusions are presented in Sec. V.

II. BASIC THEORY FOR THE QUBIT

A. A state postulate

In addition to the well-known four laws of thermodynamics, the classical theory makes use of the "state postulate," which establishes that the thermodynamic state of a system in equilibrium is determined by knowing the values of a reduced set of independent intensive properties. Typically, for a simple compressible system without magnetic or other additional effects, two independent properties completely determine the state; i.e., any other property is a function of those two properties [11].

In the framework of open quantum systems and following the same philosophy, it would be useful to choose a set of thermodynamic properties (in the sense discussed in the Introduction) such that they allow to express any other one. Since the reduced state of an open two-level system can be put in correspondence with a point in the Bloch sphere, it is clear that three parameters are necessary to fully describe the state. A natural choice are the components of the Bloch vector:

$$\vec{B} = (B_x, B_y, B_z), \tag{5}$$

which can be obtained as the expected values of the spin operators S_x, S_y, and S_z (aside from a factor $\hbar/2$):

$$\begin{aligned}
B_x &= \langle S_x \rangle = \mathrm{tr}(\rho_s \sigma_x) \\
B_y &= \langle S_y \rangle = \mathrm{tr}(\rho_s \sigma_y) \\
B_z &= \langle S_z \rangle = \mathrm{tr}(\rho_s \sigma_z),
\end{aligned} \tag{6}$$

where σ_x, σ_y, and σ_z are the Pauli matrices. Since they are expected values of local operators, they satisfy our definition of a thermodynamic property. Additionally, they completely determine the thermodynamic state, considering that the reduced density matrix can be expressed in terms of the Bloch vector components in the following way:

$$\rho_s = \frac{1}{2}[1 + \vec{B} \cdot \vec{\sigma}] = \frac{1}{2} \begin{pmatrix} 1 + B_z & B_x - iB_y \\ B_x + iB_y & 1 - B_z \end{pmatrix}, \tag{7}$$

where $\vec{\sigma}$ is the vector whose components are the Pauli matrices. This implies that any other conceivable thermodynamic property (in particular the temperature) must be a function of

them. For example, the dimensionless von Neumann entropy can be expressed in terms of the modulus of the Bloch vector B as:

$$\frac{S_{vN}}{k_B} = -\left(\frac{1+B}{2}\right)\ln\left(\frac{1+B}{2}\right) - \left(\frac{1-B}{2}\right)\ln\left(\frac{1-B}{2}\right). \tag{8}$$

B. Internal energy, heat, and work

The unitary evolution of the total system (qubit plus environment) is governed by a Hamiltonian H, which in the general case can be written as:

$$H = H_S + H_E + H_{\text{int}}, \tag{9}$$

where H_S is the qubit Hamiltonian, H_E is the Hamiltonian of the environment, and H_{int} describes the interaction between both systems. Note that the qubit Hamiltonian H_S can be written as a linear combination of the Pauli matrices, aside from a scalar multiple of the identity, without physical consequences since it represents a shift in the energy eigenvalues:

$$H_S = -\vec{v} \cdot \vec{\sigma}, \tag{10}$$

where $\vec{v}$ is a vector which can be associated to an effective magnetic field. Note also that $\pm|\vec{v}|$ are the eigenenergies of the system.

In the weak-coupling limit, the internal energy can be obtained using Eqs. (3), (7), and (10) and with the help of the identity:

$$(\vec{a} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) = (\vec{a} \cdot \vec{b})I + i\vec{\sigma} \cdot (\vec{a} \times \vec{b}), \tag{11}$$

resulting in:

$$E = -\vec{B} \cdot \vec{v}, \tag{12}$$

i.e., the projection of the Bloch vector on the effective magnetic field. If the Hamiltonian is time dependent, then we can write an infinitesimal change in the internal energy as:

$$dE = -d\vec{B} \cdot \vec{v} - \vec{B} \cdot d\vec{v}. \tag{13}$$

As usual, we identify the energy change due to variations in the reduced state as *heat* [12]:

$$\delta Q = -d\vec{B} \cdot \vec{v}. \tag{14}$$

Since an isolated qubit undergoes an unitary evolution, and therefore $d\vec{B} \perp \vec{v}$, we verify that in this case $\delta Q = 0$, as expected. We also identify the energy change associated to our possible control over the temporal evolution of the Hamiltonian, as *work*:

$$\delta W = -\vec{B} \cdot d\vec{v}. \tag{15}$$

Clearly, Eq. (13) can be considered as a statement of the first law of thermodynamics in the quantum regime:

$$dE = \delta Q + \delta W. \tag{16}$$

III. RESULTS

A. Temperature

If we assume that the von Neumann entropy, Eq. (8), is a valid extension of the statistical entropy in the quantum regime, then we can use Eq. (1) to obtain the temperature.
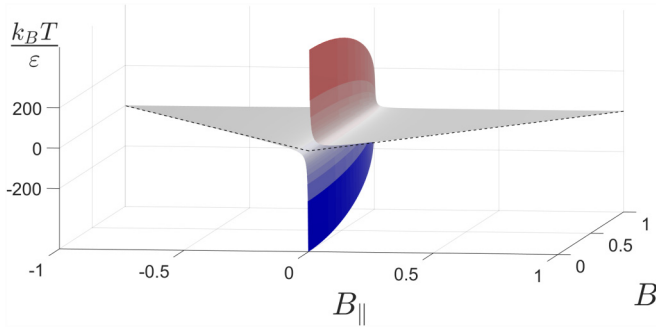
FIG. 1. Dimensionless qubit's temperature $k_B T/\varepsilon$ as a function of the modulus B and the z component $B_\parallel$ of the Bloch vector.

We note that the internal energy, Eq. (12), can be expressed in terms of the projection $B_\parallel = \vec{B} \cdot \hat{v}$ of the Bloch vector on the direction $\hat{v}$:

$$E = -|\vec{v}| B_\parallel, \qquad (17)$$

and therefore

$$\frac{1}{T} = -\frac{1}{|\vec{v}|} \frac{\partial S_{vN}}{\partial B_\parallel} \bigg|_{B_\perp}. \qquad (18)$$

Since $\frac{dS_{vN}}{dB} = -k_B \tanh^{-1}(B)$ and $\frac{\partial B}{\partial B_\parallel}|_{B_\perp} = \frac{B_\parallel}{B}$, the expression for the temperature is

$$T = \frac{\varepsilon B}{k_B B_\parallel \tanh^{-1}(B)}, \qquad (19)$$

where we have denoted the eigenenergy $|\vec{v}|$ by ε. Since entropy and energy are defined for equilibrium and out-of-equilibrium states, Eq. (19) applies in both cases, allowing us to obtain the qubit's temperature as a function of the reduced state and the instantaneous Hamiltonian.

Let us consider, as usual in physical implementations, of the qubit as a spin in a magnetic field pointing along the z direction. Therefore, the Hamiltonian adopts the form

$$H_S = -\varepsilon \sigma_z. \qquad (20)$$

In Fig. 1 we plot the qubit's temperature as a function of B and $B_\parallel$. Two branches are appreciated, one associated to positive temperature states (for $B_\parallel > 0$), and the other to negative temperature states (for $B_\parallel < 0$). This means that the spin's temperature is positive if the projection of the Bloch vector on the z direction is aligned with the field, negative in the opposite case, and undefined if the expected value is zero (in this case, the temperature diverges to $\pm\infty$ as $B_\parallel$ goes to $0^\pm$).

B. Consistency with the equilibrium temperature

If the system reaches thermal equilibrium with a reservoir at positive temperature T_E, then the time-averaged reduced state adopts the form [13,14]:

$$\overline{\rho}_S = \frac{e^{-\beta_E H_S}}{\text{tr}(e^{-\beta_E H_S})}, \qquad (21)$$

where $\beta_E = (k_B T_E)^{-1}$. In this case, Eq. (7) reduces to

$$\overline{\rho}_S = \frac{1}{2}[1 + \vec{B}_{\text{eq}} \cdot \vec{\sigma}], \qquad (22)$$
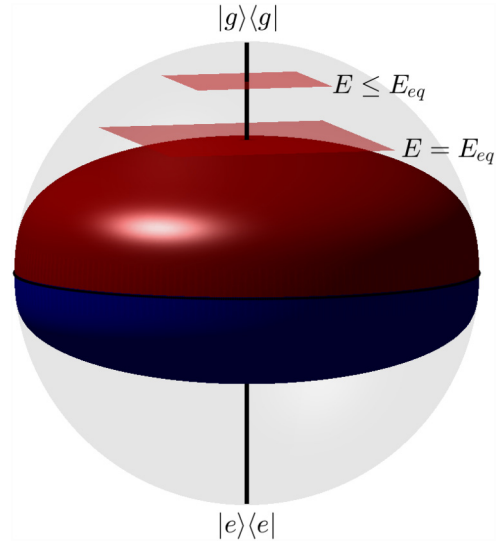

FIG. 2. Isothermal surfaces in the Bloch sphere, corresponding to the values of dimensionless temperature $k_B T_1/\varepsilon = 1.5$ (red, northern hemisphere) and $k_B T_2/\varepsilon = -2$ (blue, southern hemisphere). Two constant energy planes are also shown, one tangent to the isotherm $k_B T_1/\varepsilon = 1.5$, which is associated to the equilibrium energy E_{eq}, and another associated to an energy smaller than E_{eq}.

so the Bloch vector points along the $\hat{v}$ direction and, after some calculation we see that it has a modulus:

$$B_{\text{eq}} = \tanh\left(\frac{\varepsilon}{k_B T_E}\right), \qquad (23)$$

so the environment temperature can be expressed in terms of the modulus of the equilibrium Bloch vector as:

$$T_E = \frac{\varepsilon}{k_B \tanh^{-1}(B_{\text{eq}})}. \qquad (24)$$

Observe that since in this case $B = B_\parallel = B_{\text{eq}}$, the qubit's temperature, Eq. (19), coincides with the environment temperature, Eq. (24). In this case, considering Eq. (20), one notes that the natural populations, i.e., the eigenvalues of the reduced density matrix ($\lambda_{+/-} = 1/2 \pm B/2$) are the equilibrium populations P_g and P_e of the ground and excited states, respectively, so we reobtain the typical relation between the environment temperature and the populations:

$$T_E = T = \frac{2\varepsilon}{k_B \ln\left(\frac{P_g}{P_e}\right)}. \qquad (25)$$

The second equality of Eq. (25) and other similar relations are usually employed outside the equilibrium situation, when the introduction of an "effective temperature" is useful in order to characterize the evolution of the system [15–23].

Fixing the temperature, Eq. (24) allows to construct the isothermal surfaces on the Bloch sphere, two of which are represented in Fig. 2. The larger the value of the temperature, the lower the curvature of the corresponding isothermal surface, and as T increases, the surfaces converge to the maximum circle located in the horizontal plane. The surface of the sphere is also an isothermal surface, corresponding to temperature 0, except for the equator, located in the $z = 0$ plane, in which the temperature is not defined. There are also represented

two constant energy planes. The lower one corresponds to the energy of the system in its thermal equilibrium state, E_{eq}, when the system is embedded in an environment at temperature T_1. Such state is located at the intersection of the corresponding isothermal surface with the vertical diameter. Note that the upper plane does not intersect the isothermal surface, so energy values lower than that of the equilibrium at a certain temperature are only compatible with also lower values of the temperature.

C. Internal entropy production

At the macroscopic level irreversible processes are accompanied by a positive entropy production δS_{gen}, which for a system that undergoes an infinitesimal process exchanging only energy with the environment is defined, in terms of the entropy change dS, and the entropy flux associated to the heat exchanged, $\delta Q/T$, as follows:

$$\delta S_{\text{gen}} = dS - \frac{\delta Q}{T}, \tag{26}$$

where T is the temperature of the surface region where heat exchange takes place. Usually, heat reservoirs are modeled as internally reversible, which means that no entropy is produced in their interior. This implies that if we consider a control volume that includes the system we are studying, and whose boundary is at the temperature of the heat reservoir, application of Eq. (26) allows us to obtain the total entropy generated. This value includes the entropy produced due to irreversible heat transfer (if the temperature difference across the boundary is not infinitesimal) and eventually contributions associated to internal irreversibilities inside the system of interest. In what follows, we will see that our notion of temperature allows us to evaluate these contributions to the total entropy production.

For an arbitrary infinitesimal change in the modulus of the Bloch vector, from Eq. (8) the total entropy change of the qubit is

$$dS_{vN} = -k_B \tanh^{-1}(B)dB. \tag{27}$$

Let us consider the unit vectors $\hat{B} = \vec{B}/B$ and $\hat{v} = \vec{v}/\varepsilon$. Since $dB = \hat{B} \cdot d\vec{B}$, and expressing $\hat{B}$ in terms of its projections along the direction of $\hat{v}$ and its orthogonal complement, we obtain

$$dS_{vN} = -k_B \tanh^{-1}(B)[(\hat{v} \cdot \hat{B})\hat{v} + (\hat{B} - (\hat{v} \cdot \hat{B})\hat{v})] \cdot d\vec{B}. \tag{28}$$

Using Eqs. (14) and (19), the first term on the right-hand side of the equation above is

$$-k_B \tanh^{-1}(B)(\hat{v} \cdot \hat{B})\hat{v} \cdot d\vec{B} = \frac{\delta Q}{T}. \tag{29}$$

Thus we arrive at:

$$\delta S_{\text{gen}}^{\text{int}} = dS_{vN} - \frac{\delta Q}{T}, \tag{30}$$

where we have defined the internal entropy production $\delta S_{\text{gen}}^{\text{int}}$ as

$$\delta S_{\text{gen}}^{\text{int}} \equiv -k_B \tanh^{-1}(B)[\hat{B} - (\hat{v} \cdot \hat{B})\hat{v}] \cdot d\vec{B}. \tag{31}$$

Unlike the previous discussion, in this case the temperature appearing in Eq. (30) is the qubit's temperature instead of the environment temperature, and, consequently, the corresponding entropy production is only a fraction of the total entropy production, since the latter also includes the irreversible heat transfer contribution associated to the possible finite temperature difference between the qubit and the environment. To clarify this point, we recall that at the quantum level the total entropy produced during a process is linked to the distance, measured in a particular way, between the initial and the equilibrium states of the system, in case the latter exists [24–26]. Specifically, Ref. [24] proposes that:

$$S_{\text{gen}}^{\text{tot}}(t) = k_B \{ D(\rho_S(0) \parallel \rho_S^{\text{eq}}) - D[\rho_S(t) \parallel \rho_S^{\text{eq}}] \}, \tag{32}$$

where $D(\rho \parallel \rho') = \text{tr}(\rho \ln \rho) - \text{tr}(\rho \ln \rho')$ is the Kullbak-Leibler divergence (relative entropy) of the states ρ and ρ', and ρ_S^{eq} is the equilibrium state. Assuming that the equilibrium state is the thermal state at the environment temperature T_E, it is straightforward to see that:

$$\delta S_{\text{gen}}^{\text{tot}} = dS_{vN} - \frac{\delta Q}{T_E}. \tag{33}$$

Then, using Eqs. (30) and (33), we obtain:

$$\delta S_{\text{gen}}^{\text{tot}} = \delta S_{\text{gen}}^{\text{ht}} + \delta S_{\text{gen}}^{\text{int}}, \tag{34}$$

where we have defined

$$\delta S_{\text{gen}}^{\text{ht}} = \delta Q \left(\frac{1}{T} - \frac{1}{T_E} \right). \tag{35}$$

Equation (35) can be interpreted as the entropy production due the heat transfer at the system's boundary, since this term cancels when the temperatures of the system and the environment coincide or when the heat exchanged is zero. This confirms that the second term of Eq. (34), $\delta S_{\text{gen}}^{\text{int}}$, must be associated exclusively to internal irreversibilities. The classification of the total entropy production in the internal and boundary contributions is the standard procedure in classical thermodynamics, and it is plausible also in quantum mechanics provided that the temperatures are well defined. However, the existence of an intrinsic entropy generation even for such a simple quantum system is a rather remarkable fact, and some of its relevant aspects are discussed in Appendix.

D. Heat capacity

All qubit states located on a isothermal surface $T = \text{const}$ are out of equilibrium except for the thermal state, for which the Bloch vector points in the direction of the applied field (the vertical diameter). On the other hand, Eq. (12) shows that the constant energy surfaces are horizontal planes such that energy decreases with height. Observing Fig. 2, it is easy to conclude that from all the states at a given temperature, the equilibrium state is the one of least energy.

In order to formalize these ideas, we proceed to obtain a general expression for the heat capacity of the system, as a function of the state. Typically, the heat capacity is defined considering a process in which the relevant work is zero (for example, a constant volume process for a compressible substance; or a constant magnetization process for a magnetic substance). If the direction of $\vec{v}$ is fixed, then the zero work
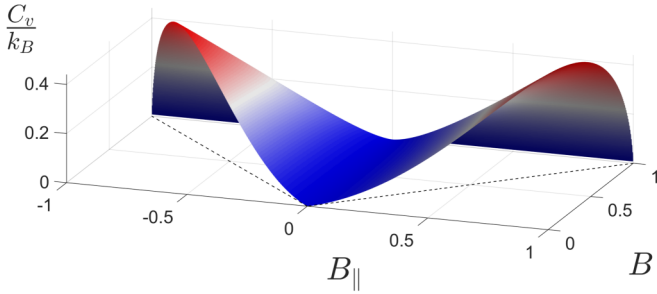
FIG. 3. Dimensionless heat capacity C_ε/k_B, as a function of the state defined through the modulus and z component of the Bloch vector.

condition implies that the eigenenergy ε is fixed, so in general it makes sense to define:

$$C_\varepsilon = \left(\frac{\partial E}{\partial T}\right)_\varepsilon. \tag{36}$$

But the energy depends only on the $B_\parallel$ component, $E = -\varepsilon B_\parallel$, so we obtain:

$$C_\varepsilon = -\varepsilon \left(\frac{\partial T}{\partial B_\parallel}\right)^{-1}. \tag{37}$$

After some algebra, the general expression for the qubit's heat capacity is

$$C_\varepsilon = \frac{k_B B(1 - B^2)[\tanh^{-1}(B)]^2 B_\parallel^2}{\tanh^{-1}(B)(B^2 - B_\parallel^2)(1 - B^2) + BB_\parallel^2}. \tag{38}$$

It is interesting to test the behavior of a well-known particular case. For the equilibrium states of the system at positive temperature we have that $B = B_\parallel$; in this case:

$$C_\varepsilon = k_B(1 - B^2)[\tanh^{-1}(B)]^2. \tag{39}$$

But as we have seen, the modulus of the equilibrium Bloch vector is defined by the environment temperature, which coincides in this case with the temperature of the qubit:

$$B = \tanh\left(\frac{\varepsilon}{k_B T}\right) \tag{40}$$

so we obtain:

$$C_\varepsilon = k_B \left[\frac{\varepsilon/k_B T}{\cosh(\varepsilon/k_B T)}\right]^2. \tag{41}$$

Equation (41) is the well-known expression for the specific heat of a two-level system at thermal equilibrium, which shows once again the consistency of the theory with the equilibrium case [27].

More in general, we note that since $|B_\parallel| \leqslant B \leqslant 1$, Eq. (38) always leads to $C_\varepsilon \geqslant 0$ (see Fig. 3).

We also notice that pure states, and those located on the plane $B_\parallel = 0$, have zero heat capacity. This implies that, for these states, very small energy variations are able to produce large temperature changes, which agrees with our previous observations on the temperature behavior.

Particularly remarkable also is the fact that, for any process starting from a zero temperature state ($B = 1$), and evolving toward an infinite temperature state ($B_\parallel = 0$), the value of

the heat capacity increases from zero, reaches a maximum value, and then diminishes and tends asymptotically to zero. This effect, known as the *Schottky anomaly* is well known in equilibrium statistical mechanics and typically occurs in systems with a finite number of energy levels [28]. The analysis of Fig. 3 shows that the effect is present even in the out-of-equilibrium situation. In particular, C_ε presents two global maxima in the regions $B = B_\parallel$ and $B = -B_\parallel$, with values:

$$C_\varepsilon^{\max} \simeq 0.4392, \tag{42}$$

in agreement with the known result for a two level system in thermal equilibrium [27].

In the following section we will apply these results to some simple two-level models, with emphasis in the behavior of the temperature and the internal entropy production.

IV. APPLICATIONS

A. Two two-level atoms exchanging photons

Let us consider a system S composed of two two-level atoms separated a distance R and embedded in a common thermostat at zero temperature. If we focus on the case where only spontaneous emission is taken into account, then the system undergoes a dissipative process governed by the Markovian master equation [29]

$$\frac{\partial \rho}{\partial t} = \frac{1}{2} \sum_{k,l=A,B} \gamma_{kl}(2\sigma_-^k \rho \sigma_+^l - \sigma_+^k \sigma_- \rho - \rho \sigma_+^k \sigma_-^k), \tag{43}$$

where

$$\sigma_\pm^A = \sigma_\pm \otimes \mathbb{I}_2, \quad \sigma_\pm^B = \mathbb{I}_2 \otimes \sigma_\pm \quad \sigma_\pm = \tfrac{1}{2}(\sigma_x + i\sigma_y). \tag{44}$$

Above, $\gamma_{AA} = \gamma_{BB} = \gamma_0$ is the single atom spontaneous emission rate, and $\gamma_{AB} = \gamma_{BA} = \gamma = g(R)\gamma_0 \leqslant \gamma_0$ is the photon-exchange relaxation constant, where the function $g(R)$ approaches 1 as $R \to 0$.

The explicit solution of Eq. (43) for an arbitrary initial density matrix can be found in Ref. [29], where it is used to evaluate the level of transient entanglement produced between the atoms due to the photons exchange. Here we are interested in the thermodynamic aspects of the evolution, so we consider such exchange as a heat transfer process between the atoms, with losses to the environment. This is so because considering the atoms at different locations implies that $\gamma < \gamma_0$, and consequently, the system composed of both atoms loses energy and asymptotically relaxes toward the product of the ground states, $|0\rangle \otimes |0\rangle$, regardless of the initial state. This kind of process is adequate to study the behavior of the temperature definition proposed in this work.

In Fig. 4 we present the comparative time evolution of the temperatures and internal energies for both atoms. The global initial state is a product state, with atom a in its ground state ($E_a/\varepsilon = -1$, $T_a = 0$), and atom b in a mixed state such that $E_b = -0.8$, $T_2 > 0$. Initially atom a absorbs a fraction of the energy emitted by atom b, while its own emission is negligible, since it starts from the ground state, so both its energy and temperature grow. Meanwhile, atom b releases energy and its temperature decreases. At some point, T_a is large enough, and T_b low enough, so that the emission by atom
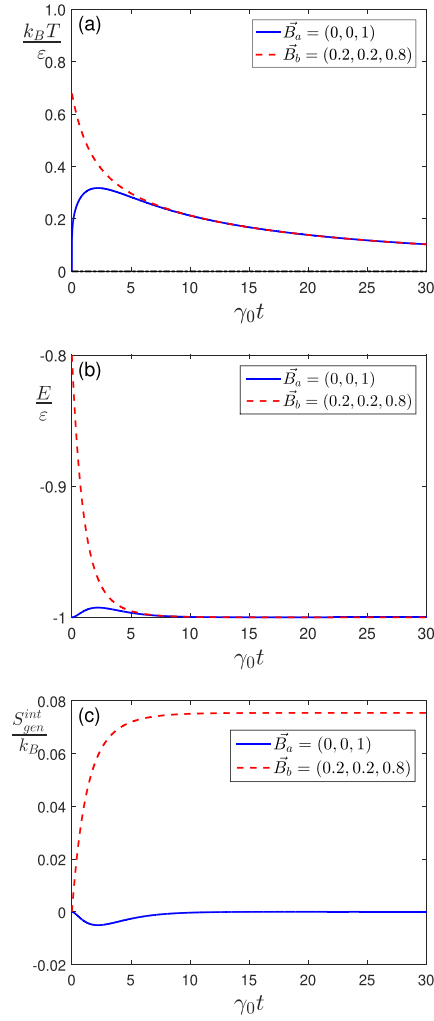
FIG. 4. Temperature, internal energy, and entropy production time evolutions, as a function of $\gamma_0 t$ for two interacting two-level atoms a and b. (a) Dimensionless temperature $k_B T/\varepsilon$. (b) Dimensionless internal energies E/ε. (c) Dimensionless internal entropy production. The initial reduced state is a product state of local densities defined by the Bloch vectors $\vec{B}_a = (0, 0, 1)$ and $\vec{B}_b = (0.2, 0.2, 0.8)$, and $g(R) = \gamma/\gamma_0 = 0.5$. The environment temperature is zero (black dash-dotted line.)

a exceeds its absorption, so T_a and E_a reach a maximum value simultaneously and subsequently start to decrease. Finally, we observe that thermal equilibrium between the atoms occurs before thermal equilibrium with the environment. In fact, once T_a equals T_b, no energy flux occurs between the atoms and the composed system behaves as a unique system since the temperature and energy of both atoms are the same for all subsequent times. From this moment onward, they cool together and thermalize with the environment. This behavior is reminiscent of the one that undergo two macroscopic bodies at different temperatures in thermal contact between them, and with an environment at a temperature less than or equal to the lowest of those of the systems involved.

Note that, although the internal entropy generated associated to atom a has a negative initial transient, the sum of the contributions of both atoms is monotonically increasing. The

decrease in entropy of atom a is associated to the fact that it was initially in thermal equilibrium, so when it interacts with atom b it starts moving away from the z axis. Since the variation of the distance to this axis is a measure of the internal entropy generated (see Appendix), this explains the excursion into negative entropy values in the case of this atom.

B. Two-level system interacting with a heat reservoir: The Jaynes-Cummings model

The interaction between a two-level atom and the electromagnetic field is described by the multimode Jaynes-Cummings Hamiltonian:

$$H = \frac{\hbar}{2}\omega_0 \sigma_z + \hbar \sum_k [\omega_k b_k^\dagger b_k + \lambda_k \sigma_+ b_k + \lambda_k^* \sigma_- b_k^\dagger], \quad (45)$$

where b_k and $b_k^\dagger$ are the creation and annihilation operators associated to the kth mode of the field with frequency ω_k and coupling constant λ_k, and w_0 is the atomic transition frequency.

For thermal radiation at temperature T_E, explicit expressions for the elements of the atom's reduced density matrix, in the weak-coupling and low-temperature approximation, can be found in Ref. [30]. The analysis of this expression shows that, independently of the initial state, the atom reaches thermal equilibrium with the field at the temperature

$$k_B T_{\text{eq}} = \frac{\hbar\omega_0}{\tanh^{-1}\left[1 - 2\exp\left(-\frac{\hbar\omega_0}{k_B T_E}\right)\right]}. \quad (46)$$

The transition to equilibrium is shown in Fig. 5, where we plot the atom's temperature, its internal energy, and the internal entropy production. Since the temperature of the environment changes during the evolution in an unknown way, the evaluation of the total entropy production cannot be performed. Nevertheless, the growing behavior of the internal entropy production can be appreciated.

More interesting conclusions arise if one studies the system under the Markovian approximation, valid in the limit of high temperature. In Ref. [24] it is shown that the master equation for the atom in the interaction picture is

$$\frac{\partial \rho_s}{\partial t} = \gamma_0(\mathcal{N}+1)\left(\sigma_-\rho\sigma_+ - \frac{1}{2}\sigma_+\sigma_-\rho - \frac{1}{2}\rho\sigma_+\sigma_-\right)$$
$$+ \gamma_0\mathcal{N}\left(\sigma_+\rho\sigma_- - \frac{1}{2}\sigma_-\sigma_+\rho - \frac{1}{2}\rho\sigma_-\sigma_+\right), \quad (47)$$

where γ_0 is the spontaneous emission rate and $\mathcal{N}$ is the Planck distribution at the transition frequency ω_0:

$$\mathcal{N} = \frac{1}{e^{\beta_E \hbar\omega_0} - 1}. \quad (48)$$

The master equation can be solved with the help of Pauli matrices algebra, and the explicit components of the Bloch vector can be found in Ref. [24]. With the time dependence of the three basic thermodynamic properties at hand, we can implement the thermodynamic analysis of the model.

In Fig. 6 we plot the dimensionless atom's temperature, Eq. (19), and the dimensionless internal energy for two different initial states. Note that if the initial temperature is greater than the environment temperature T_E, the internal energy
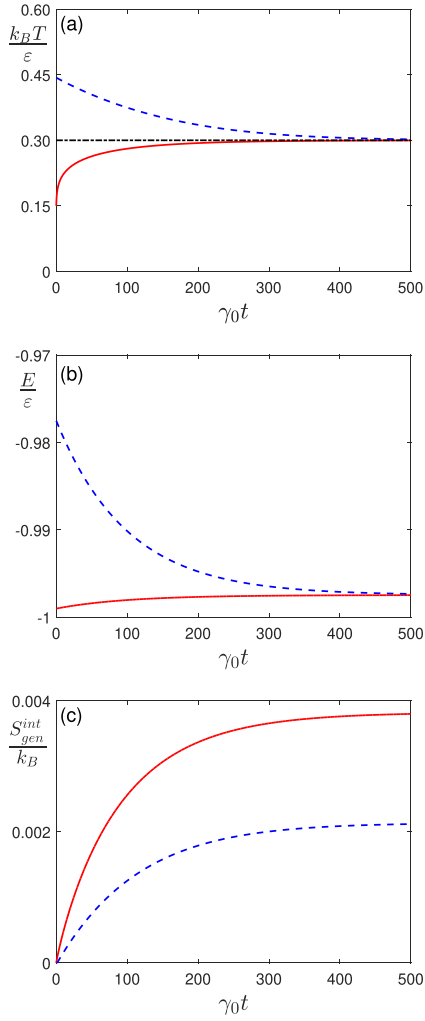
FIG. 5. Temperature, internal energy, and entropy time evolutions for a two level-system interacting with a heat reservoir. (a) Dimensionless temperature $\frac{k_B T}{\varepsilon}$, as a function of $\gamma_0 t$. (b) Dimensionless internal energy $\frac{E}{\varepsilon}$. (c) Internal entropy production, in units of k_B. The temperatures of the initial states considered are $0.5 T_{eq}$ (red full line) and $1.5 T_{eq}$ (blue dashed line). The initial environment temperature is $k_B T_e / \varepsilon = 0.15$. The equilibrium temperature of the system is represented by the black dash-dotted line.
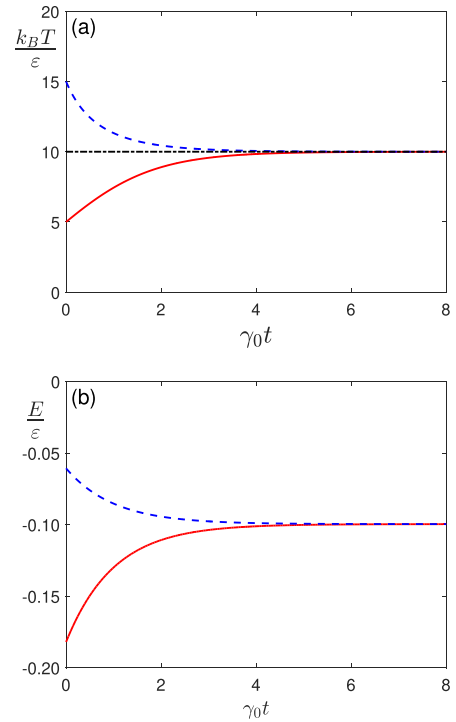

FIG. 6. Temperature and internal energy evolution of a two-level system interacting with the reservoir within the Markovian approximation. (a) Dimensionless temperature $\frac{k_B T}{\varepsilon}$. (b) Dimensionless internal energy $\frac{E}{\varepsilon}$ as a function of $\gamma_0 t$. The time evolution of the internal entropy generated for this system is shown in Fig. 6(a). The dimensionless environment temperature is 10 (black dash-dotted line), and the initial states considered are selected in such a way that the qubit's initial dimensionless temperatures are 5 (red full line) and 15 (blue dashed line).

decreases in time. This implies that the system releases heat to the environment. On the other hand, for an initial temperature lower that T_E, the internal energy increases, so the system receives heat from the reservoir. As expected, when the asymptotic state is reached, in all cases the qubit's temperature coincides with the environment temperature. These observations leads to consider Eq. (19) as a real indicator of how "warm" the qubit finds itself in the corresponding reduced state.

In this case, a complete entropy balance is possible since the environment remains at constant, finite temperature during the process. This allows to separate the total entropy production into its internal [Eq. (31), Fig. 7(a)] and boundary [Eq. (35), Fig. 7(b)] contributions, as well as their sum [Fig. 7(c)]. The monotonically increasing behavior of these three quantities is verified in Fig. 7.

The situation in which the system starts with the same temperature as the environment but in an out-of-equilibrium

state was also studied. For all initial states considered satisfying this condition, the evolution of the system is essentially isothermal, as can be seen in Fig. 8. This results, as in the classical case, in the reversibility of the heat transfer, and as a consequence, that the boundary contribution to the total entropy production is negligible. In this case, the growing behavior of the total entropy production, and of the correlations between the system and the bath, can be understood in a purely geometrical way, since they are due exclusively to the tendency of the Bloch vector to point along the z direction, reducing the Euclidean distance between the point representing the reduced state, and the z axis.

The fact that systems in out-of-equilibrium states with a temperature given by Eq. (19) that coincides with the environment temperature, evolve on isothermal surfaces is rather remarkable, and in our opinion is a strong argument in favor of adopting that expression as the qubit's temperature.

V. FINAL REMARKS AND CONCLUSIONS

In this work we have presented a natural extension of the temperature concept, valid for two-dimensional open quantum systems in generic out-of-equilibrium processes, under the hypothesis of weak interaction with the environment. The construction is based on the fact that the von Neumann
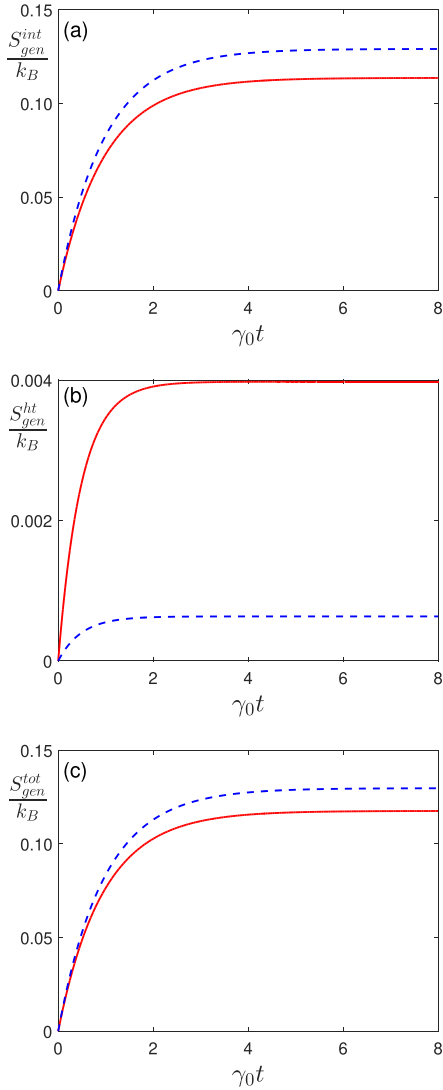
FIG. 7. Components of the entropy production for a two-level system interacting with a heat reservoir. (a) Internal entropy production. (b) Entropy production due to heat transfer. (c) Total entropy production, in units of k_B. The initial states and respective illustration codes are the same of Fig. 6.
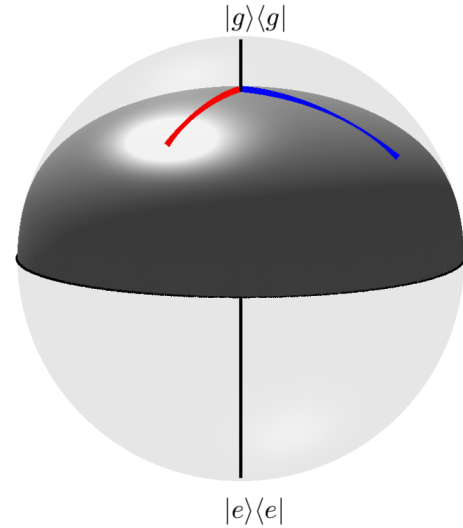

FIG. 8. Isothermal trajectories in the Bloch sphere. The trajectories represented correspond to the initial value $k_B T/\varepsilon = 1$ and remain very close to the isothermal surface. For large t they reach the thermal state located on the z axis.

entropy and the expected value of the Hamiltonian are well-defined in the out-of-equilibrium situation.

The use of the von Neumann entropy guarantees consistency with the equilibrium temperature when thermal equilibrium states are considered. In the model systems analyzed, this temperature has a behavior that is reminiscent of the classical behavior, correctly indicating the senses of the heat fluxes between initially uncorrelated systems.

We have observed that the adoption of this temperature allows to identify the internal and heat transfer contributions to the total entropy production. Although the geometrical interpretation of the internal entropy generated is clear, the understanding of the physical reasons associated to the existence of internal irreversibilities requires further analysis, as well as its interpretation from the information-theoretical perspective. A first step in this study is given in Appendix A 1, where we show that, for a system of two qubits, the total

entropy generated can be directly put into correspondence with the change in quantum mutual information between the qubits. Furthermore, in Appendix A 2 we show that the internal entropy contribution to the total generated entropy can be measured through the loss of quantum coherence in each of the qubits.

We have also obtained an explicit expression for the heat capacity of the system as a function of the state. The resulting expression is non-negative for all possible states, assuring the standard relation between heat fluxes and temperature when no work is involved. It also allows to recover the results obtained in the thermal equilibrium situation, such as the Schottky anomaly, and to show the existence of a similar behavior outside equilibrium.

The exploration of this theoretical framework for other two-level models is currently under investigation, as well as its implications in relevant tasks, such as work extraction. Generalizations to quantum systems with a more complex structure are also been considered.

ACKNOWLEDGMENTS

APPENDIX: ABOUT THE INTERNAL ENTROPY PRODUCTION, EQ. (31)

1. Entropy production and correlations in a two-qubit system

Note that Eq. (34) does not include internal entropy production associated to the reservoir. It is an approximation valid in the limit of a large heat bath, so that it is reasonable to assume that it remains in the canonical state at temperature T_E during the process (which is consistent with the internal

reversibility hypothesis of thermal reservoirs in macroscopic systems). But in the case of interactions with a finite environment, the existence of an additional term of internal entropy production is expected. This can be illustrated considering the limit case: a system composed of two qubits. We start from the following identity for the von Neumann entropy (denoted by S) of a bipartite system AB:

$$S_A + S_B - S_{AB} = I(A:B) \geqslant 0, \qquad (A1)$$

where $I(A:B)$ is the *quantum mutual information*:

$$I(A:B) = D(\rho_{AB} \parallel \rho_A \otimes \rho_B), \qquad (A2)$$

and represents a measure of the total correlations (quantum and classical) between A and B [31].

Each system satisfies the relation:

$$dS_{A/B} = \frac{\delta Q_{A/B}}{T_{A/B}} + \delta S^{\text{int}}_{\text{gen}(A/B)}, \qquad (A3)$$

so integrating in time and replacing in Eq. (A1), we obtain:

$$\int_0^t \frac{\delta Q_A}{T_A} + S^{\text{int}}_{\text{gen}(A)}(t) + \int_0^t \frac{\delta Q_B}{T_B} + S^{\text{int}}_{\text{gen}(B)}(t)$$
$$= I(A:B)(t) - [S_A(0) + S_B(0) - S_{AB}(t)]. \qquad (A4)$$

Since entropy is preserved by the unitary evolution of the global system, we have that $S_{AB}(t) = S_{AB}(0)$, and we can identify the terms between brackets on the right-hand side of the last equation as the initial mutual information: $I(A:B)(0) = S_A(0) + S_B(0) - S_{AB}(0)$. Then, using that $\delta Q_A = -\delta Q_B \equiv \delta Q$, it follows that:

$$S^{\text{int}}_{\text{gen}(A)}(t) + \int_0^t \delta Q\left(\frac{1}{T_A} - \frac{1}{T_B}\right) + S^{\text{int}}_{\text{gen}(B)}(t)$$
$$= I(A:B)(t) - I(A:B)(0). \qquad (A5)$$

As before, we can interpret the second term as the entropy production due to heat transfer, $S^{\text{ht}}_{\text{gen}}$. So we conclude that the total entropy production can be obtained by adding the internal contributions produced in each system plus the boundary term, and it equals the change of mutual information:

$$S^{\text{tot}}_{\text{gen}} = S^{\text{int}}_{\text{gen}(A)} + S^{\text{int}}_{\text{gen}(B)} + S^{\text{ht}}_{\text{gen}} = \Delta I(A:B). \qquad (A6)$$

Equation (A6) establishes, for the present system, the equivalence between the production of entropy and the creation of correlations. The relation between both phenomena has been reported in Ref. [32], for a system placed in contact with one (or several) reservoirs, each one of them in a thermal state.

Observe that if $I(A:B)(0) = 0$, i.e., in absence of initial correlations, then the non-negativity of the mutual information leads to:

$$S^{\text{tot}}_{\text{gen}} = S^{\text{int}}_{\text{gen}(A)} + S^{\text{int}}_{\text{gen}(B)} + S^{\text{ht}}_{\text{gen}} \geqslant 0 \qquad (A7)$$

and the non-negativity of the entropy production is guaranteed. The observation that previous correlations (i.e., before the systems are placed in interaction) must be negligible for the second law to be true in its classical form can be tracked to Boltzmann himself [33].

Nevertheless, in the case of initially correlated systems, it is known that mutual information can decrease, and violations of the classical statements of the second law are expected. In

particular, the existence of an anomalous heat flow (from a low temperature to a high temperature) has been predicted [34,35], and experimentally demonstrated in the case of a two-qubit system, prepared in a correlated initial state such that the marginal states are thermal [36]. Such anomalous heat flow does not necessarily imply an inversion of the arrow of time, since the system can be understood as acting as a refrigerator, using the work potential stored in the correlations [37]. Moreover, it has been shown that no system-bath correlations are necessary in order to reverse the heat flow, but only internal correlations associated to quantum coherences [38].

The interplay between correlations, entropy production and work extraction in quantum systems is an active field of research, with major implications in our theoretical understanding of the physical world [39–44].

2. Internal entropy production as coherence loss

In order to give a physical interpretation to the internal entropy production, it is convenient to express Eq. (31) in spherical coordinates. Choosing the z axis in the direction $\hat{v}$ (now considered fixed), and setting $d\vec{B} = dB\hat{B} + Bd\theta\hat{e}_\theta + B\sin\theta d\varphi\hat{e}_\varphi$, we obtain:

$$\delta S^{\text{int}}_{\text{gen}} = -k_B \tanh^{-1}(B)\sin\theta[dB\sin\theta + B\cos\theta d\theta]. \quad (A8)$$

Since $dB\sin\theta + B\cos\theta d\theta = d(B\sin\theta)$, and $B\sin\theta$ is the Euclidean distance between the point representing the reduced state and the z axis, which coincides with the value of the coherence of the state measured using the l_1 norm, C_{l_1} [45]:

$$C_{l_1} \equiv \sum_{i \neq j} |\rho_{S_{ij}}| = B\sin\theta, \qquad (A9)$$

we can write:

$$\delta S^{\text{int}}_{\text{gen}} = -k_B \tanh^{-1}(B)\sin\theta dC_{l_1}. \qquad (A10)$$

We note that in the case that the system evolves over incoherent states, $\vec{B} \propto \vec{v}$, $\sin\theta = 0$, no entropy is produced. In this case total reversibility is not assured, since the temperatures of the system and the environment may be different, which would imply an irreversible heat transfer. However, if the system is initially in thermal equilibrium, and the temperature of the environment changes slowly enough for the system to stay in thermal equilibrium throughout the process, then the heat transfer contribution to the total entropy production will be also zero. Such processes are frequently employed in the theoretical construction of quantum power cycles [46].

A second case of interest is when the evolution is unitary. In this case the Bloch vector rotates around $\hat{v}$ at constant angular speed, keeping its modulus and angle θ fixed. This implies that the coherence is constant, $dC_{l_1} = 0$, and consequently, $\delta S^{\text{int}}_{\text{gen}} = 0$, as in the previous case.

These two cases suggest that internal reversibility can be considered as equivalent to the preservation of the coherence. On the other hand, we note, considering Eq. (A10), that whenever coherence is lost, $dC_{l_1} < 0$, entropy is produced $\delta S^{\text{int}}_{\text{gen}} > 0$. This is typically the case when the system evolves toward an equilibrium state. The relation between entropy production and quantum coherence has been recently studied from a more general perspective in Ref. [47].

[1] A. Puglisi, A. Sarracino, and Vulpiani, Phys. Rep. **709–710**, 1 (2017).

[2] A. Abragam and W. G. Proctor, Phys. Rev. **109**, 1441 (1958).

[3] A. Romanelli, Phys. Rev. A **85**, 012319 (2012).

[4] J. Gemmer, M. Michel, and G. Mahler, *Quantum Thermodynamics: The Emergence of Thermodynamic Behavior within Composite Quantum Systems*, Lecture Notes in Physics (Springer, Berlin, 2004).

[5] M. Hartmann and G. Mahler, Europhys. Lett. **70**, 579 (2005).

[6] N. Brunner, N. Linden, S. Popescu, and P. Skrzypczyk, Phys. Rev. E **85**, 051117 (2012).

[7] C. L. Latune, I. Sinayskiy, and F. Petruccione, Quant. Sci. Technol. **4**, 025005 (2019).

[8] Md. Manirul Ali, W.-M. Huang, and W.-M. Zhang, arXiv:1803.04658v3 [quant-ph].

[9] S. Ghonge and D. Can Vural, J. Stat. Mech. (2018) 073102.

[10] H. J. D. Miller and J. Anders, Phys. Rev. E **95**, 062123 (2017).

[11] Y. A. Cengel and M. A. Boles, *Thermodynamics: An Engineering Approach*, 4th ed. (McGraw-Hill, New York, 2001), pp. 1056.

[12] T. D. Kieu, Phys. Rev. Lett. **93**, 140403 (2004).

[13] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghi, Phys. Rev. Lett. **96**, 050403 (2006).

[14] S. Popescu, A. Short, and A. Winter, Nat. Phys. **2**, 754 (2006).

[15] H. T. Quan, Y.-x. Liu, C. P. Sun, and F. Nori, Phys. Rev. E **76**, 031105 (2007).

[16] I. Serban, M. I. Dykman, and F. K. Wilhelm, Phys. Rev. A **81**, 022305 (2010).

[17] X. L. Huang, T. Wang, and X. X. Yi, Phys. Rev. E **86**, 051105 (2012).

[18] L. Du, Y. Yu, and D. Lan, Low Temp. Phys. **39**, 111 (2013).

[19] X. Y. Jin, A. Kamal, A. P. Sears, T. Gudmundsen, D. Hover, J. Miloshi, R. Slattery, F. Yan, J. Yoder, T. P. Orlando, S. Gustavsson, and W. D. Oliver, Phys. Rev. Lett. **114**, 240501 (2015).

[20] P. Doyeux, B. Leggio, R. Messina, and M. Antezza, Phys. Rev. E **93**, 022134 (2016).

[21] S. Das, A. Misra, A. Kumar Pal, A. Sen (De) and U. Sen, Europhys. Lett. **125**, 20007 (2019).

[22] M. O. Scully, M. Suhail Zubairy, G. S. Agarwal, and H. Walther, Science **299**, 862 (2003).

[23] H. T. Quan, P. Zhang, and C. P. Sun, Phys. Rev. E **73**, 036122 (2006).

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

[25] M. Brunelli, L. Fusco, R. Landig, W. Wieczorek, J. Hoelscher-Obermaier, G. Landi, F. L. Semiao, A. Ferraro, N. Kiesel, T.

Donner, G. De Chiara, and M. Paternostro, Phys. Rev. Lett. **121**, 160604 (2018).

[26] A. Vallejo, A. Romanelli, R. Donangelo, and R. Portugal, Phys. Rev. A **99**, 032319 (2019).

[27] S.-Y. Kim, J. Korean Phys. Soc. **65**, 970 (2014).

[28] S. Mahdavifar and A. Akbari, J. Phys. Soc. Jpn. **77**, 024710 (2008).

[29] L. Jakóbczyk and A. Jamróz, Phys. Lett. A **318**, 318 (2003).

[30] S. Shresta, C. Anastopoulos, A. Dragulescu, and B. L. Hu, Phys. Rev. A **71**, 022109 (2005).

[31] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).

[32] M. Esposito, K. Lindenberg, and C. Van den Broeck, New J. Phys. **12**, 013013 (2010).

[33] G. Vitagliano, C. Klöckl, M. Huber and N. Friis, Trade-off between work and correlations in quantum thermodynamics, in *Thermodynamics in the Quantum Regime*, edited by F. Binder, Fundamental Theories of Physics (Springer, Cham, 2019), Vol. 195.

[34] M. H. Partovi, Phys. Rev. E **77**, 021110 (2008).

[35] D. Jennings and T. Rudolph, Phys. Rev. E **81**, 061130 (2010).

[36] K. Micadei, J. P. S. Peterson, A. M. Souza, R. S. Sarthour, I. S. Oliveira, G. T. Landi, T. B. Batalhao, R. M. Serra, and E. Lutz, Nat. Commun. **10**, 2456 (2019).

[37] M. N. Bera, A. Riera, M. Lewenstein, and A. Winter, Nat. Commun. **8**, 2180 (2017).

[38] C. L. Latune, I. Sinayskiy, and F. Petruccione, Phys. Rev. Research **1**, 033097 (2019).

[39] P. Skrzypczyk, A. Short, and J. Popescu, Nat. Commun. **5**, 4185 (2014).

[40] J. M. R. Parrondo, J. M. Horowitz, and T. Sagawa, Nat. Phys. **11**, 131 (2015).

[41] F. Brandão, M. Horodecki, N. Ng, J. Oppenheim, and S. Wehner, Proc. Natl. Acad. Sci. USA **112**, 3275 (2015).

[42] J. Goold, M. Huber, A. Riera, L. del Rio, and P. Skrzypczyk, J. Phys. A **49**, 143001 (2016).

[43] S. Alipour, F. Benatti, F. Bakhshinezhad, M. Afsary, S. Marcantoni, and A. T. Rezakhani, Sci. Rep. **6**, 35568 (2016).

[44] G. Manzano, F. Plastina, and R. Zambrini, Phys. Rev. Lett. **121**, 120602 (2018).

[45] T. Baumgratz, M. Cramer, and M. B. Plenio, Phys. Rev. Lett. **113**, 140401 (2014).

[46] X. L. Huang, X. Y. Niu, X. M. Xiu, and X. X. Yi, Eur. Phys. J. D **68**, 32 (2014).

[47] J. P. Santos, L. C. Céleri, G. T. Landi, M. Paternostro, npj Quant. Info. **5**, 23 (2019).