Non-Markovianity through entropy-based quantum thermodynamics

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We introduce a generalized approach to characterize the non-Markovianity of quantum dynamical maps via breakdown of monotonicity of thermodynamic functions. By adopting an entropy-based formulation of quantum thermodynamics, we use the relationship between heat and entropy to propose a measure of non-Markovianity based on the heat flow for single-qubit quantum evolutions. This measure can be applied for unital dynamical maps that do not invert the sign of the internal energy. Under certain conditions, it can also be extended for other thermodynamic functions, such as internal energy and work flows. In this context, a natural connection between heat and quantum coherence can be identified for dynamical maps that are both unital and incoherent. As applications, we explore dissipative and nondissipative quantum dynamical processes, illustrating the compatibility between our thermodynamic quantifiers and the well-establish measure defined via quantum coherence.

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I. INTRODUCTION

Quantum thermodynamics [1,2] is a research field in the making, with fruitful conceptual implications and a potential range of applications, mainly in the field of quantum technologies (see, e.g., Ref. [3]). It aims at generalizing the laws of thermodynamics to the quantum domain, rewriting thermodynamic state functions and processes from the bottom up so that the laws of thermodynamics can be consistently applied to small systems and scaled up to the classical world [4-9]. Remarkably, the definitions of thermodynamic variables, such as work and heat, have been challenging, since they cannot be taken as observables described by Hermitian operators [10]. In the standard framework of quantum thermodynamics [11], the internal energy change due to state population rearrangement induced by the external environment has been defined as heat. On the other hand, the internal energy change due to energy gap variations induced by the coherent dynamics has been defined as work. This framework has recently been revisited through an entropy-based formulation for heat and work [12-14], with heat identified as the entropy-related contribution to the internal energy change and work taken as the part unrelated to the entropy change. In particular, this has been applied to the study of the thermodynamics of a single qubit far from equilibrium [15], where a notion of temperature compatible with the classical limit was introduced. The alternative entropy-based view turns out to motivate an interplay with quantum information, with the interpretation of thermodynamic variables in terms of resources and correlations in a quantum system.

Indeed, quantum thermodynamics is intrinsically connected with quantum information theory, with quantum resources strongly affecting thermodynamic variables and processes. This is manifested in a number of situations, such as measurements and their influence on the work performed on or by a quantum system [10,16–19], efficiency of thermodynamic tasks in quantum correlated devices [6,20–22], and coherence effects on work and heat [23–30], among others. By looking at information-based quantifiers, it is known that quantum coherence plays a relevant role in the characterization of system-bath memory effects. In particular, quantum coherence can be associated with a measure of non-Markovianity for incoherent dynamical maps [31–34]. Notice that a memoryless (Markovian) behavior is always an idealization, with non-Markovian quantum dynamics being non-negligible in a number of different scenarios (see, e.g., Refs. [35–37]). From an applied point of view, non-Markovian dynamics may also be a resource for certain quantum tasks [38,39].

In this work we adopt the entropy-based formulation of quantum thermodynamics to introduce a measure of non-Markovianity based on the heat flow for single-qubit quantum evolutions. This measure can be applied for unital dynamical maps that do not invert the sign of the internal energy (energy sign-preserving maps), which is rooted in the idea that von Neumann entropy itself can be used to build a non-Markovianity measure for unital maps [40]. Under certain conditions, we can also extend this approach to other thermodynamic functions, such as internal energy and work flows. Then a natural connection between heat and quantum coherence can be observed for dynamical maps that are both unital and incoherent. In particular, we show that heat and work are monotonically related to quantum coherence for nondissipative processes. Consequently, both heat and work can witness non-Markovianity for nondissipative unital maps as well as nondissipative incoherent maps. Moreover, we establish and illustrate the conditions over the system purity and the Hamiltonian such that the thermodynamic variables can be used to provide non-Markovianity measures throughout the evolution in a decohering environment.

The paper is organized as follows. In Sec. II we briefly introduce the entropy-based formulation of quantum thermodynamics, expressing the first law of thermodynamics and its corresponding thermodynamic variables for a single-qubit system. In Sec. III we discuss the non-Markovian dynamics, where we propose measures of non-Markovianity via generalized sign-preserving functions. In Sec. IV we consider applications in dissipative and nondissipative evolutions, illustrating the use of thermodynamic variables as measures of non-Markovianity. In Sec. V we summarize and present our conclusions.

II. QUANTUM THERMODYNAMICS

According to the standard framework for quantum thermodynamics [11], the internal energy U of a system described by a density operator ρ is provided by the expected value of its Hamiltonian H, i.e., $U = \text{tr}[\rho H]$. In this formalism, the first law of thermodynamics emerges from an infinitesimal change in the internal energy $dU = \delta Q + \delta W$, with $\delta Q = \text{tr}[d\rho H]$ and $\delta W = \text{tr}[\rho dH]$ defining the heat absorbed by system and the work performed on system, respectively. Considering the density operator as expressed in its spectral decomposition, we have $\rho = \sum_k r_k |r_k\rangle \langle r_k|$, where $|r_k\rangle$ denotes an eigenvector of ρ and r_k the corresponding eigenvalue. Then the thermodynamic quantities U, δQ , and δW can be rewritten as

$$U = \sum_{k} r_k \langle r_k | H | r_k \rangle, \tag{1}$$

$$\delta Q = \sum_{k} dr_k \langle r_k | H | r_k \rangle + \sum_{k} r_k (\langle r_k | H d | r_k \rangle + \text{H.c.}), \quad (2)$$

$$\delta W = \sum_{k} r_k \langle r_k | dH | r_k \rangle. \tag{3}$$

Note that the first term on the right-hand side of Eq. (2) is responsible for changes in the von Neumann entropy $S = -k_B \text{tr}[\rho \ln \rho]$ since $dS = -k_B \sum_k dr_k \ln r_k$. Therefore, in order to connect the heat flow with the entropy change as in classical thermodynamics, an entropy-based formulation of quantum thermodynamics has recently been introduced in Refs. [12–14]. In this framework, heat and work are redefined through

$$\delta \mathbb{Q} = \delta Q - \delta \mathbb{W}^* \tag{4}$$

and

$$\delta \mathbb{W} = \delta W + \delta \mathbb{W}^*, \tag{5}$$

where $\delta \mathbb{W}^*$ is an additional work contribution given by

$$\delta \mathbb{W}^* = \sum_k r_k (\langle r_k | Hd | r_k \rangle + \text{H.c.}).$$
(6)

The work $\delta \mathbb{W}^*$ is related to the variation $d|r_k\rangle$ of the density operator eigenvectors. Note that the entropy-based formalism satisfies the first law of thermodynamics, i.e., $dU = \delta \mathbb{Q} + \delta \mathbb{W}$, being then equivalent to the standard framework for $\delta \mathbb{W}^* = 0$. Remarkably, it can be shown that the existence of quantum coherence in ρ in the energy eigenbasis $\{|h_k\rangle\}$ is a necessary ingredient for a nonzero work $\delta \mathbb{W}^*$ if the energy eigenvectors are fixed, i.e., for $d|h_k\rangle = 0 \forall k$. Here we will define coherence through the l_1 -norm [31] of ρ in the energy eigenbasis, reading

$$C(\rho) = \sum_{k \neq l} |\langle h_k | \rho | h_l \rangle|.$$
(7)

Indeed, observe that if *H* is constant and ρ and *H* have a common basis of eigenvectors, then $d|h_k\rangle = d|r_k\rangle = 0$. This leads to $\delta \mathbb{W}^* = 0$. Moreover, since a common basis for *H* and ρ implies that ρ is diagonal in the energy eigenbasis $\{|h_k\rangle\}$, we will have $C(\rho) = 0$.

For an arbitrary single-qubit system, the density operator can be written in the Pauli basis $\{I, \vec{\sigma}\}$ as

$$\rho = \frac{1}{2}(I + \vec{r} \cdot \vec{\sigma}), \tag{8}$$

where $\vec{r} = (x, y, z)$ is the Bloch vector. For the Hamiltonian, we have $H = -\vec{h} \cdot \vec{\sigma}$. We observe that $\vec{r} = (x, y, z)$ can be interpreted as a classical magnetic dipole moment immersed in an external magnetic field \vec{h} . Indeed, the quantities in Eqs. (1)–(7) reduce to [15]

$$U = -\vec{h} \cdot \vec{r},\tag{9}$$

$$\delta Q = -\vec{h} \cdot d\vec{r},\tag{10}$$

$$\delta W = -\vec{r} \cdot d\vec{h},\tag{11}$$

$$\delta \mathbb{Q} = U_r dr, \tag{12}$$

$$\delta \mathbb{W} = r d U_r, \tag{13}$$

$$\delta \mathbb{W}^* = -rh\hat{h} \cdot d\hat{r},\tag{14}$$

$$C = r \sqrt{1 - \frac{U_r^2}{h^2}},$$
 (15)

where $r \equiv |\vec{r}|$ is the purity, $U_r \equiv U/r$ is the internal energy per unit of purity, $h \equiv |\vec{h}|$ is the positive energy eigenvalue, $\hat{r} \equiv \vec{r}/r$ is the dipole direction, and $\hat{h} \equiv \vec{h}/h$ is the external field direction. Note that heat and work in the entropy-based qubit formalism, namely, $\delta \mathbb{Q}$ and $\delta \mathbb{W}$, are necessarily associated with changes in *r* (and consequently in *S*) and U_r , respectively. On the other hand, the standard contributions for these thermodynamic quantities, δQ and δW , are required to be associated with variations in \vec{r} and \vec{h} , respectively.

An interpretation for $\delta \mathbb{W}^*$ in terms of the behavior of \vec{r} can be obtained through the relation between $\delta \mathbb{W}^*$ and $C(\rho)$. First, a change in the eigenvectors of ρ is required for nonzero $\delta \mathbb{W}^*$. By imposing $d\hat{h} = 0$, i.e., a fixed energy eigenbasis, we can express $\delta \mathbb{W}^*$ in Eq. (14) as $\delta \mathbb{W}^* = hCd\theta$, where $hC = |\vec{r} \times \vec{h}|$ denotes the absolute value of the torque on \vec{r} induced by \vec{h} and $\theta = \arccos(\hat{h} \cdot \hat{r})$ is the angle between \vec{r} and \vec{h} [15]. Therefore, $\delta \mathbb{W}^*$ is equivalent to the energy cost required to rotate a magnetic dipole moment immersed in an external magnetic field, being proportional to coherence. More generally, $\delta \mathbb{W}^*$ represents the departure from the quasistatic dynamics [12,13].

III. CHARACTERIZING NON-MARKOVIANITY

Let us suppose an open-system dynamical evolution governed by a time-local master equation

$$\dot{\rho} = \mathcal{L}_{i}\rho(t) = -i[H(t), \rho(t)] + \sum_{i} \gamma_{i}(t)[A_{i}(t)\rho(t)A_{i}^{\dagger}(t) - \frac{1}{2}\{A_{i}^{\dagger}(t)A_{i}(t), \rho(t)\}], \quad (16)$$

where \mathcal{L}_t is the time-dependent generator, H(t) is the effective Hamiltonian of the system, $A_i(t)$ are the Lindblad operators, $\gamma_i(t)$ are the relaxation rates, and the overdot denotes time derivative. By taking $\gamma_i(t) \ge 0$, \mathcal{L}_t assumes the Lindblad form at each instant of time [41]. Consequently, the master equation solution $\rho(t) = \Phi_{t,\tau}\rho(\tau)$ is obtained through a completely positive and trace-preserving (CPTP) map $\Phi_{t,\tau}$ = $\mathcal{T} \exp(\int_{\tau}^{t} dt' \mathcal{L}_{t'})$, with \mathcal{T} representing the chronological timeordering operator. In this case, the dynamical map $\Phi_{t,\tau}$ satisfies the divisibility condition, i.e., $\Phi_{t,\tau} = \Phi_{t,\tau} \Phi_{r,\tau}$ $(t \ge$ $r \ge \tau \ge 0$), which characterizes the Markovianity of the dynamical evolution. On the other hand, for $\gamma_i(t) < 0$, the corresponding dynamical map $\Phi_{t,\tau}$ may not be CPTP for intermediate time intervals and the divisibility property of the overall CPTP dynamics is violated, which characterizes a non-Markovian behavior [42–44].

Now assume that $F_{\alpha}(t) = F_{\alpha}(\rho(t))$ represents an arbitrary monotonic function of t under divisible dynamical maps, where $\alpha = +1$ and $\alpha = -1$ indicate increasing and decreasing behaviors, respectively. Then a sign change in $F_{\alpha}(t)$ works as a witness of non-Markovianity. From this breakdown of monotonicity, we propose a measure of non-Markovianity as

$$N_{F_{\alpha}}[\Phi] = \max_{\rho_0} \int_{\operatorname{sgn}\dot{F_{\alpha}} = -\alpha} |\dot{F_{\alpha}}(t)| dt.$$
 (17)

The maximization in Eq. (17) is performed over all sets of possible initial states ρ_0 and the integration extends over all time intervals for which the sign of $\dot{F}_{\alpha}(t)$ is $\operatorname{sgn}\dot{F}_{\alpha} = -\alpha$. If $\{(t_i^k, t_f^k)\}$ represents the set of all time intervals for which $\operatorname{sgn}\dot{F}_{\alpha} = -\alpha$, then we can write

$$N_{F_{\alpha}}[\Phi] = \max_{\rho_0} \sum_{k: \operatorname{sgn} \dot{F_{\alpha}} = -\alpha} \left| F_{\alpha}(t_f^k) - F_{\alpha}(t_i^k) \right|.$$
(18)

Note that $N_{F_{\alpha}}[\Phi]$ quantifies the departure from the map divisibility. It has been previously adopted for several functions $F_{\alpha}(t)$, such as in Refs. [42,44]. Here we use the terminology *measure* for $N_{F_{\alpha}}[\Phi]$ in the way it has been employed in the seminal work in Ref. [42] and not as it is properly used in resource theories (see, e.g., Refs. [26,45]). The choice for $F_{\alpha}(t)$ will depend on the dynamical map. First, let us consider the case of operations over incoherent states. By choosing a fixed basis $\{|i\rangle\}$ in a *d*-dimensional Hilbert space, incoherent states are defined by density operators ρ_{inc} that are diagonal when expressed in the basis $\{|i\rangle\}$, namely, $\rho_{inc} = \sum_{i} c_i |i\rangle \langle i|$, with c_i denoting an arbitrary complex amplitude. Then it follows the notion of an incoherent map, which is a dynamical map leading any incoherent state to another incoherent state. For the case of incoherent quantum operations, it can be shown that quantum coherence $C(\rho(t))$ can witness non-Markovianity through $F_{-1}(t) = C(\rho(t))$ [32]. We can also consider the case of a unital map, which maps the identity operator to itself, $\Phi(I) = I$. In this case, it can be shown

that the von Neumann entropy can witness non-Markovianity through $F_{+1}(t) = S(\rho(t))$ [40]. An operational approach to determine whether or not a dynamical map is unital or incoherent can be established through the sufficient conditions obtained from Eq. (16): (i) If $[A_i, A_i^{\dagger}] = 0$ then Φ is a unital map; (ii) if $\langle h_n | A_i | h_k \rangle \langle h_k | A_i^{\dagger} | h_m \rangle = 0$ for all k and $n \neq m$ then Φ is an incoherent map in the energy eigenbasis $\{|h_k\rangle\}$ [32]. There are several well-known quantum channels that are both incoherent and unital, such as phase flip, bit flip, and bit-phase flip, among others [46]. For further applications of Eq. (18) as a non-Markovianity measure and its relationship with correlation measures, see also Ref. [47]. Note that, in this generalized approach, α may depend on the initial state, enabling the use of thermodynamic quantities such as internal energy, heat, and work to characterize non-Markovianity.

The use of the von Neumann entropy to witness non-Markovianity for unital maps suggests that heat flow, as defined by the entropy-based formulation of quantum thermodynamics, is also able to detect non-Markovian processes for unital maps. Indeed, the expression $\dot{\mathbb{Q}} = U_r \dot{r}$ obtained from Eq. (12) reveals that heat is monotonically related to the purity (consequently to the entropy) for single-qubit energy sign-preserving dynamics, i.e., quantum evolutions such that the internal energy U is either a non-negative or a nonpositive function of the time t. Note that the purity does not increase under unital Markovian quantum processes [48]. Then we can establish the following measure of non-Markovianity.

(a) $N_{\mathbb{Q}}[\Phi]$ is a measure of non-Markovianity if Φ is a single-qubit energy sign-preserving unital map.

In this case, heat can witness non-Markovianity via $F_{\alpha}(t) = \mathbb{Q}(\rho(t))$ with $\alpha = \operatorname{sgn} U \neq 0$. As an illustration, the sign of U does not change under isochoric processes, with heat a monotonic function of the purity

$$\mathbb{Q} = \Delta U = U_r(r - r_0) \quad (\dot{U}_r = 0), \tag{19}$$

where r_0 represents the initial purity. Then we can employ either \mathbb{Q} or U to quantify the degree of non-Markovianity for isochoric unital maps. Other examples include nondissipative processes, where heat and work are monotonically related to the quantum coherence,

$$\mathbb{Q} = -\mathbb{W} = U \ln \sqrt{\frac{C^2 + U^2/h^2}{C_0^2 + U^2/h^2}} \quad (\dot{U} = 0), \qquad (20)$$

with C_0 the initial quantum coherence. Consequently, we can use either \mathbb{Q} or \mathbb{W} to characterize the non-Markovianity of nondissipative unital maps as well as nondissipative incoherent maps. Regardless of \mathbb{Q} , we can use U and \mathbb{W} for characterization of non-Markovianity if $\vec{h}(t) \cdot \vec{r}(t)$ and $U_r(t)$ are monotonic functions of t for $\gamma_i(t) \ge 0$ ($\forall t \ge 0$), respectively. As a special case, let us provide sufficient conditions for the thermodynamical variables to witness non-Markovianity for a time-independent Hamiltonian. In this scenario, we take $H = \omega_0 \sigma_z$ and define $\vec{r} = [x(t), y(t), z(t)]$. Moreover, let us define $z_r \equiv z/r = \cos\theta$. Then it follows that

$$U(t) = \omega_0 z(t), \tag{21}$$

$$\hat{\mathbb{Q}}(t) = \omega_0 z_r(t) \dot{r}(t), \qquad (22)$$

$$\dot{\mathbb{W}}(t) = \dot{\mathbb{W}}^*(t) = \omega_0 r(t) \dot{z}_r(t).$$
(23)

Hence, from Eq. (22), we can establish the following.

(b) $N_{\mathbb{Q}}[\Phi]$ is a measure of non-Markovianity for a timeindependent Hamiltonian $H = \omega_0 \sigma_z$ if Φ is a single-qubit unital map that does not invert the sign of z(t).

Furthermore, it follows from Eqs. (21) and (23) that N_U and N_W are measures of non-Markovianity if z(t) and $z_r(t)$ are monotonic functions of time for $\gamma_i(t) \ge 0$ ($\forall t \ge 0$), respectively.

IV. APPLICATIONS

A. Dissipative quantum evolution

Let us first consider a dissipative single-qubit dynamics described by a time-local master equation given by Eq. (16), with $H = \omega_0 \sigma_z$, $A_i = \delta_{1,i} \sigma_x$, and $\gamma_i = \delta_{1,i} \gamma$, such that $\omega_0 > 0$ and $\gamma > 0$. Then

$$\dot{\rho}(t) = -i\omega_0[\sigma_z, \rho(t)] + \gamma[\sigma_x \rho(t)\sigma_x - \rho(t)].$$
(24)

This master equation generates a Markovian quantum process $\rho(t) = \Phi_M \rho_0 = [I + \vec{r}(t) \cdot \vec{\sigma}]/2$, where $\vec{r}(t) = [x(t), y(t), z(t)]$, whose solution for the Bloch vector is given by

$$x(t) = \frac{e^{-\gamma t}}{2\omega} [\alpha_x e^{\omega t} + \beta_x e^{-\omega t}], \qquad (25)$$

$$y(t) = \frac{e^{-\gamma t}}{2\omega} [\alpha_y e^{\omega t} + \beta_y e^{-\omega t}], \qquad (26)$$

$$z(t) = z_0 e^{-2\gamma t}, \qquad (27)$$

where

$$\alpha_x = \omega x_0 + \gamma x_0 - 2\omega_0 y_0, \qquad (28)$$

$$\beta_x = \omega x_0 - \gamma x_0 + 2\omega_0 y_0, \qquad (29)$$

$$\alpha_y = \omega y_0 - \gamma y_0 + 2\omega_0 x_0, \tag{30}$$

$$\beta_{\mathbf{y}} = \omega y_0 + \gamma y_0 - 2\omega_0 x_0, \tag{31}$$

with

$$\omega = \sqrt{\gamma^2 - 4\omega_0^2} \tag{32}$$

and $\vec{r}_0 = [x_0, y_0, z_0]$ denoting the initial state. The Markovian map Φ_M is both unital and incoherent, since the Lindblad operators $A_i = \delta_{1,i}\sigma_x$ satisfy the conditions (i) and (ii) described in Sec. III. Moreover, Φ_M is also a map that preserves the sign of z(t) [note that $\text{sgn}z(t) = \text{sgn}z_0 \forall t \ge 0$]. Consequently, we can use the monotonicity of $\mathbb{Q}(t)$ or C(t) as a function of t to observe the Markovianity of Eq. (24). Then

$$N_{F_{\alpha}}[\Phi_M] = 0, \tag{33}$$

where $F_{\alpha} = \mathbb{Q}$ with $\alpha = \operatorname{sgn}_{z_0} \neq 0$ or $F_{\alpha} = C$ with $\alpha = -1$. Indeed, Fig. 1 illustrates the sign preservation of $\dot{F}_{\alpha}(t)$ for the initial state $\vec{r}_0 = [1/2, 0, 1/2]$, where the heat and coherence

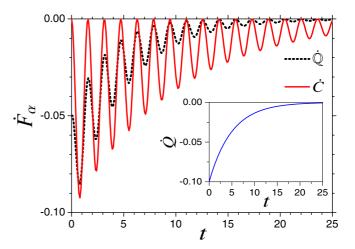


FIG. 1. Heat (black dotted line) and quantum coherence (red solid line) flows as a function of time for $\vec{r}_0 = [1/2, 0, 1/2]$, in units such that $\gamma = 0.1$ and $\omega_0 = 1$. The inset shows \dot{Q} as a function of t.

flows reduce to

$$\dot{\mathbb{Q}}(t) = \frac{\omega_0 \gamma \left\{ 2\omega_0^2 [1 - \cosh\left(2\omega t\right)] - \omega^2 e^{-2\gamma t} \right\} e^{-2\gamma t}}{\omega^2 e^{-2\gamma t} + \gamma^2 \cosh\left(2\omega t\right) + \omega\gamma \sinh\left(2\omega t\right) - 4\omega_0^2},\tag{34}$$

$$\dot{C}(t) = \frac{2\omega_0^2 \gamma e^{-\gamma t} (1 - \cosh 2\omega t)}{\omega \sqrt{\gamma^2 \cosh (2\omega t) + \omega \gamma \sinh (2\omega t) - 4\omega_0^2}}.$$
 (35)

The Markovianity of Eq. (24) can also be witnessed from the behavior of the internal energy and work (see plots for Uand \mathbb{W} for $\vec{r}_0 = [1/2, 0, 1/2]$ in Ref. [12]). Concerning the standard thermodynamic quantities, we have that the conventional heat flow Q is equal to the internal energy flow U. This holds for an arbitrary time-independent Hamiltonian, since the conventional work flow \dot{W} is zero in this case. From Eqs. (21) and (27) we then obtain $\dot{Q} = \dot{U} = -2\gamma z_0 \omega_0 e^{-2\gamma t}$. Since the map Φ_M preserves the sign of \dot{Q} (see the inset in Fig. 1), we can also conclude that $N_{F_{\alpha}}[\Phi_M] = 0$ for $F_{\alpha} = Q$ with $\alpha =$ $sgn z_0 \neq 0$. From the inset in Fig. 1 we observe that the monotonicity between the heat flow and the coherence flow is lost in the conventional framework, but the identification of the Markovian behavior still works. In order to investigate a non-Markovian scenario, we may take temporary negative constant rates γ . In this case, Eqs. (25)–(27) are kept for either positive or negative piecewise constant γ . This fact implies that the signs of internal energy, heat, and coherence flows will not be preserved throughout the dynamics, then identifying the non-Markovian behavior. Notice that the equivalence observed in this example between the conventional and entropy-based formalisms to characterize non-Markovianity is far from general. Indeed, we will consider next a nondissipative quantum evolution for a time-independent Hamiltonian. As we will show for that case, both internal energy and conventional heat flow fail as non-Markovianity witnesses since $\dot{Q} = \dot{U} = 0 \forall t \ge 0$.

B. Nondissipative quantum evolution

Let us consider now the dynamics of a single qubit under dephasing, whose master equation is given by

$$\dot{\rho}(t) = -i\omega_0[\sigma_z, \rho(t)] + \gamma(t)[\sigma_z\rho(t)\sigma_z - \rho(t)].$$
(36)

This master equation can be derived from Eq. (16) by taking $H = \omega_0 \sigma_z$, $A_i = \delta_{1,i} \sigma_z$, and $\gamma_i = \delta_{1,i} \gamma$. The solution is given by a map Φ_D such that $\rho(t) = \Phi_D \rho_0 = [I + \vec{r}(t) \cdot \vec{\sigma}]/2$ with [32]

$$\vec{r}(t) = [x_0 \Gamma(t), y_0 \Gamma(t), z_0], \tag{37}$$

where

$$\Gamma(t) = \exp\left(-\int_0^t \gamma(t)dt\right).$$
 (38)

The non-Markovianity measure in Eq. (18) then reads

In this case, the internal energy and the quantum coherence are given by

$$U(t) = U_0, \tag{39}$$

with $U_0 = \omega_0 z_0$, and

$$C(t) = C_0 \Gamma(t), \tag{40}$$

with $C_0 = \sqrt{r_0^2 - z_0^2}$, respectively. The map Φ_D is both nondissipative unital and nondissipative incoherent. Consequently, we can use $\mathbb{Q}(t)$, $\mathbb{W}(t)$, or C(t) to characterize the non-Markovianity of Eq. (36). Inserting Eqs. (39) and (40) in Eq. (20), we can express heat in the form

$$\mathbb{Q}(t) = \omega_0 z_{r0} r_0 \ln \sqrt{\Gamma(t)^2 + [1 - \Gamma(t)^2] z_{r0}^2}.$$
 (41)

$$N_{\mathbb{Q}}[\Phi_{D}] = \max_{\rho_{0}} \sum_{k: \operatorname{sgn}\dot{\mathbb{Q}} = \operatorname{sgn}U_{0}} \left| \mathbb{Q}(t_{f}^{k}) - \mathbb{Q}(t_{i}^{k}) \right| = \omega_{0} \max_{|z_{r0}|, r_{0}} r_{0} \sum_{k: \gamma < 0} |z_{r0}| \ln \sqrt{\frac{\Gamma(t_{f}^{k})^{2} + (1 - \Gamma(t_{f}^{k})^{2})|z_{r0}|^{2}}{\Gamma(t_{i}^{k})^{2} + (1 - \Gamma(t_{i}^{k})^{2})|z_{r0}|^{2}}}} = \omega_{0} \max_{|z_{0}|} \sum_{k: \gamma < 0} |z_{0}| \ln \sqrt{\frac{\Gamma(t_{f}^{k})^{2} + (1 - \Gamma(t_{f}^{k})^{2})|z_{0}|^{2}}{\Gamma(t_{i}^{k})^{2} + (1 - \Gamma(t_{i}^{k})^{2})|z_{0}|^{2}}}}.$$
(42)

Note that a pure initial state, i.e., $r_0 = 1$, results from the maximization procedure in Eq. (42). In order to enable a numerical comparison with the coherence-based measure of non-Markovianity, let us consider a typical example of a zero-temperature bosonic reservoir with an Ohmic-like spectral density, where the time-dependent dephasing rate presents the specific form [32,49,50]

$$\gamma(t,s) = [1 + (\omega_c t)^2]^{-s/2} \Gamma_*(s) \sin[s \arctan(\omega_c t)], \quad (43)$$

with $s \ge 0$ the Ohmicity parameter, $\Gamma_*(s)$ the Euler Gamma function, and ω_c the cutoff spectral frequency. In this case, $\gamma(t, s) < 0$ occurs for $t_i^k = t_{2k-1}$ and $t_f^k = t_{2k}$, where $t_k = \tan(k\pi/2s)/\omega_c$, with *k* an integer such that $0 \le k \le \lfloor s \rfloor (\lfloor s \rfloor)$ is the floor function of *s*). Thus, we can conclude that $0 \le s \le 2$ and s > 2 correspond to the Markovian and non-Markovian regimes of this model. In terms of the Ohmicity parameter, $N_{\mathbb{Q}}[\Phi_D]$ takes the form

$$N_{\mathbb{Q}}(s) = \omega_0 \ln \left[\prod_{k=1}^{\lfloor s/2 \rfloor} \frac{\Gamma(t_{2k})^2 + [1 - \Gamma(t_{2k})^2] z_{\max}^2}{\Gamma(t_{2k-1})^2 + [1 - \Gamma(t_{2k-1})^2] z_{\max}^2} \right]^{z_{\max}/2},$$
(44)

where z_{max} represents the value of $|z_0|$ that maximizes the last expression in Eq. (42). The coherence-based measure $N_C[\Phi]$ has been employed to quantify the degree of non-Markovianity of the incoherent map Φ_D for the dephasing rate described in Eq. (43) [32]. As a function of the parameter *s*,

 $N_C[\Phi_D]$ reduces to

$$N_{C}(s) = \max_{\rho_{0}} \sum_{\substack{k: \text{sgn}\dot{C} = +1 \\ k: \text{sgn}\dot{C} = +1}} |C(t_{f}^{k}) - C(t_{i}^{k})|$$
$$= \sum_{k=1}^{\lfloor s/2 \rfloor} [\Gamma(t_{2k}) - \Gamma(t_{2k-1})],$$
(45)

where a maximally coherent state (i.e., $C_0 = 1$) emerges from the maximization process.

In order to witness non-Markovianity, Fig. 2 shows the time evolution of the heat \mathbb{Q} for an initial pure state under the single-qubit dephasing channel in both Markovian and

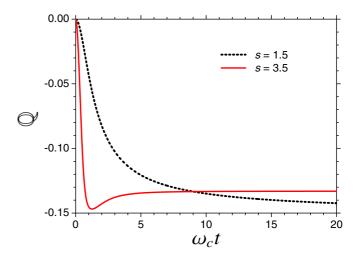


FIG. 2. Plot of \mathbb{Q} as a function of $\omega_c t$ for s = 1.5 (black dotted line) and s = 3.5 (red solid line), with $\omega_0 = 1$, $r_0 = 1$, and $z_0 = 0.05$.

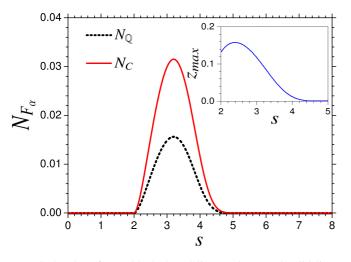


FIG. 3. Plot of $N_{\mathbb{Q}}$ (black dotted line) and N_C (red solid line) as functions of *s* for $\omega_0 = 1$ and $\omega_c = 1$. The inset shows z_{max} as a function of *s*.

non-Markovian regimes. Note that \mathbb{Q} is a monotonically decreasing function of time for s = 1.5. On the other hand, a nonmonotonic behavior arises due to the backflow of heat from the environment to the system for s = 3.5. The behaviors of the non-Markovianity measures $N_{\mathbb{Q}}$ and N_C as functions of s are illustrated in Fig. 3, with the inset showing z_{max} versus s. These measures are monotonically related, i.e., $N_C(s) \approx 2.0N_{\mathbb{Q}}(s)$, with both assuming nonzero values only for s > 2, a maximum value at s = 3.2, and negligible values for s > 5. From the behavior of $z_{\text{max}}(s)$, note that a maximally coherent state (where $z_0 = 0$) does not optimize the expression in Eq. (44) for all s.

- S. Deffner and S. Campbell, *Quantum Thermodynamics: An Introduction to the Thermodynamics of Quantum Information* (Morgan & Claypool, San Rafael, 2019).
- [2] J. Gemmer, M. Michel, and G. Mahler, Quantum Thermodynamics: Emergence of Thermodynamic Behavior within Composite Quantum Systems (Springer, Berlin, 2009).
- [3] A. Auffeves, PRX Quantum 3, 020101 (2022).
- [4] R. Kosloff, Entropy 15, 2100 (2013).
- [5] L. Masanes and J. Oppenheim, Nat. Commun. 8, 14538 (2017).
- [6] T. D. Kieu, Phys. Rev. Lett. 93, 140403 (2004).
- [7] Y. Xu, Entropy 24, 180 (2022).
- [8] F. G. S. L. Brandão, M. Horodecki, N. H. Ying, J. Oppenheim, and S. Wehner, Proc. Natl. Acad. Sci. USA 112, 3275 (2015).
- [9] H. Hossein-Nejad, E. J O'Reilly, and A. Olaya-Castro, New J. Phys. 17, 075014 (2015).
- [10] P. Talkner, E. Lutz, and P. Hänggi, Phys. Rev. E 75, 050102(R) (2007).
- [11] R. Alicki, J. Phys. A: Math. Gen. 12, L103 (1979).
- [12] S. Alipour, A. T. Rezakhani, A. Chenu, A. del Campo, and T. Ala-Nissila, Phys. Rev. A 105, L040201 (2022).
- [13] S. Alipour, A. T. Rezakhani, A. Chenu, A. del Campo, and T. Ala-Nissila, Quantum 4, 336 (2020).

V. CONCLUSION

We have introduced a characterization of non-Markovianity by using the entropy-based formulation of quantum thermodynamics. Specifically, by looking at the divisibility property of the overall CPTP dynamics, we derived a measure of non-Markovian behavior through the relationship between entropy and heat in a thermodynamic process. This result supports the entropy-based approach, since it provides utility for the definition of heat by exclusively taking the entropy change contribution in the internal energy balance.

The analysis of the heat flow can be a useful tool from an experimental point of view to provide a thermodynamic assessment of the memory effects of the bath. Based on the heat flow behavior, we can design an environment engineering approach to induce the desired amount of memory in a system-bath interaction for a suitable physical architecture, from a conceptual point of view, it would be interesting to establish to what extent a thermodynamic characterization of non-Markovianity beyond single-qubit maps can be achieved. These are left as perspectives for future investigations.

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- [14] B. Ahmadi, S. Salimi, and A. S. Khorashadl, arXiv:1912.01983.
- [15] A. Vallejo, A. Romanelli, and R. Donangelo, Phys. Rev. E 103, 042105 (2021).
- [16] W. T. B. Malouf, Thermodynamics and information in linear quantum lattices, M.Sc. thesis, University of São Paulo, 2019.
- [17] C. Jarzynski and D. K. Wojcik, Phys. Rev. Lett. 92, 230602 (2004).
- [18] J. Oppenheim, M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Rev. Lett. 89, 180402 (2002).
- [19] J. Chen, G. Su, J. Chen, and S. Su, arXiv:2201.12202.
- [20] T. Zhang, W.-T. Liu, P.-X. Chen, and C.-Z. Li, Phys. Rev. A 75, 062102 (2007).
- [21] J. Roßnagel, O. Abah, F. Schmidt-Kaler, K. Singer, and E. Lutz, Phys. Rev. Lett. **112**, 030602 (2014).
- [22] C. L. Latune, I. Sinayskiy, and F. Petruccione, Sci. Rep. 9, 3191 (2019).
- [23] M. O. Scully, M. S. Zubairy, G. S. Agarwal, and H. Walther, Science 299, 862 (2003).
- [24] P. Kammerlander and J. Anders, Sci. Rep. 6, 22174 (2016).
- [25] K. Brandner, M. Bauer, and U. Seifert, Phys. Rev. Lett. 119, 170602 (2017).
- [26] A. Streltsov, G. Adesso, and M. B. Plenio, Rev. Mod. Phys. 89, 041003 (2017).

- [27] B. L. Bernardo, Phys. Rev. E 102, 062152 (2020).
- [28] C. L. Latune, I. Sinayskiy, and F. Petruccione, Eur. Phys. J. Spec. Top. 230, 841 (2021).
- [29] Y. Ma, C. L. Liu, and C. P. Sun, arXiv:2110.04550.
- [30] K. Hammam, H. Leitch, Y. Hassouni, and G. De Chiara, New J. Phys. 24, 113053 (2022).
- [31] T. Baumgratz, M. Cramer, and M. B. Plenio, Phys. Rev. Lett. 113, 140401 (2014).
- [32] T. Chanda and S. Bhattacharya, Ann. Phys. (NY) **366**, 1 (2016).
- [33] M. H. M. Passos, P. C. Obando, W. F. Balthazar, F. M. Paula, J. A. O. Huguenin, and M. S. Sarandy, Opt. Lett. 44, 2478 (2019).
- [34] K. Wu, Z. Hou, G. Xiang, C. Li, G. Guo, D. Dong, and F. Nori, npj Quantum Inf. 6, 55 (2020).
- [35] Tony J. G. Apollaro, C. Di Franco, F. Plastina, and M. Paternostro, Phys. Rev. A 83, 032103 (2011).
- [36] P. Haikka, J. Goold, S. McEndoo, F. Plastina, and S. Maniscalco, Phys. Rev. A 85, 060101(R) (2012).
- [37] H.-B. Chen, N. Lambert, Y.-C. Cheng, Y.-N. Chen, and F. Nori, Sci. Rep. 5, 12753 (2015).
- [38] D. Aharonov, A. Kitaev, and J. Preskill, Phys. Rev. Lett. 96, 050504 (2006).

- [39] B. Bylicka, D. Chruscinski, and S. Maniscalco, Sci. Rep. 4, 5720 (2014).
- [40] S. Haseli, S. Salimi, and A. S. Khorashad, Quantum Inf. Process. 14, 3581 (2015).
- [41] V. Gorini, A. Kossakowski, and E. C. G. Sudarshan, J. Math. Phys. 17, 821 (1976).
- [42] H.-P. Breuer, E.-M. Laine, and J. Piilo, Phys. Rev. Lett. 103, 210401 (2009).
- [43] A. Rivas, S. F. Huelga, and M. B. Plenio, Phys. Rev. Lett. 105, 050403 (2010).
- [44] D. Chruscinski and S. Maniscalco, Phys. Rev. Lett. 112, 120404 (2014).
- [45] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Rev. Mod. Phys. 81, 865 (2009).
- [46] M. Nielsen and I. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).
- [47] F. M. Paula, P. C. Obando, and M. S. Sarandy, Phys. Rev. A 93, 042337 (2016).
- [48] A. Streltsov, H. Kampermann, S. Wolk, M. Gessner, and D. Bruß, New J. Phys. 20, 053058 (2018).
- [49] P. Haikka, T. H. Johnson, and S. Maniscalco, Phys. Rev. A 87, 010103(R) (2013).
- [50] H. S. Dhar, M. N. Bera, and G. Adesso, Phys. Rev. A 91, 032115 (2015).