Gauge quantum thermodynamics of time-local non-Markovian evolutions

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Dealing with a generic time-local non-Markovian master equation, we define current and power to be process-dependent as in classical thermodynamics. Each process is characterized by a symmetry transformation, a gauge of the master equation, and is associated with different amounts of heat and/or work. Once the symmetry requirement fixes the thermodynamical quantities, a consistent gauge interpretation of the laws of thermodynamics emerges. We also provide the necessary and sufficient conditions for a system to have a gauge-independent thermodynamical behavior and show that systems satisfying quantum detailed balance conditions are gauge-independent. Applying the theory to quantum thermal engines, we show that gauge transformations can change the machine efficiency, however, yet constrained by the classical Carnot bound.

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I. INTRODUCTION

One of the challenges of nonequilibrium quantum thermodynamics is to provide a consistent description of the dynamics underlying processes of interaction between small- or big-scale quantum systems by means of thermodynamical quantities [1–22]. In classical thermodynamics, work and heat are process-dependent quantities that change the state of the physical system [23]. Two states, characterized by their own set of variables (pressure, temperature, volume, ...), can be linked in infinitely many ways, each one differing from the other by a chosen process, which can also vary by amounts of work and heat exchanged by the system.

In a well-established scenario for interacting quantum systems [24–35], the dynamics is modeled through a master equation. The association of the nonunitary part of this master equation with "heat" currents dates back to Alicki's paper [3], leaving work as a manifestation of the unitary piece [2]. However, this dichotomy is not clear as just stated [10,11]. As we will show, these master equations have a well-known gauge symmetry [24], which merges the generators of the unitary part (a Hamiltonian) with those of the dissipation part (the Lindblad operators), while the evolution of the system is kept invariant. Since their standard definitions depend on the generators, energy, heat currents, and power are not invariant, contrary to the system state, which misleads and intertwines their notions. From a logical viewpoint, there is no physical reason to withdraw any of these ingredients, and the only way to deal with the gauge issues is to interpret their implications on the physical laws while respecting the dynamical invariance.

In this work, we interpret gauge transformations as conceivable thermodynamical processes keeping the system's evolution unchanged. The intertwining of current and power is naturally incorporated in our findings when we recognize that each process has its distinctive fraction of these quantities. Incorporating the gauge-freedom into thermodynamics, the thermodynamical functions turn themselves process-dependent, enabling a gauge-consistent definition of a quantum first law.

Although gauge-induced contributions will give rise to a component of work performed on (by) the system by (on) the reservoir [11,16], the first law will consider only two possible ways of energy variation, as in classical thermodynamics, throughout heat and work, both described by Alicki's formulas [3] and their gauge transformations. We will also explore the existence of systems thermodynamically unresponsive to gauges when we write the necessary and sufficient conditions for the invariance of the thermodynamical quantities. Notwithstanding, they constitute a small set among all physical systems governed by a master equation, which enforces the necessity of a gauge-dependent interpretation.

A general theory for the entropy production for generic master equations is still missing [7] and would provide a complete thermodynamical description for systems governed by such equations. Notwithstanding, a recent result [11] is used to describe quantum thermal machines constituted by a system strongly coupled to thermal reservoirs and, interestingly enough, we show that the Carnot bound [23] limits the efficiency of these machines for the work and heat provided by Alicki definitions and for any of their gauge-transformations.

In Sec. II, we review the main hypothesis of our approach, i.e., the time-local master equation and the first law of quantum thermodynamics. Then, we present formal expressions for the gauge transformations and, in the sequence, we explore the behavior of work and heat rates under gauges. Conditions for the invariance of all thermodynamical quantities are derived in Sec. III, where we also show that quantum detailed balance is sufficient for thermodynamical invariance. Section IV provides our interpretation of a gauge-dependent thermodynamics, where each gauge is associated with a thermodynamical path followed by the system and explores the

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gauge freedom for particular processes. Remarks about the entropy production are in Sec. V, while in Sec. VI, all presented theory is exemplified within the pure decoherence model. In Sec. VII, quantum thermal machines and the Carnot bound are studied under the developed approach. As an example, we apply all results for a three-level maser. We discuss and contextualize our achievements in Sec. VIII with final remarks and outlooks.

II. SYSTEM DYNAMICS AND THERMODYNAMICS

The open-system scenario, see Ref. [24] for instance, considers the evolution of the state of a system S, initially described by the density operator $\hat{\rho}_0$, as the partial trace

$$\hat{\rho}(t) = \mathrm{Tr}_{\mathrm{E}}(\hat{U}_t \hat{\rho}_0 \otimes \hat{\rho}_{\mathrm{E}} \hat{U}_t^\dagger) =: \Phi_t[\hat{\rho}_0] \tag{1}$$

over the Hilbert space of another system E, where the evolution of the joint system SE is ruled by the unitary operator $\hat{U}_t$, which is the solution of $i\hbar\partial_t \hat{U}_t = \hat{H}_{\mathrm{SE}}\hat{U}_t$ for the Hamiltonian $\hat{H}_{\mathrm{SE}}$ of the global system. This Hamiltonian includes a term relative to the system S, another relative to the system E dynamics, as well as a coupling energy term.

When the completely positive trace-preserving (CPTP) map Φ_t is differentiable with respect to t and invertible, i.e., Φ_t^{-1} exists [30], a time-local master equation (ME) [25,26] rules the evolution of the system S (see note [36]):

$$\partial_t \hat{\rho} = \frac{i}{\hbar}[\hat{\rho}, \hat{H}] - \frac{g_{\mu\nu}}{2\hbar}(\{\hat{L}_\mu^\dagger \hat{L}_\nu, \hat{\rho}\} - 2\hat{L}_\mu \hat{\rho} \hat{L}_\nu^\dagger), \tag{2}$$

where all the remaining influence from E are represented by Lindblad operators $\hat{L}_\mu$ $(\mu = 1, \dots, M)$ and a Hermitian operator $\hat{H}$, an effective Hamiltonian. None of these operators necessarily are pieces of $\hat{H}_{\mathrm{SE}}$, since they crucially depend also on $\hat{\rho}_{\mathrm{E}}$. The matrix $\mathbf{g}$, whose elements are $g_{\mu\nu}$, is a $M \times M$ diagonal matrix defined as

$$\mathbf{g} = \mathrm{Diag}(\underbrace{1, \dots, 1}_{m_+ \text{ times}}, \underbrace{-1, \dots, -1}_{m_- \text{ times}}), \quad M = m_+ + m_-,$$

and the Einstein convention is employed throughout this text. It should be mentioned that $\mathbf{g}$ may also depend on time,[1] that is, $m_\pm$ can change, however, this is irrelevant to our results. Sometimes it will be useful to write Eq. (2) generically as $\partial_t \hat{\rho} = \mathfrak{L}(\hat{\rho})$ and also to split the generator into a unitary and nonunitary part, respectively, defined as the superoperators

$$\mathfrak{U} := \frac{i}{\hbar}[\bullet, \hat{H}], \;\; \mathfrak{D} := -\frac{g_{\mu\nu}}{2\hbar}(\{\hat{L}_\mu^\dagger \hat{L}_\nu, \bullet\} - 2\hat{L}_\mu \bullet \hat{L}_\nu^\dagger), \tag{3}$$

such that $\mathfrak{L} = \mathfrak{U} + \mathfrak{D}$.

In principle, we consider all the operators in (2) *time-dependent*, where memory effects may not be negligible, and the non-Markovianity can take place despite the absence of a memory kernel [24–26]. The strict Markovian Lindblad ME, the one which generates a quantum dynamical semigroup [28], will be treated as the particular instance of an autonomous ME[2] with $m_- = 0$. Between this and that, the evolution of a generic ME (2) may be Markovian with time-dependent operators [24–26]. However, it is only possible to ensure complete positivity for the dynamics for all times if $m_- = 0\, \forall\, t$. For any other m_- values, complete positivity may or may not be preserved depending on the case [25,26].

As described in Ref. [26], the time-local ME (2) is obtained analytically from the CPTP map (1). Surprisingly enough, there is no approximations at all, nor *a priori* assumptions about the state (or the nature) of subsystem E, see Ref. [36] for further comments. Examples of non-Markovian ME are [30,31], some of them highlight the utility of Eq. (2) in dealing with a strong coupling between S and E; see also the examples and references contained in Refs. [25–27].

The operators $\hat{H}_{\mathrm{SE}}$ and $\hat{\rho}_{\mathrm{E}}$ determine the evolution of $\hat{\rho}$, however, they do not uniquely fix the operators in the ME, which is manifested by the gauge transformations [24]:

$$\begin{aligned} \hat{L}_\mu &\longrightarrow \hat{L}'_\mu = U_{\mu\nu}\hat{L}_\nu + \gamma_\mu \;(\mu = 1, \dots, M), \\ \hat{H} &\longrightarrow \hat{H}' = \hat{H} + \delta\hat{H}, \end{aligned} \tag{4}$$

with $\nu = 1, \dots, M$, $\gamma_\mu : t \in \mathbb{R} \mapsto \gamma_\mu(t) \in \mathbb{C}$, and $U_{\mu\nu} : t \in \mathbb{R} \mapsto U_{\mu\nu}(t) \in \mathbb{C}$ are the matrix elements of the pseudo-unitary $M \times M$ matrix $\mathbf{U}$ satisfying $\mathbf{U}^\dagger \mathbf{g} \mathbf{U} = \mathbf{g}$. While each Lindblad operator undergoes an affine transformation in (4), the Hamiltonian is translated by the Hermitian operator

$$\delta\hat{H} := \frac{g_{\mu\nu}}{2i}(\gamma_\mu^* U_{\nu\kappa}\hat{L}_\kappa - \gamma_\mu U_{\nu\kappa}^* \hat{L}_\kappa^\dagger) + \phi, \tag{5}$$

keeping the ME in (2) unchanged; in above $\phi : t \in \mathbb{R} \mapsto \phi(t) \in \mathbb{R}$. In fact, the action of gauge (4) upon (3), after simple calculations, is

$$\begin{aligned} \mathfrak{U} &\longrightarrow \mathfrak{U}' = \frac{i}{\hbar}[\bullet, \hat{H}'] = \mathfrak{U}(\hat{\rho}) + \frac{i}{\hbar}[\bullet, \delta\hat{H}], \\ \mathfrak{D} &\longrightarrow \mathfrak{D}' = -\frac{g_{\mu\nu}}{2\hbar}(\{\hat{L}_\mu'^\dagger \hat{L}'_\nu, \bullet\} - 2\hat{L}'_\mu \bullet \hat{L}_\nu'^\dagger) \\ &= \mathfrak{D} - \frac{i}{\hbar}[\bullet, \delta\hat{H}], \end{aligned} \tag{6}$$

which express the invariance of the global generator: $\mathfrak{L}' := \mathfrak{U}' + \mathfrak{D}' = \mathfrak{U} + \mathfrak{D} = \mathfrak{L}$.

The set of all transformations in (4) is the symmetry group of the Lindblad equation, defined by the product rule [11] $(\gamma''_\mu, \mathbf{U}'', \phi'')(\gamma'_\mu, \mathbf{U}', \phi') = (\gamma_\mu, \mathbf{U}, \phi)$, where

$$\begin{aligned} \gamma_\mu &= \gamma''_\mu + U''_{\mu\nu}\gamma'_\nu, \quad \mathbf{U} = \mathbf{U}''\mathbf{U}', \\ \phi &= \phi' + \phi'' + \mathrm{Im}(\gamma_\mu''^* g_{\mu\nu} U''_{\nu\kappa}\gamma'_\kappa). \end{aligned}$$

These symmetries are inherently associated with the origin of a ME, which is only justified when, whatever the reason, there is a lack of knowledge or control about the system and its surroundings, this lack manifests as the gauges. In other words, if one has complete control over the global system ($\hat{H}_{\mathrm{SE}}$, $\hat{\rho}_{\mathrm{E}}$, and $\hat{\rho}_0$), the dynamics will be promptly described by the global unitary evolution, and the gauges are as useless as an ME.

[1] When all Lindblad operators can be written as $\hat{L}_\mu = \omega_\mu(t)\hat{A}_\mu$ for time-independent $\hat{A}_\mu$, then $g_{\mu\nu} = \mathrm{sign}(\omega_\mu)\delta_{\mu\nu}$. Throughout the text, we denote time-independent Lindblad operators by $\hat{A}_\mu$.

[2] Autonomous means $\partial_t \hat{H} = \partial_t \hat{L}_\mu = \partial_t g_{\mu\nu} = 0$. To gain generality, an autonomous ME may be different from a strict Lindblad ME, since it is possible to have $g_{\mu\nu} \neq \delta_{\mu\nu}$ or, equivalently, $m_- \neq 0$.

When an experimentalist does not know the microscopic details about the whole system-environment state, he or she is left with standard tomographic procedures for measurements of the system state or of the generator $\mathfrak{L}$, both gauge-invariant. The obtained generator will fit with any operators connected by a gauge transformation (4). See Chap. 8 of the book [37] for a description of tomography for quantum state and processes and its experimental references.

The dichotomy heat-work naturally emerges [3] for the ME (2) if the internal energy of the system is taken as the mean value $\langle\hat{H}\rangle := \mathrm{Tr}(\hat{H}\hat{\rho})$, once a temporal derivative reads

$$\partial_t\langle\hat{H}\rangle = \mathcal{J} + \mathcal{P}, \tag{7}$$

with the *Lindblad total current* and the *Lindblad power* defined, respectively, as

$$\mathcal{J} := \mathrm{Tr}(\hat{H}\partial_t\hat{\rho}) = \mathrm{Tr}[\hat{H}\mathfrak{D}(\hat{\rho})], \quad \mathcal{P} := \langle\partial_t\hat{H}\rangle. \tag{8}$$

The expression for the total current above is a consequence of $\mathrm{Tr}[\hat{H}\mathfrak{U}(\hat{\rho})] = 0$, which shows that there is no contribution of the unitary part and that the current is proper to the interaction with subsystem E. Writing $\mathfrak{D}$ explicitly as in (3),

$$\mathcal{J} = \sum_{\mu=1}^{M}\mathcal{J}_\mu = -\frac{1}{\hbar}g_{\mu\nu}\mathrm{Re}\langle\hat{L}_\mu^\dagger[\hat{L}_\nu,\hat{H}]\rangle, \tag{9}$$

i.e., the total current is the sum of the currents due to each Lindblad operator

$$\mathcal{J}_\mu := -\frac{1}{\hbar}\delta_{\mu\kappa}g_{\kappa\nu}\mathrm{Re}\langle\hat{L}_\kappa^\dagger[\hat{L}_\nu,\hat{H}]\rangle. \tag{10}$$

The above formulas, established by Alicki in Ref. [3], constitute the standard definitions for the thermodynamical quantities associated with the ME [38]. However, the invariance of the ME under any gauge (4) does not apply to the thermodynamical functions [10], which is the starting point of our work.

A. Energy noninvariance

The first step towards understanding the relation between gauges and thermodynamics is to consider the energy of the system. Applying the gauge transformation (4) in the mean energy, $\langle\hat{H}\rangle \longrightarrow \langle\hat{H}'\rangle = \langle\hat{H}\rangle + \langle\delta\hat{H}\rangle$, taking the temporal derivative and using (7), one obtains

$$\partial_t\langle\hat{H}'\rangle = \partial_t\langle\hat{H}\rangle + \partial_t\langle\delta\hat{H}\rangle = \mathcal{J} + \mathcal{P} + \partial_t\langle\delta\hat{H}\rangle. \tag{11}$$

We can thus already conclude that the mean energy of the system, as well as its variation, changes for an applied gauge. In the sequence, we perform the remaining derivative in (11):

$$\begin{aligned}\partial_t\langle\delta\hat{H}\rangle &= \mathrm{Tr}(\delta\hat{H}\partial_t\hat{\rho}) + \langle\partial_t\delta\hat{H}\rangle\\ &= \mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}} + \langle\partial_t\delta\hat{H}\rangle,\end{aligned} \tag{12}$$

where the last equality is obtained by inserting the ME (2), using (3), and defining

$$\begin{aligned}\mathcal{J}_{\delta\hat{H}} &:= \mathrm{Tr}[\delta\hat{H}\mathfrak{D}(\hat{\rho})] = -\frac{g_{\mu\nu}}{\hbar}\mathrm{Re}\langle\hat{L}_\mu^\dagger[\hat{L}_\nu,\delta\hat{H}]\rangle,\\ \mathcal{C}_{\delta\hat{H}} &:= \mathrm{Tr}[\delta\hat{H}\mathfrak{U}(\hat{\rho})] = \frac{i}{\hbar}\langle[\hat{H},\delta\hat{H}]\rangle.\end{aligned} \tag{13}$$

Finally, collecting all these calculations,

$$\partial_t\langle\hat{H}'\rangle = \mathcal{J} + \mathcal{P} + \mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}} + \langle\partial_t\delta\hat{H}\rangle, \tag{14}$$

which is the action of the gauge transformations into Eq. (7).

While the dynamics governed by the ME is invariant, the quantum counterpart of the first law—provided by Alicki's definitions in Eq. (7)—is not invariant and acquires other components. Fortunately, all gauge-induced contributions in (14) have a precise physical meaning. Compared with $\mathcal{P}$ in (8), $\langle\partial_t\delta\hat{H}\rangle$ is a power component due to the Hamiltonian $\delta\hat{H}$, as well as, $\mathcal{J}_{\delta\hat{H}}$ in (13) is a current with the same structure as $\mathcal{J}$ in (9). In Eq. (13), $\mathcal{C}_{\delta\hat{H}}$ is the mean value of the unitary evolution (the commutator with the system Hamiltonian $\hat{H}$) of the operator $\delta\hat{H}$, thus another power component. Noteworthy, all these gauge contributions are mean values of Hermitian operators (observables), as well as $\mathcal{J}$ and $\mathcal{P}$.

B. Covariance of the first law

To go deeper into our analysis, the individual behavior of each thermodynamical quantity in Eq. (7) will be explored in order to give a precise meaning to formula (14).

Each of the system currents (10) under a gauge (4) becomes

$$\mathcal{J}_\mu \longrightarrow \mathcal{J}'_\mu = -\frac{1}{\hbar}\delta_{\mu\kappa}g_{\kappa\nu}\mathrm{Re}\langle\hat{L}_\kappa'^\dagger[\hat{L}'_\nu,\hat{H}+\delta\hat{H}]\rangle, \tag{15}$$

where $\hat{L}'_\mu$ is defined in (4) and $\delta\hat{H}$ in (5). Summing up for all μ, after tedious but straightforward manipulations, the transformed current reads

$$\mathcal{J} \longrightarrow \mathcal{J}' := \sum_{\mu=1}^{M}\mathcal{J}'_\mu = \mathcal{J} + \mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}}, \tag{16}$$

i.e., the total current, which itself is noninvariant, accounts for both quantities (13), see Eq. (12). For the Lindblad power $\mathcal{P}$ in (8), applying the symmetry transformation (4), one gets

$$\mathcal{P} \longrightarrow \mathcal{P}' = \langle\partial_t\hat{H}'\rangle = \langle\partial_t(\hat{H}+\delta\hat{H})\rangle = \mathcal{P} + \langle\partial_t\delta\hat{H}\rangle, \tag{17}$$

and the remaining gauge contribution $\langle\partial_t\delta\hat{H}\rangle$ in (12) comes from the noninvariance of the power.

Consistently, it should be noted that $\mathcal{J}'$ in (16) is equal to

$$\mathcal{J}' = \mathrm{Tr}(\hat{H}'\partial_t\hat{\rho}) = \mathrm{Tr}[\hat{H}\mathfrak{D}(\hat{\rho})] + \mathrm{Tr}(\delta\hat{H}\partial_t\hat{\rho}), \tag{18}$$

in accordance with $\mathcal{J}$ in Eq. (8) and $\mathrm{Tr}(\delta\hat{H}\partial_t\hat{\rho}) = \mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}}$ from (12).

Summing the above expression for $\mathcal{J}'$ with $\mathcal{P}'$ in (17), one attains a gauge *covariant* expression for the first law:

$$\partial_t\langle\hat{H}'\rangle = \mathrm{Tr}(\hat{H}'\partial_t\hat{\rho} + \hat{\rho}\partial_t\hat{H}') = \mathcal{J}' + \mathcal{P}', \tag{19}$$

which is simply a consequence of the linearity of both temporal derivative and trace operations in Eqs. (7) and (8).

The noninvariance of the mean energy $\langle\hat{H}'\rangle \neq \langle\hat{H}\rangle$ is the root of all gauge-induced contributions, see Eqs. (11) and (12), and deserves some comments regarding the energy-conservation. Gauges are ascribed to information lack owing to the trace in (1) [24], which means that many operators $\hat{H}_{\mathrm{SE}}$ and $\hat{\rho}_{\mathrm{E}}$ raise the same ME (2), which only contains information about the system state $\hat{\rho}$. The noninvariance of the energy, $\langle\hat{H}'\rangle = \langle\hat{H}\rangle + \langle\delta\hat{H}\rangle$, is thus a comparison between two different global systems SE. For each of these, the mean value of the global Hamiltonian, say $\hat{H}_{\rm SE}$ or $\hat{H}'_{\rm SE}$, determines the total energy, and the partial trace in (1) selects the corresponding part of the system, determined by $\hat{H}$ or $\hat{H}'$, which does not contradict the global energy conservation for each global system.

C. The interplay among generators

Ultimately, a gauge transformation is an interplay of the operator $\delta\hat{H}$ between the generators $\mathfrak{U}$ and $\mathfrak{D}$, see Eq. (6). To explore this observation thermodynamically, we make a digression and consider a slightly different situation without gauge transformations.

Consider a ME given by

$$\partial_t\hat{\rho} = \mathfrak{L}_1(\hat{\rho}) := \mathfrak{U}'(\hat{\rho}) + \mathfrak{D}(\hat{\rho}), \quad \mathfrak{U}' = \mathfrak{U} + \frac{i}{\hbar}[\bullet, \hat{V}], \quad (20)$$

with $\mathfrak{U}$ and $\mathfrak{D}$ as in (3), i.e., the dynamics is described by a ME (2) with the Hamiltonian $\hat{H}' = \hat{H} + \hat{V}$ and Lindblad operators $\hat{L}_\mu$. Equivalently, it is possible to write for the same ME that

$$\partial_t\hat{\rho} = \mathfrak{L}_2(\hat{\rho}) := \mathfrak{U}(\hat{\rho}) + \mathfrak{D}''(\hat{\rho}), \quad \mathfrak{D}'' := \mathfrak{D} + \frac{i}{\hbar}[\bullet, \hat{V}]. \quad (21)$$

If and only if the potential term $\hat{V}$ is a Hermitian linear combination of $\hat{L}_\mu$, the same Lindblad operators appearing in the generator $\mathfrak{D}$, it is possible to write $\hat{V} = \delta\hat{H}$ for some set of functions $\{U_{\mu\nu}, \gamma_\mu, \phi\}$ in (5). As learned in (6), for $\hat{V}$ written as (5), it is possible to regroup the generator $\mathfrak{D}''$ in (21) as

$$\mathfrak{D}''(\hat{\rho}) = -\frac{g_{\mu\nu}}{2\hbar}(\{\hat{L}''^{\dagger}_\mu\hat{L}''_\nu, \hat{\rho}\} - 2\hat{L}''_\mu\hat{\rho}\hat{L}''^{\dagger}_\nu),$$

with $\hat{L}''_\mu = U_{\mu\nu}\hat{L}_\mu - \gamma_\mu$; note the different signs in (21) and in (6). Therefore, the same evolution is ruled by an equivalent ME, $\partial_t\hat{\rho} = \mathfrak{L}_2(\hat{\rho})$, with $\hat{L}''_\mu$ and $\hat{H} = \hat{H}' - \hat{V}$.

From the thermodynamical point of view, energy, currents, and power definitions are corrupted by the interplay of $\hat{V} = \delta\hat{H}$, and the reason is the same as before: the mean energy of the system changes, as well as, its distribution among heat and work. For the generator $\mathfrak{L}_1$ in (20), we have $\mathrm{Tr}[\hat{H}'\mathfrak{U}'(\hat{\rho})] = 0$, thus

$$\partial_t\langle\hat{H}'\rangle = \mathrm{Tr}[\hat{H}'\mathfrak{L}_1(\hat{\rho})] + \langle\partial_t\hat{H}'\rangle = \mathcal{J} + \mathcal{J}_{\delta\hat{H}} + \mathcal{P}'$$

for $\mathcal{J}$ in (8), $\mathcal{J}_{\delta\hat{H}}$ in (13), and $\mathcal{P}'$ in (17). However, the generator $\mathfrak{L}_2$ in (21) reads

$$\partial_t\langle\hat{H}\rangle = \mathrm{Tr}[\hat{H}\mathfrak{L}_2(\hat{\rho})] + \langle\partial_t\hat{H}\rangle = \mathcal{J} - \mathcal{C}_{\delta\hat{H}} + \mathcal{P},$$

for $\mathcal{J}$ and $\mathcal{P}$ both in (8), and $\mathcal{C}_{\delta\hat{H}}$ in (13). Therefore, like for a gauge transformation, a simple redistribution of the potential $\hat{V}$ among the ME generators breaks the dichotomy heat-work given by Alicki's definitions in (8). Besides, the gauge-induced terms in (12) appear on both versions of the first law above as a consequence of the redistribution, which indicates that those terms need to be correctly accounted when considering the thermodynamics of a quantum system governed by a ME.

Far from pure theoretical curiosity, this interplay may happen in truly physical systems, which is the case of the infamous phenomenon of resonance fluorescence, see for instance Refs. [8,24]. In such cases, the dynamics is modeled by a Markovian Lindblad ME (2) with $M = 2$, $\mu \in \{+, -\}$, $g_{\mu\nu} = \delta_{\mu\nu}$ and

$$\hat{H}' = \frac{1}{2}\hbar\omega_0\hat{\sigma}_z + \hat{V}, \quad \hat{V} := \hbar\Omega(e^{-i\omega t}\hat{\sigma}_+ + e^{+i\omega t}\hat{\sigma}_-),$$
$$\hat{L}_\pm = \lambda_\pm\hat{\sigma}_\pm, \quad \lambda_\pm := \sqrt{\hbar\Gamma(\bar{n} \mp 1/2 + 1/2)},$$

where $\hat{\sigma}_z$ and $\hat{\sigma}_\pm$ are the standard SU(2) matrices, ω_0 is an atomic frequency transition, ω is a coherent laser frequency, the Rabi frequency is Ω, the decaying rate is Γ, and $\bar{n}$ is the mean-occupation number of a reservoir. The interaction term can be written as $\hat{V} = \delta\hat{H}$ in Eq. (5) using the functions

$$\gamma_\pm = -i\hbar\Omega\lambda_\pm^{-1}e^{\pm i\omega t}, \quad \phi = 0, \quad U_{\mu\nu} = \delta_{\mu\nu}.$$

The ME can thus be written as in (20) with $\hat{H}'$ and $\hat{L}_\mu$ above or equivalently by (21) for the operators

$$\hat{H} = \tfrac{1}{2}\hbar\omega_0\hat{\sigma}_z, \quad \hat{L}''_\pm = \lambda_\pm\hat{\sigma}_\pm - \gamma_\pm.$$

Remarkably the atom-field interaction $\hat{V} = \hat{H}' - \hat{H} = \delta\hat{H}$ manifests itself as an affine transformation of the Lindblad operators, as in Eq. (4).

After all, although we start saying that we were not dealing with gauges to treat the interplay, it can be understood as such. Consider the evolution given by (20) with $\hat{H} = \hat{H}_0 + \hat{V}$ and $\hat{V}$ written as (5). The gauge transformation $\hat{L}'_\mu = U_{\mu\nu}\hat{L}_\nu - \gamma_\mu$ translates the Hamiltonian $\hat{H}$ by $\delta\hat{H} = -\hat{V}$, see Eq. (4), and the transformed Hamiltonian is $\hat{H}' = \hat{H}_0$. After the gauge, the same dynamics will be governed by an ME with generators written as (6).

D. Statistical interpretation of heat and work

As established by statistical physics [39], *work* is associated with changes in the system energy levels $\hat{H} \to \hat{H} + \Delta\hat{H}$, and *heat* to variation of populations $\hat{\rho} \to \hat{\rho} + \Delta\hat{\rho}$. This dichotomy is naturally accomplished by the ME (2) in terms of the power $\mathcal{P}$ and of the current $\mathcal{J}$, both in (8), since $d(\hat{\rho}\hat{H}) = \hat{\rho}d\hat{H} + d\hat{\rho}\hat{H}$. However, despite the covariance of the first law in (19), the dichotomy is not so clear when we consider gauge transformations, and the reason is the acquired contributions for the power $\mathcal{P}'$ in (17) and for the current $\mathcal{J}'$ in (16). In what follows, we explore their physical meaning and their relations with this statistical interpretation.

The component $\mathcal{C}_{\delta\hat{H}}$ in (16) is a remarkable consequence of gauge transformations. The origin of this piece, defined in (13), is fundamentally related to the change in the energy-eigenstates[3] by the gauge transformation, it is thus a genuine quantum effect without a classical counterpart. Not for nothing, it is a power contribution that appears in the current (16) or a power piece provided by the interaction with the environment. In detail, if we consider a transformation in (4), which preserves the energy eigenstates, i.e., one gauge such that $[\hat{H}', \hat{H}] = 0$, then $\mathcal{C}_{\delta\hat{H}} = 0$. Otherwise, if $[\hat{H}', \hat{H}] \neq 0$, the gauges change the eigenstates, which is the origin of $\mathcal{C}_{\delta\hat{H}}$. The

[3]From the spectral decomposition $\hat{H} = \sum_n E_n|n\rangle\langle n|$, the variation of the energy has a contribution from the eigenvalues and another from the eigenvectors: $d\hat{H} = \sum_n dE_n|n\rangle\langle n| + E_n d[|n\rangle\langle n|]$.

discrimination of a term directly in the first law (7) related to eigenvectors variation is performed in works [15,17].

If the ME has operators satisfying $[\hat{L}_\mu, \hat{H}] = 0\ \forall\ \mu$, all the individual currents (10) are null, consequently $\mathcal{J} = 0$ in (9). The Lindblad operators, which are diagonal in the energy eigenbasis, do not promote energy transitions, i.e. $\hat{L}_\mu|n\rangle$ belongs to the same ray as the energy eigenket $|n\rangle$, which is the reason behind $\mathrm{Tr}[\mathfrak{D}(\hat{\rho})\hat{H}] = 0$, see (8). This can also be seen in writing $\mathrm{Tr}[\mathfrak{D}(\hat{\rho})\hat{H}] = \langle \mathfrak{D}^+(\hat{H})\rangle$, for the adjoint operator $\mathfrak{D}^+$ [24]. The above commutation relations are equivalent to $\mathfrak{D}^+(\hat{H}) = 0$, which annihilates the heat contribution $d\hat{\rho}\hat{H}$ to the mean energy variation. Besides, the only gauge contribution to $\mathcal{J}'$ in (16) is the current $\mathcal{J}_{\delta\hat{H}}$, since $\mathcal{C}_{\delta\hat{H}} = 0$ due to $[\hat{H}', \hat{H}] = [\delta\hat{H}, \hat{H}] = 0$ for $\delta\hat{H}$ in (5).

In a system described by an ME with Lindblad operators such that $[\hat{L}_\mu, \hat{L}_\nu] = [\hat{L}_\mu, \hat{L}_\nu^\dagger] = 0\ \forall\ \mu, \nu$, from Eq. (5), $[\hat{L}_\mu, \delta\hat{H}] = [\hat{L}_\mu^\dagger, \delta\hat{H}] = 0\ \forall\ \mu$, then $\mathcal{J}_{\delta\hat{H}} = 0$ in (13) by the same physical reason of the nullity of $\mathcal{J}$. In this case, the gauge contributions are the power in (17) and $\mathcal{C}_{\delta\hat{H}}$ in (16). Even when the system in question further satisfies $[\hat{L}_\mu, \hat{H}] = 0\ \forall\ \mu$, the power $\mathcal{P}'$ is still given by (17) and the system is still gauge-dependent, despite $\mathcal{J}_{\delta\hat{H}} = \mathcal{C}_{\delta\hat{H}} = 0$. In Sec. VI, as an example, we present a system satisfying all these commutation relations. Consider an *autonomous system*, the one in which the evolution is governed by (2) with time-independent operators: $\partial_t\hat{H} = \partial_t\hat{L}_\mu = 0\ \forall\ \mu$. For this class of systems, which contains the Lindblad ME, the power is always null, $\mathcal{P} = 0$, see Eq. (8). However, $\mathcal{P}'$ in (17) may not be, due to the temporal dependence of the parameters in (5). Even for a gauge described by time-independent functions $\{U_{\mu\nu}, \gamma_\mu, \phi\}$, where now it is also true that $\mathcal{P}' = 0$ due to $\partial_t\delta\hat{H} = 0$, the current (16) is not invariant, as well as the first law, since $\mathcal{J}_{\delta\hat{H}}$ and $\mathcal{C}_{\delta\hat{H}}$ in (13) does not vanish for an autonomous system.

Even the thermodynamics of a noninteracting system is gauge-dependent. If $\hat{L}_\mu = 0\ \forall\ \mu$, the ME (2) becomes the Liouville-von Neumann unitary evolution

$$\partial_t\hat{\rho} = \mathfrak{U}(\hat{\rho}) = \frac{i}{\hbar}[\hat{\rho}, \hat{H}], \tag{22}$$

which warrants $\mathcal{J} = 0$, as expected for an isolated system, see Eq. (8). The addition of a dynamical phase, $\hat{H} \to \hat{H}' = \hat{H} + \phi(t)$, is a gauge symmetry of the unitary evolution, which generates a power contribution for the system energy:

$$\partial_t\langle\hat{H}'\rangle = \mathcal{P}' = \mathcal{P} + \partial_t\phi,$$

according to Eq. (14) with $\delta\hat{H} = \phi(t)$, see Eq. (5), and $\mathcal{J}_{\delta\hat{H}} = \mathcal{C}_{\delta\hat{H}} = 0$, due to $\hat{L}_\mu = 0$, see Eq. (13). Note that this very same gauge symmetry is also present in the dynamical map (1) through the unitary evolution associated with the global Hamiltonian $\hat{H}_{\mathrm{SE}}$.

III. THERMODYNAMICAL INVARIANCE

In the scenario described so far, gauges influence the thermodynamics of a system, raising the question about the existence of a possible invariant thermodynamical behavior and under what conditions this invariance is manifested.

Following the description in Eq. (16), the invariance of the Lindblad total current is attained when

$$\mathcal{J}' = \mathcal{J} \iff \mathrm{Tr}(\partial_t\hat{\rho}\delta\hat{H}) = \mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}} = 0, \tag{23}$$

and from (17) the invariance of the Lindblad power is such that

$$\mathcal{P}' = \mathcal{P} \iff \langle\partial_t\delta\hat{H}\rangle = 0. \tag{24}$$

In this way, the first law in (7) is invariant provided the conditions of invariance of the current in (23) and of power in (24) are met, as it should be. However, the condition for the invariance of the mean energy (or its rate) is

$$\langle\hat{H}'\rangle = \langle\hat{H}\rangle \iff \langle\delta\hat{H}\rangle = 0 \implies \partial_t\langle\delta\hat{H}\rangle = 0, \tag{25}$$

which is only a necessary condition for both current and power invariances, since $\langle\delta\hat{H}\rangle = 0$ means neither (23) nor (24).

Let us give a closer look to condition (24). Using the definition in (5), one writes

$$\langle\partial_t\delta\hat{H}\rangle = \mathrm{Im}\langle g_{\mu\nu}\dot{\gamma}_\mu^* U_{\nu\kappa}\hat{L}_\kappa\rangle + \mathrm{Im}\langle g_{\mu\nu}\gamma_\mu^*\dot{U}_{\nu\kappa}\hat{L}_\kappa\rangle + \mathrm{Im}\langle g_{\mu\nu}\gamma_\mu^* U_{\nu\kappa}\partial_t\hat{L}_\kappa\rangle + \partial_t\phi.$$

Consequently, the invariance in (24) for any gauge (4), i.e., for arbitrary functions γ_μ, $U_{\mu\nu}$, and ϕ, becomes

$$\langle\partial_t\delta\hat{H}\rangle = 0 \iff \partial_t\phi = \langle\hat{L}_\mu\rangle = \langle\partial_t\hat{L}_\mu\rangle = 0\ \forall\ \mu. \tag{26}$$

The invariance condition in (23), using $\delta\hat{H}$ from (5), becomes $\mathrm{Im}[g_{\mu\nu}\gamma_\mu^* U_{\nu\kappa}\mathrm{Tr}(\hat{L}_\kappa\partial_t\hat{\rho})] = 0$. For arbitrary gauge functions, this is the same as

$$\mathrm{Tr}(\hat{L}_\mu\partial_t\hat{\rho}) = \partial_t\langle\hat{L}_\mu\rangle - \langle\partial_t\hat{L}_\mu\rangle = 0\ \forall\ \mu. \tag{27}$$

Finally, one can write

$$\mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}} = 0 \iff \partial_t\langle\hat{L}_\mu\rangle = \langle\partial_t\hat{L}_\mu\rangle\ \forall\ \mu. \tag{28}$$

The statements in (26) and in (28) are, in principle, independent of each other. However, to obtain a consistent description for the first law, expressed as (7), where each term (energy, power, and current) is invariant under all possible gauges of the ME, it is necessary and sufficient to have

$$\partial_t\phi = \langle\hat{L}_\mu\rangle = \langle\partial_t\hat{L}_\mu\rangle = 0\ \forall\ \mu. \tag{29}$$

For an autonomous system, these reduce to $\partial_t\phi = \langle\hat{L}_\mu\rangle = 0$.

The standard first law (7) works well for invariant systems since $\mathcal{J}$ and $\mathcal{P}$ are not affected by any possible gauge of the system. Notwithstanding, the invariance conditions (29) are very restrictive: they must be satisfied at any time, including system initial state. We are thus led to conclude that the thermodynamics of the vast majority of systems is influenced by the gauge symmetries of the ME and requires a consistent interpretation based on Eqs. (16), (17), and (19). We provide this interpretation in Sec. IV, but, before, we spend some words discussing the conditions and presenting an important class of invariant systems.

A. Invariance conditions

Here we will explore the physical meaning of the invariance conditions in Eq. (29) and its relation with the system thermodynamics.

A time-dependent phase $\phi(t)$ would continuously change the energy of the system. Since it appears as part of the Hamiltonian through $\delta\hat{H}$, see Eq. (5), it will be properly quantified by work. Therefore, $\partial_t\phi = 0$ in (29) is related to the invariance of power, see (24). For a constant phase, all the system energy levels will be shifted as a mere redefinition of the ground-state energy, as in the Schrödinger equation. We return to this point in Sec. IV A.

Condition $\langle\hat{L}_\mu\rangle = 0$ implies that the energy contribution $\delta\hat{H}$ promoted by any gauge, see Eqs. (4) and (5), does not impact the internal energy of the system on average, $\langle\hat{H}'\rangle = \langle\hat{H}\rangle$. Assuming that $\hat{\rho}$ is expanded in the eigenbasis of the system Hamiltonian $\hat{H}$, and that $\hat{L}_\mu$ stands for a projector operator at some definite level of this Hamiltonian, then the mean value $\langle\hat{L}_\mu\rangle$ will be the time-dependent occupation probability of this level. Condition $\langle\hat{L}_\mu\rangle = 0$ will be fulfilled for a vanishing occupation probability, which can occur solely for specific initial states. Furthermore, if $\hat{L}_\mu$ stands for some energy transition, i.e., it is a jump operator, then $\langle\hat{L}_\mu\rangle$ becomes a probability amplitude. The invariance condition requires the vanishing of this amplitude for all time, which again depends on the particular initial state.

For a generic time-dependent Lindblad operator, the invariance conditions must include $\langle\partial_t\hat{L}_\mu\rangle = 0$. From Eq. (17) and $\delta\hat{H}$ in (5), this condition ensures the power invariance due to $\langle\partial_t\delta\hat{H}\rangle = 0$. Note that, if the energy and power are invariant, logically the current will either be, mathematically this is expressed in Eqs. (27) and (28) when the former conditions $\partial_t\phi = \langle\hat{L}_\mu\rangle = 0$ are valid.

Among many possibilities for the temporal dependence of the Lindblad operators, the particular case $\hat{L}_\mu = \omega_\mu(t)\hat{A}_\mu$ for a time-independent $\hat{A}_\mu$ turns the third invariance condition into $\langle\partial_t\hat{L}_\mu\rangle = \dot{\omega}_\mu\hat{A}_\mu = 0$, which is analogous to the previous discussion in terms of probabilities. Actually, even for a generic time-dependence, when the condition $\langle\hat{L}_\mu\rangle = 0$ is met, the condition $\langle\partial_t\hat{L}_\mu\rangle = 0$ is subsidiary since applying (27) implies $\langle\partial_t\hat{\rho}\hat{L}_\mu\rangle = 0$, which, for an infinitesimal evolution, shows that $\langle\hat{\rho}(t+dt)\hat{L}_\mu\rangle = \langle\hat{\rho}(t)\hat{L}_\mu\rangle$, i.e., $\langle\hat{L}_\mu\rangle$ is constant. Although subsidiary, this condition is necessary for the invariance of the current through (27).

B. Quantum detailed balance

Although specific, a significant property of some MEs is their ability to drive the system toward thermal equilibrium. In analogy with classical stochastic processes, this property is mathematically expressed by the so-called quantum detailed balance conditions (QDBCs) [32].

For a time-independent Hamiltonian $\hat{H}_{\rm S}$ with non-null Bohr frequencies $\omega_1,\dots,\omega_n$ and an autonomous Lindblad ME, governing the evolution of the system, composed by Lindblad operators $\hat{A}_\mu$ and by another Hamiltonian $\hat{H}$, the QDBCs are

(a) $[\hat{H}_{\rm S},\hat{H}] = 0$;

(b) $\hat{U}_{\rm S}^\dagger\hat{A}_\mu\hat{U}_{\rm S} = e^{-i\omega_\mu t}\hat{A}_\mu, \quad \hat{U}_{\rm S} := e^{-\frac{i}{\hbar}\hat{H}_{\rm S}t}$;

(c) $\hat{A}_{\mu+n} = e^{-\frac{1}{2}\beta\hbar\omega_\mu}\hat{A}_\mu^\dagger, \quad 1\leqslant\mu\leqslant n$.

The physical consequence of these conditions will be described in a while, just after we show the main result of this part: a ME satisfying these QDBC is thermodynamically invariant under gauges transformations.

Under condition (c), the generator $\mathfrak{D}$ in (3) becomes

$$\tilde{\mathfrak{D}}(\hat{\rho}) = -\frac{1}{2\hbar}\sum_{\mu=1}^{n}(\{\hat{A}_\mu^\dagger\hat{A}_\mu,\hat{\rho}\} - 2\hat{A}_\mu\hat{\rho}\hat{A}_\mu^\dagger)(1-e^{-\hbar\beta\omega_\mu}).$$

Note that condition (c) imposes $M = 2n$ in (2).

Using condition (b) in the above generator $\tilde{\mathfrak{D}}$, it is possible to show that $\hat{U}_{\rm S}\tilde{\mathfrak{D}}(\hat{\rho})\hat{U}_{\rm S}^\dagger = \tilde{\mathfrak{D}}(\hat{U}_{\rm S}\hat{\rho}\hat{U}_{\rm S}^\dagger)$; from condition (a), immediately one has $\hat{U}_{\rm S}\mathfrak{U}(\hat{\rho})\hat{U}_{\rm S}^\dagger = \mathfrak{U}(\hat{U}_{\rm S}\hat{\rho}\hat{U}_{\rm S}^\dagger)$ for the generator $\mathfrak{U}$ in (3). Thus, the ME $\partial_t\hat{\rho} = \mathfrak{U}(\hat{\rho}) + \tilde{\mathfrak{D}}(\hat{\rho})$ satisfies $\hat{U}_{\rm S}(\partial_t\hat{\rho})\hat{U}_{\rm S}^\dagger = \partial_t(\hat{U}_{\rm S}\hat{\rho}\hat{U}_{\rm S}^\dagger)$, which implies $[\hat{\rho},\hat{H}_{\rm S}] = 0$ and $\hat{U}_{\rm S}\hat{\rho}\hat{U}_{\rm S}^\dagger = \hat{\rho}$.

Since $[\hat{\rho},\hat{H}_{\rm S}] = 0$, $\partial_t\hat{A}_\mu = 0$, and $\partial_t\omega_\mu = 0$, condition (b) is equivalently written as [32,33]

$$\hat{\chi}_{\rm S}^+\hat{A}_\mu\hat{\chi}_{\rm S}^- = e^{-\beta\hbar\omega_\mu}\hat{A}_\mu, \quad \hat{\chi}_{\rm S}^\pm := \exp[\pm\beta\hat{H}_{\rm S}],$$

which is nothing but a Wick-rotated version of (b). With this in hands, the cyclicity of the trace readily gives

$$\langle\hat{A}_\mu\rangle = \mathrm{Tr}(\hat{\rho}\hat{A}_\mu) = \mathrm{Tr}(\hat{\chi}_{\rm S}^-\hat{\rho}\hat{\chi}_{\rm S}^+\hat{A}_\mu) = e^{-\beta\hbar\omega_\mu}\langle\hat{A}_\mu\rangle,$$

from where $(e^{-\beta\hbar\omega_\mu}-1)\langle\hat{A}_\mu\rangle = 0$. As required by the QDBC $\omega_\mu \neq 0$, thus $\langle\hat{A}_\mu\rangle = 0\ \forall\ \beta\neq 0$.

Instead of using $\hat{\chi}_{\rm S}^\pm$, the same steps for the (unrotated) unitary operator $\hat{U}_{\rm S}$ would give $(e^{-i\omega_\mu t}-1)\langle\hat{A}_\mu\rangle = 0$, which certifies that the instant $t = 0$ corresponds to the value $\beta = 0$. Finally, we can conclude that $\langle\hat{A}_\mu\rangle = 0\ \forall\ t\neq 0$, which is the requisite in (29) for the thermodynamical invariance of an autonomous system, except for two facts: the initial state $\hat{\rho}(t=0)$ and the condition over ϕ. The discussion about the phase and its meaning in (29) will be postponed to Sec. IV A, till then, it will be taken for granted.

The invariance of currents, power, and energy of a system satisfying QDBC for the whole evolution will only be valid if its initial state is such that $\langle\hat{A}_\mu\rangle = 0$. If not, the thermodynamical invariance can possibly occur only for fixed points of the ME, these can be an asymptotic state, or even thermal equilibrium states, which move us back to the physical consequence of the QDBC.

For some dynamical semigroups, the QDBCs are necessary and sufficient conditions to

$$\lim_{t\to\infty}\hat{\rho}(t) = \hat{\chi}_{\rm S}^-/\mathrm{Tr}(\hat{\chi}_{\rm S}^-) = e^{-\beta\hat{H}_{\rm S}}/\mathrm{Tr}(e^{-\beta\hat{H}_{\rm S}}),$$

which means that the asymptotic state of the ME, also a fixed point, is the Gibbs state of the Hamiltonian $\hat{H}_{\rm S}$. As far as we know, this is only proved for dynamical semigroups of finite-dimensional quantum systems [32] and for Gaussian dynamical semigroups of continuous variables systems [33]—a very small set in the universe of MEs. Nonetheless, a generic ME that does not belong to this set can satisfy the QDBC and will be thermodynamically invariant throughout the whole evolution for a suitable choice of the initial state, as proved.

Examples of Markovian systems satisfying the QDBCs are the infamous quantum optics master equations for bosonic systems and discrete systems, including the decay of a two-level atom; for instance, see Sec. 3.4 of Ref. [24].

IV. GAUGE-DEPENDENT THERMODYNAMICS

From the dynamical point of view, it is impossible to discriminate what would be the proper gauge of the evolution since the dynamics is governed by a gauge-invariant ME. The only plausible way to distinguish between gauges, or to determine the amount of work and heat in a certain process, is a choice of measurements to be performed on the system. The internal energy $\langle \hat{H}' \rangle$ can be determined after the measurement of the corresponding operator $\hat{H}'$ in Eq. (4), associated with an infinite set of possible operators $\hat{L}'_\mu$, through the choice of $\delta\hat{H}$ in (5), one piece of $\hat{H}'$. A choice for the Hamiltonian is precisely the first step in modern tomographic methods [40].

Instead of considering the symmetries of the ME as an impossibility to determine the thermodynamical quantities correctly, we place our analysis on the classical interpretation ground: Each possible gauge defined by a choice of the functions $\{\gamma_\mu, U_{\mu\nu}, \phi\}$ in (4) represents a particular thermodynamical process (or path) with its own amount of heat and work.

Contrasting with classical thermodynamics, the energy is not a "state function", it varies according to the gauge (a thermodynamical path), $\langle \hat{H}' \rangle = \langle \hat{H} \rangle + \langle \delta\hat{H} \rangle$. In our scenario, state functions are gauge-invariant quantities, which depend solely on the system state $\hat{\rho}$; therefore, any function with domain in the space of density matrices is invariant, e.g., the von Neumann entropy and measures of non-Markovianity based on divisibility of quantum maps or on distinguishability of quantum states [25].

The thermodynamics embodied in the system evolution is only properly described by an ME written as $\partial_t \hat{\rho} = \mathfrak{L}'(\hat{\rho}) = \mathfrak{U}'(\hat{\rho}) + \mathfrak{D}'(\hat{\rho})$, for the generators in (6), where $\hat{H}'$ and $\hat{L}'_\mu$ are the operators in (4), which are defined by the set

$$\ell = \{\hat{H}, \hat{L}_\mu, \gamma_\mu, U_{\mu\nu}, \phi;\ \mu, \nu = 1, \dots, M\}, \tag{30}$$

the thermodynamical path or process. The projection of all paths sharing the same operators $\hat{H}$ and $\hat{L}_\mu$ is the path

$$\ell_0 = \{\hat{H}, \hat{L}_\mu;\ \mu = 1, \dots, M\}, \tag{31}$$

corresponding to the system evolution through the invariant ME, as pictorially represented in Fig. 1. Formally, the set ℓ_0 in (31) is an equivalence class of invariant dynamics under the group of transformations in (4). This class contains all sets ℓ defined by Eq. (30).

The heat Q_ℓ and the work W_ℓ along a path ℓ, thus gauge-dependent, are determined by $\mathcal{J}'$ in (16) and $\mathcal{P}'$ in (17):

$$\begin{aligned} Q_\ell &= \int_\ell \mathcal{J}' dt = \int_\ell (\mathcal{J} + \mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}}) dt, \\ W_\ell &= \int_\ell \mathcal{P}' dt = \int_\ell (\mathcal{P} + \langle \partial_t \delta\hat{H} \rangle) dt, \end{aligned} \tag{32}$$

for $\mathcal{P}$ and $\mathcal{J}$ both defined in (8), and $\mathcal{J}_{\delta\hat{H}}$ and $\mathcal{C}_{\delta\hat{H}}$ both defined in (13). Needless to say, $Q_\ell + W_\ell = \Delta\langle \hat{H}' \rangle$ is the integral representation of the first law in (19).

For thermodynamical-invariant systems, those satisfying the invariance conditions (29), all thermodynamical paths (30) collapse into ℓ_0, the path identified with the system evolution,

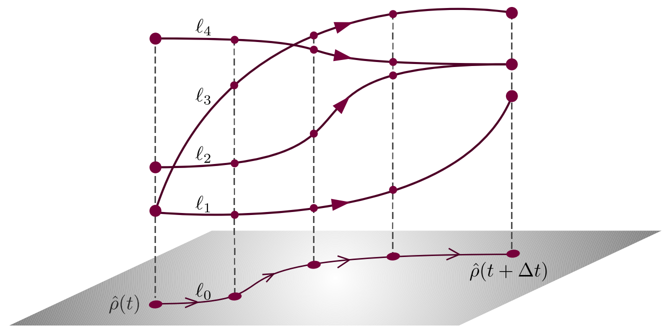

FIG. 1. Schematic representation of thermodynamical paths. Each of curves ℓ_1, ℓ_2, ℓ_3, and ℓ_4 represents a specific thermodynamical process, with its amount of heat and work. The covariance of the mean energy rate in (19) ensures the validity of the first law along each path since the sum of heat and work gives the variation of the (gauge-dependent) mean energy. These paths differ by the gauge parameters $\{\gamma_\mu, U_{\mu\nu}, \phi\}$ and are projected into a unique curve ℓ_0 in the state space, representing the system evolution and its invariance under gauge transformations. A gauge can even change during the evolution due to the temporal dependence of $\{\gamma_\mu, U_{\mu\nu}, \phi\}$, a situation depicted by the crossing curves.

thus $Q_\ell = Q_{\ell_0}$ and $W_\ell = W_{\ell_0}\ \forall\ \ell$, with

$$Q_{\ell_0} = \int_{\ell_0} \mathcal{J} dt, \quad W_{\ell_0} = \int_{\ell_0} \mathcal{P} dt, \quad \Delta\langle \hat{H} \rangle = Q_{\ell_0} + W_{\ell_0}. \tag{33}$$

For noninvariant systems, the differences

$$\begin{aligned} Q_\ell - Q_{\ell_0} &= \int_{\ell_0} (\mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}}) dt, \\ W_\ell - W_{\ell_0} &= \int_{\ell_0} \langle \partial_t \delta\hat{H} \rangle dt, \end{aligned} \tag{34}$$

are the gauge contributions for the heat and work and, of course, are related through $\Delta\langle \hat{H}' \rangle - \Delta\langle \hat{H} \rangle = \Delta\langle \delta\hat{H} \rangle$.

Path ℓ_0 is not special compared with the other paths ℓ, it is actually only a didactic reference, a choice for operators of the system, which can be anyone in (4) or any path (30). The only fixed quantity is the generator $\mathcal{L}$ of the ME since it is the same for any path. Once ℓ_0 is chosen, all the other paths, and all thermodynamical quantities, will be related to this one by gauge transformations (4).

In the end, we must say that there is nothing new regarding a path-dependence in quantum thermodynamics since two quantum states can be connected by the temporal evolution ruled by different MEs; in our description, these MEs are associated with different curves ℓ_0 in the state space (equivalence classes), see Fig. 1. Our interpretation resides on the association of different paths ℓ to the same state evolution.

A. Unitary dynamics and noninteracting systems

The analysis of this simple situation may be enlightening and paves the way to discussing the remaining point about the invariance condition $\partial_t \phi = 0$ in (26).

Regarding the unitary dynamics ruled by (22), mathematically the phase addition $\hat{H} \to \hat{H}' = \hat{H} + \phi(t)$ is a U(1) symmetry of the Liouville-von Neumann equation and a thermodynamical path $\ell = \{\hat{H}, \phi\}$ is the one-dimensional manifold of the unitary operator $\hat{U}_t'$, the solution of the Schrödinger equation $i\hbar\partial_t\hat{U}_t' = \hat{H}'\hat{U}_t'$. Two paths, say $\ell_1 = \{\hat{H}, \phi_1\}$ and $\ell_2 = \{\hat{H}, \phi_2\}$, are members of the equivalence class $\ell_0 = \{\hat{H}\}$, the manifold of the unitary operator satisfying $i\hbar\partial_t\hat{U}_t = \hat{H}\hat{U}_t$.

Of course, the phase $\phi(t)$ is a global and instantaneous shift of the energy levels, which does not change the system dynamics (22), however, it does cause a change in system energy, thermodynamically accounted by the work in (32) with $\delta\hat{H} = \phi(t)$, $\mathcal{C}_{\delta\hat{H}} = 0$, and $\mathcal{P} = \langle\partial_t\hat{H}\rangle$. As a trivial example, the phase $\phi(t) = \frac{1}{2}\hbar\omega(t)$ is a power source appearing in the time-dependent Hamiltonian $\hat{H} = \hbar\omega(t)\hat{n} + \phi(t)$ of the harmonic oscillator; some thermodynamical properties of this system were described in Ref. [12].

We now return to the point regarding the phase and the thermodynamical invariance. Whereas ϕ has its origin in a gauge transformation, the condition $\partial_t\phi = 0$ in Eq. (26), and also in Eq. (29), is awkward. Nevertheless, ϕ appears as a source of power for a system governed by a ME through $\delta\hat{H}$, see Eqs. (17) and (5), in the same way as it appears in the unitary evolution, where the power is unequivocally defined and addition of phases simply describes the gauge group. Strictly speaking, there is no thermodynamical invariance at all if one is free to add a time-dependent phase to the Hamiltonian. As in the unitary dynamics, the phase will change the energy of a system governed by a ME (2). Besides $\langle\hat{L}_\mu\rangle = \langle\partial_t\hat{L}_\mu\rangle = 0$, imposing the invariance condition for ϕ in (29) is actually a restriction of the allowed gauge functions.

B. Analysis of particular processes

Among all possible gauges, it is interesting to pinpoint some particular thermodynamical features associated with specific processes for generic noninvariant systems.

(i) *Energy preservation.* The internal energy of a system is not gauge-invariant, $\langle\hat{H}'\rangle = \langle\hat{H}\rangle + \langle\delta\hat{H}\rangle$, see Eq. (14). Notwithstanding, there are many paths ℓ in (30) such that $\langle\hat{H}'\rangle = \langle\hat{H}\rangle$: these are the ones such that $\langle\delta\hat{H}\rangle = 0$, of course.[4]

Considering the ME with the transformed generators (6), the suitable choice $\gamma_\mu = U_{\mu\nu}\langle\hat{L}_\nu\rangle$ and $\phi = 0$ designs a path ℓ such that $\delta\hat{H} = \frac{g_{\mu\nu}}{2i}[\langle\hat{L}_\mu^\dagger\rangle\hat{L}_\nu - \langle\hat{L}_\mu\rangle\hat{L}_\nu^\dagger]$, according to (5). Consequently, $\langle\delta\hat{H}\rangle = 0$ and $\langle\hat{H}'\rangle = \langle\hat{H}\rangle$. For the chosen gauge, the current is given by (16) and the power by (17) for the above $\delta\hat{H}$ and, following (12), these are related through $\mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}} = -\langle\partial_t\delta\hat{H}\rangle$. Note that this is true for any matrix $\mathbf{U}$, since the attained $\delta\hat{H}$ does not depend on it.

For the same purpose, another path ℓ is determined by the choice

$$\phi = -\frac{g_{\mu\nu}}{2i}(\gamma_\mu^* U_{\nu\kappa}\langle\hat{L}_\kappa\rangle - \gamma_\mu U_{\nu\kappa}^*\langle\hat{L}_\kappa^\dagger\rangle),$$

which, according to (5), is such that $\langle\delta\hat{H}\rangle = 0$. Now Eq. (14) gives $\mathcal{J} + \mathcal{P} = \mathcal{J}' + \mathcal{P}'$ for any γ_μ and any $\mathbf{U}$.

If in ℓ_0, the work exactly balances heat, *i.e.*, $\mathcal{P} = -\mathcal{J}$, the energy of the system following ℓ_0 will be conserved, $\partial_t\langle\hat{H}\rangle = 0$, according to (7). Above designed gauges are specifically useful to preserve this conservation since another generic gauge transformation will generate a path with nonconserved internal energy $\langle\hat{H}'\rangle$ such that $\partial_t\langle\hat{H}'\rangle = \partial_t\langle\delta\hat{H}\rangle$, obtained from Eqs. (12) and (14) with $\mathcal{P} = -\mathcal{J}$.

(ii) *Power preservation.* Consider the following phase:

$$\phi = -\frac{1}{2i}\int_0^t \langle\partial_\tau(g_{\mu\nu}\gamma_\mu^* U_{\nu\kappa}\hat{L}_\kappa - g_{\mu\nu}\gamma_\mu U_{\nu\kappa}^*\hat{L}_\kappa^\dagger)\rangle d\tau,$$

which defines a path ℓ_1 such that $\mathcal{P}' = \mathcal{P}$, see (17), since $\langle\partial_t\delta\hat{H}\rangle = 0$. The current will be the one in Eq. (16) with $\mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}} = \partial_t\langle\delta\hat{H}\rangle$. Beyond that, one can choose a path ℓ_2 for the same phase above and also take $\gamma_\mu = U_{\mu\nu}\langle\hat{L}_\nu\rangle$ for a generic $\mathbf{U}$, then $\langle\delta\hat{H}\rangle = \phi$. However $\mathcal{J}' = \mathcal{J} + \partial_t\phi$ and $\langle\hat{H}'\rangle = \langle\hat{H}\rangle + \phi$ in ℓ_2. Even in the particular case of an autonomous ME, $\mathcal{J}' \neq \mathcal{J}$, despite $\mathcal{P}' = \mathcal{P} = 0$, since ϕ is in general a time-dependent function.

(iii) *Current preservation.* Since $\det\mathbf{U} \neq 0$, it is possible to choose γ_μ as a "**g**-orthogonal" vector to $\mathrm{Tr}[U_{\nu\kappa}\hat{L}_\kappa\partial_t\hat{\rho}]$, such that $g_{\mu\nu}\gamma_\mu^* U_{\nu\kappa}\mathrm{Tr}[\hat{L}_\kappa\partial_t\hat{\rho}] = 0$, according to which $\mathcal{J}' = \mathcal{J}$, as can be seen by inserting (5) into (18) and comparing with (16). Additionally, by choosing a phase ϕ such that $\langle\delta\hat{H}\rangle = 0$, like in (*i*), one obtains $\langle\hat{H}'\rangle = \langle\hat{H}\rangle$ and thus $\mathcal{P} = \mathcal{P}'$. This choice for the functions $\{\gamma_\mu, \phi\}$ designs infinite paths $\ell \neq \ell_0$, see Eq. (30), in which all thermodynamical quantities are preserved, i.e., they have the same value as in ℓ_0.

(iv) *Minimal dissipation.* For systems described by finite-dimensional Hilbert spaces, the gauge fixed by $U_{\mu\nu} = \delta_{\mu\nu}$ and $\gamma_\mu = -\mathrm{Tr}(\hat{L}_\mu)$ ensures $\mathrm{Tr}(\hat{L}_\mu') = 0$ in (4), which is the minimal dissipation condition postulated in Ref. [11].

V. ENTROPY PRODUCTION AND SECOND LAW

The von Neumann entropy $\mathcal{S} := -\langle\ln\hat{\rho}\rangle$ is a state function, an exclusive function of the density operator, thus invariant under gauge transformations. According to (2), its evolution is

$$\partial_t\mathcal{S} = -\mathrm{Tr}(\ln\hat{\rho}\,\partial_t\hat{\rho}) = \frac{g_{\mu\nu}}{\hbar}\mathrm{Re}\langle\hat{L}_\mu^\dagger[\hat{L}_\nu, \ln\hat{\rho}]\rangle, \tag{35}$$

which is also a state function. For concreteness, this conclusion can be achieved by inserting (4) into (35). The similarity of the above equation with the current in Eq. (8) is not a coincidence, it actually refers to the statistical interpretation [39]: currents are bonded to entropy changes since heat is associated with the variation of populations $d\hat{\rho} = \partial_t\hat{\rho}dt$, see Sec. II D.

The contraction of the relative entropy $S(\Phi_t[\hat{\rho}_0]|\Phi_t[\hat{\rho}_\star]) \leqslant S(\hat{\rho}_0|\hat{\rho}_\star)$ [6] under the CPTP map Φ_t in (1) associated with the ME in (2) enables us to define, as in the strictly Markovian case [4,24], the entropy production (EP)

$$\Sigma := S(\hat{\rho}_0|\hat{\rho}_\star) - S(\hat{\rho}_t|\hat{\rho}_\star) \geqslant 0, \tag{36}$$

and its rate

$$\mathcal{E} := \partial_t\Sigma = \partial_t\mathcal{S} + \partial_t\mathrm{Tr}(\hat{\rho}_t\ln\hat{\rho}_\star), \tag{37}$$

where $\partial_t\mathcal{S}$ is in (35), while the remaining term is related to the entropy flux due to heat exchange between S and E. In the above formulas, $\hat{\rho}_\star$ is a fixed point of the CPTP map, i.e., a solution of $\Phi_t[\hat{\rho}_\star] = \hat{\rho}_\star$.

[4]The system energy invariance by $\langle\delta\hat{H}\rangle = 0$ is the necessary condition expressed in (25).

Since $\mathcal{S}$ and $\partial_t\mathcal{S}$ are state functions, one can easily gather that both Σ and $\mathcal{E}$ are gauge-invariant, or also state functions. For a non-Markovian evolution, the EP rate in Eq. (37) can be momentarily negative, a feature associated with the break of P-divisibility of Φ_t [25], while Σ is always non-negative. The (non)positivity of the EP rate, as stated in this paragraph, is a vocable for the second law of thermodynamics in the quantum realm, and its violation (break of P-divisibility) is associated with non-Markovian effects [25].

Another formula for an EP rate found in Ref. [11] considers a situation in which system S is strongly coupled with a thermal bath (system E) at inverse temperature β:

$$\tilde{\mathcal{E}} = \partial_t\mathcal{S} - \beta\mathcal{J} = \frac{g_{\mu\nu}}{\hbar}\mathrm{Re}\langle\hat{L}_\mu^\dagger[\hat{L}_\nu, \beta\hat{H} + \ln\hat{\rho}]\rangle, \tag{38}$$

where $\beta\mathcal{J}$ is the flux associated with the total current in (8). Despite positive for a P-divisible map (equivalent to a Markovian ME) Φ_t [11,25], the expression for $\tilde{\mathcal{E}}$ will be invariant if and only if conditions (29) are satisfied, due to its dependence on $\mathcal{J}$. On another side, choosing a gauge like (iii) in Sec. IV B ensures the preservation of $\tilde{\mathcal{E}}$. Interestingly enough, $\tilde{\mathcal{E}}$ changes according to the current, see Eq. (16),

$$\tilde{\mathcal{E}}' = \tilde{\mathcal{E}} - \beta(\mathcal{J}' - \mathcal{J}) = \tilde{\mathcal{E}} - \beta(\mathcal{J}_{\delta\hat{H}} + \mathcal{C}_{\delta\hat{H}}), \tag{39}$$

in order to keep the invariance of $\partial_t\mathcal{S}$.

The expression in (38) was deduced from a specific gauge choice in Ref. [11], the minimal dissipation gauge, item (iv) in Sec. IV B, therefore there is no strangeness on its gauge dependence. The authors there consider an instantaneous Gibbs state of the Hamiltonian $\hat{H}$ present in the ME, the gauge-transformed version in (39) is obtained considering the evolution of the system governed by the transformed Hamiltonian $\hat{H} + \delta\hat{H}$.

The universal formulation of the EP, i.e., for arbitrary subsystems (E and S) and arbitrary dynamics, considers the system, the environment, and their joint unitary evolution [13]. Part of this information is suppressed by the trace in (1) and the expressions $\mathcal{E}$ and $\tilde{\mathcal{E}}$ were developed for specific ME scenarios. While Eq. (37) simply raises from the contraction of Φ_t, it requires explicitly a fixed point $\hat{\rho}_\star$, which is not a generic property of MEs. On another side, assuming that system E is a thermal environment, Eq. (38) deduced for the ME [11] coincides with the thermodynamical EP in Ref. [14].

VI. EXAMPLE: PURE DECOHERENCE MODEL

In the wake of open quantum systems, decoherence has a special appeal due to its relation with the quantum-classical border [27]. In this section, we study the gauge-thermodynamical behavior of the simpler non-Markovian system that captures the essence of this phenomenon, the pure decoherence model [24,25].

Let us consider the ME (2) for a two-level system with only one Lindblad operator and a Hamiltonian, respectively, given by

$$\hat{L} = \sqrt{\hbar|\Gamma(t)|}\hat{\sigma}_z, \quad \hat{H} = \frac{\hbar}{2}\omega\hat{\sigma}_z, \tag{40}$$

where $\hat{\sigma}_z$ is the standard Pauli matrix, ω is the transition frequency, and $\Gamma(t) \in \mathbb{R}$ is the decay rate, in principle, a generic time-dependent function. For this system, Eq. (2) has $M = 1$ and $\mathbf{g} =: g = \mathrm{sign}[\Gamma(t)]$.

The solution for the ME is easily obtained,

$$\rho_{00} = p = 1 - \rho_{11}, \quad \rho_{01}(t) = \rho_{01}e^{-i\omega t}D(t), \tag{41}$$

where $\rho_{ij}(t) = \langle i|\hat{\rho}(t)|j\rangle$ are the matrix elements of the density operator and we denote $\rho_{ij} = \rho_{ij}(t = 0)$. The initial populations $0 \leqslant p \leqslant 1$ and $1 - p$ are constant, which is not true for the coherence term $\rho_{01} = \rho_{10}^* \in \mathbb{C}$, the latter evolves according to the decoherence function $D(t) := \exp\{-\int_0^t \Gamma(s)ds\}$, which encapsulates all the decoherence properties of the system [24,27].

Directly from the solution above, for a given initial state with elements $\rho_{00} = p$ and ρ_{01}, the state

$$\hat{\rho}_\star = p|0\rangle\langle 0| + (1 - p)|1\rangle\langle 1| \tag{42}$$

is a fixed point of the dynamics. The long-term solution of the ME will converge as $\hat{\rho}(t \to \infty) = \hat{\rho}_\star$, if the decoherence effects destroy completely the initial-state coherence ρ_{01}, which will happen for $\lim_{t\to\infty} D(t) = 0$. The evolution will be Markovian if $D(t)$ decreases monotonically since the environment will progressively erase the coherences. Otherwise, the nonmonotonic behavior of $D(t)$ will raise non-Markovian effects since the environment will create coherence in the system [24,25,27]. Recalling that, to represent a physical system, $\hat{\rho}$ must be a positive operator, which implies $|\rho_{01}(t)| \leqslant (p - p^2)\ \forall\ t$, thus $|D(t)| \leqslant 1$. At least theoretically, one can consider any function $D(t)$ satisfying the positivity restriction; nevertheless, the system may not converge to $\hat{\rho}_\star$, which will still be a fixed point of the ME.

For the thermodynamical analysis, we first consider the path ℓ_0 defined in (31) for the operators in (40). The current in (9) is null, $\mathcal{J} = -\frac{g}{\hbar}\,\mathrm{Re}\langle\hat{L}_\mu^\dagger[\hat{L}_\nu, \hat{H}]\rangle = 0$, once $[\hat{H}, \hat{L}] = 0$. The power in (8) is also null, $\mathcal{P} = 0$, since $\partial_t\hat{H} = 0$. Consequently, the energy $\langle\hat{H}\rangle = \frac{1}{2}\hbar\omega(2p - 1)$ is constant for any initial state, according to (7). This clearly agrees with (33), which says that there is no heat exchange and no work performed by/on the system in path ℓ_0.

Using the expressions in (41), we find

$$\langle\hat{L}\rangle = (2p - 1)\sqrt{|\Gamma(t)|}, \quad \langle\partial_t\hat{L}\rangle = (2p - 1)\partial_t\sqrt{|\Gamma(t)|}.$$

Hence, according to conditions (29), nonequilibrium thermodynamical invariance is fulfilled solely for states with equally populated levels, i.e., $p = 1/2$. Since ρ_{00} and ρ_{11} are constant throughout the whole evolution, if the initial state is equally populated, the system will be thermodynamically invariant for any time. For such an initial state, the values of the thermodynamical quantities in ℓ_0, $\partial_t\langle\hat{H}\rangle = \mathcal{J} = \mathcal{P} = 0$, are the same for any gauge transformation (4) with $\partial_t\phi = 0$, which for this system is written as

$$\hat{L}' = e^{i\theta(t)}\hat{L} + \gamma(t), \quad \delta\hat{H} = g\sqrt{|\Gamma(t)|}\mathrm{Im}[\gamma(t)]\hat{\sigma}_z + \phi.$$

Each of the above gauge transformations defines a path ℓ according to (30), for simplicity in what follows we will consider paths such that $\theta(t) = 0$ and that $\gamma(0) = 0$.

For a noninvariant initial state, the internal energy in ℓ is

$$\langle\hat{H}'\rangle = \langle\hat{H}\rangle + \langle\delta\hat{H}\rangle = \left(\frac{1}{2}\hbar\omega + g\sqrt{|\Gamma(t)|}\mathrm{Im}[\gamma(t)]\right)(2p-1) + \phi,$$

which is no longer constant, $\partial_t\langle\hat{H}'\rangle \neq 0$. Heat current also vanishes in ℓ, $\mathcal{J}' = \mathcal{J} = 0$, because $\mathcal{J}_{\delta\hat{H}} = \mathcal{C}_{\delta\hat{H}} = 0$ in Eq. (13); therefore, within this generic path, the work is equal to the change in internal energy:

$$W_\ell = \int_0^t \partial_t\langle\delta\hat{H}\rangle dt = (2p-1)g\sqrt{|\Gamma(t)|}\mathrm{Im}[\gamma(t)], \tag{43}$$

see Eq. (32). Its rate provides the power $\mathcal{P}' = \partial_t\langle\delta\hat{H}\rangle$ along ℓ.

The EP in (36) is a state function, meaning that it has the same value for any path ℓ, which is equal to its value in ℓ_0. Diagonalizing the operator $\hat{\rho}(t)$ in (41), its eigenvalues are $\frac{1}{2} \pm R(t)$, where

$$R(t) := \sqrt{\left(p - \frac{1}{2}\right)^2 + |\rho_{01}D(t)|^2} \leqslant 1/2 \;\forall\, t \geqslant 0$$

is a real bounded function as a consequence of the positivity of $\hat{\rho}(t)$; note that $D(0) = 1$ and $|D(t)| \leqslant 1$. Using (42) and the eigenvalues of $\hat{\rho}(t)$, it is possible to write the EP as

$$\Sigma = \mathrm{H}[R(t)] - \mathrm{H}[R(0)] \geqslant 0,$$
$$\mathrm{H}(x) := -\left(\tfrac{1}{2} + x\right)\ln\left(\tfrac{1}{2} + x\right) - \left(\tfrac{1}{2} - x\right)\ln\left(\tfrac{1}{2} - x\right).$$

The function H is Schur-concave [41] for $0 \leqslant x \leqslant \frac{1}{2}$, which implies $\mathrm{H}[R(t)] \geqslant \mathrm{H}[R(0)]$, thus $\Sigma \geqslant 0$, as expected.

The EP rate becomes

$$\mathcal{E} = -\partial_t\mathrm{H}[R(t)] = -\frac{|\rho_{01}|^2}{R(t)}\mathrm{Arctgh}[2R(t)]\partial_t[D(t)]^2,$$

which is positive whenever $\partial_t D < 0$. Recalling that a monotonically decreasing $D(t)$ corresponds to a Markovian dynamics, non-Markovianity emerges for functions $D(t)$ with $\partial_t D > 0$, which will also give rise to a negative EP rate and is associated with violations of the second law for quantum systems [11,25].

The thermodynamical behavior of decoherence is similar to the classical experiment of "free expansion" [23], where a gas irreversibly expands without exchanging heat or performing work, due exclusively to positive entropy production. This is the same behavior of the example for an invariant initial state, or even for the system following the path ℓ_0, where there are no energetic changes, only entropic ones associated with $\Sigma \geqslant 0$. Furthermore, for the same classical experiment, when isolated and expanding against a piston, there will be entropy production and work will be realized by the gas. This situation is comparable to any path other than ℓ_0 followed by the quantum system, where the power is not null and provides work in (43). Noteworthy, this analogy is lawful even when non-Markovianity takes place in the dynamics of the quantum system since $\Sigma \geqslant 0$ regardless of the sign of $\mathcal{E}$.

VII. APPLICATION TO THERMAL MACHINES

A quantum thermal machine is nothing but a system evolving cyclically with period τ, while interacting with reservoirs. The whole system evolution, a closed thermodynamical path ℓ_0, see Eq. (31), is described by periodic operators, i.e., $\hat{H}(t+\tau) = \hat{H}(\tau)$, $\hat{L}_\mu(t+\tau) = \hat{L}_\mu(t)\;\forall\,\mu$. For this path, heat and work in one period are given by (33), which in this case are closed integrals,

$$Q_{\ell_0} = \oint_{\ell_0} \mathcal{J}dt, \quad W_{\ell_0} = \oint_{\ell_0} \mathcal{P}dt, \tag{44}$$

for $\mathcal{J}$ and $\mathcal{P}$ in (8) written for the Hamiltonian and Lindblad operators governing the system evolution.

For a machine composed of two thermal reservoirs, a colder c and a hotter h, as in the classical Carnot system [23], the total current in (8) will be the sum (9). However, each reservoir may be described by more than one Lindblad operator, which leads us to define $\mathcal{J}_\mathrm{c}$ and $\mathcal{J}_\mathrm{h}$ as sums of the currents of the respective Lindblad operators and write the total current as $\mathcal{J} = \mathcal{J}_\mathrm{c} + \mathcal{J}_\mathrm{h}$. Consequently, the heat entering the system from the hotter reservoir and the heat leaving the system to the colder are, respectively, written as

$$Q_0^\mathrm{h} := \oint_{\ell_0} \mathcal{J}_\mathrm{h}dt, \quad Q_0^\mathrm{c} := \oint_{\ell_0} \mathcal{J}_\mathrm{c}dt, \tag{45}$$

and, according to (44), $Q_0^\mathrm{c} + Q_0^\mathrm{h} = Q_{\ell_0}$.

As the system returns to the initial state, the mean energy assumes its initial value, since the Hamiltonian is periodic. Consequently, $W_{\ell_0} + Q_{\ell_0} = 0$ is the integral expression of the first law (7) for a whole cycle of the machine. The efficiency of the machine, as in a classical cycle, will be defined by the ratio

$$\eta = |W_{\ell_0}|/Q_0^\mathrm{h} = 1 - |Q_0^\mathrm{c}|/Q_0^\mathrm{h}. \tag{46}$$

The von Neumann entropy also returns to its initial value after a cycle due to the periodicity of the Lindblad operators, see (35). Using Eq. (38),

$$\Delta\mathcal{S} = \oint_{\ell_0} (\tilde{\mathcal{E}} + \beta\mathcal{J})dt = 0.$$

Defining the EP as $\tilde{\Sigma} := \oint_{\ell_0}\tilde{\mathcal{E}}dt$, using (44) and (45), and performing the integration, one finds

$$\tilde{\Sigma} + \beta_\mathrm{h}Q_0^\mathrm{h} + \beta_\mathrm{c}Q_0^\mathrm{c} = 0. \tag{47}$$

The positivity of the EP, $\tilde{\Sigma} \geqslant 0$, implies $\beta_\mathrm{c}|Q_\mathrm{c}^0| \geqslant \beta_\mathrm{h}Q_\mathrm{h}^0$, which replaced in (46) shows that the efficiency is bounded by the Carnot limit, i.e.,

$$\eta = 1 - |Q_0^\mathrm{c}|/Q_0^\mathrm{h} \leqslant 1 - \beta_\mathrm{h}/\beta_\mathrm{c}. \tag{48}$$

To take into account the gauge effects, we choose a closed thermodynamical path ℓ, see Eq. (30), described by periodic gauge functions $\{\gamma_\mu, U_{\mu\nu}, \phi\}$. In this way, the Hamiltonian $\hat{H}' = \hat{H} + \delta\hat{H}$ and the Lindblad operators $\hat{L}'_\mu$ will be also periodic operators. Nonperiodic gauge functions (open paths ℓ), could be equally considered, although thermodynamical quantities will not return to their initial value after one period, a necessary requisite for a proper machine.

The heat Q_ℓ and work W_ℓ will be given by (32) and formulas (34) remain valid for the closed integral. The current after a gauge (16) is the sum of the currents of each reservoir, $\mathcal{J}' = \mathcal{J}'_\mathrm{c} + \mathcal{J}'_\mathrm{h}$, as well $Q_\mathrm{c}^\ell + Q_\mathrm{h}^\ell = Q_\ell$ will be the total heat with

$$Q_\ell^{\rm h} := \oint_\ell \mathcal{J}_{\rm h}' dt, \quad Q_\ell^{\rm c} := \oint_\ell \mathcal{J}_{\rm c}' dt. \tag{49}$$

As before, after a period $W_\ell + Q_\ell = 0$, although $W_{\ell_0} + Q_{\ell_0} = 0$. Consequently, using (34) and (11),

$$\oint \partial_t \langle \delta \hat{H} \rangle dt = 0$$

is in agreement with the periodicity of $\delta\hat{H}$ and is independent of the path ℓ.

For the EP, the periodicity of the von Neumann entropy gives

$$\oint_\ell (\tilde{\mathcal{E}}' + \beta \mathcal{J}')dt = \tilde{\Sigma}' + \beta_{\rm h} Q_\ell^{\rm h} + \beta_{\rm c} Q_\ell^{\rm c} = 0, \tag{50}$$

which, from the positivity of the EP $\tilde{\Sigma}' := \oint_\ell \tilde{\mathcal{E}}' dt \geqslant 0$, ensures that the efficiency, despite not gauge-invariant, is also bounded by the Carnot limit for any gauge:

$$\eta' = |W_\ell|/Q_\ell^{\rm h} = 1 - |Q_\ell^{\rm c}|/Q_\ell^{\rm h} \leqslant 1 - \beta_{\rm h}/\beta_{\rm c}. \tag{51}$$

A. General comments

Despite the lack of a general theory for the EP for ME, see Sec. V, the obtainment of (47) or (50) was only possible due to the recent developments in Ref. [11], which derives the EP for a system strongly coupled to a thermal reservoir. In some sense, excepting the gauges, the machine description and treatment is commonly found in the literature on Markovian machines, see Refs. [5,22] and the references therein.

While Eq. (48) refers to a machine where the dynamics is ruled by a ME (2), but describing the evolution of a system (strongly) coupled to thermal reservoirs, see Ref. [11], its particular Markovian version [38] is identical and was derived in Ref. [3], including the limitation by the Carnot bound. The efficiency and the Carnot bound have also been studied for quantum machines which do not fit in both of these scenarios, for instance, generic Markovian master equations with fixed points [42], the replacement of a thermal bath by a squeezed version [43], and also a machine governed by a global unitary evolution [21].

The formulas for the EP, Eqs. (47) or (50), are promptly obtained if the closed path is composed, as in a Carnot machine, by strokes: an isothermal at a definite temperature, representing the coupling with a reservoir, followed by an isentropic, in which the evolution is unitary. An evolution like this may be devised using periodic Lindblad operators becoming cyclically null throughout the isentropics. The EP in each isothermal will be given by Eq. (38), while it will be null throughout the isentropic since the unitary evolution ensures $\mathcal{J} = 0$ and $\partial \mathcal{S}_t = 0$. For the whole cycle, the EP will be (47) with $Q_0^{\rm h}$ and $Q_0^{\rm c}$, the heat exchanged along the hot and the cold isotherms, respectively. The positivity of $\tilde{\Sigma}$ in each isotherm, given by (38), is ensured if the evolution is Markovian [11], which gives the limitation by the Carnot bound.

Reciprocating machines, those in which combined strokes describes the evolution, are suitable for analytical calculations due to the convenient separation between the generators of the ME [5], as described by the Carnot-like machine above. "Continuous-time" quantum machines [5] are those in which the path cannot be separated in strokes. In this case, the integral of $(\tilde{\mathcal{E}} + \beta\mathcal{J})$ can be split as a sum of many infinitesimal connected paths, in which each alternate path represents the evolution of the system interacting with only one reservoir, and Eq. (38) can be applied in each piece. This scenario can be theoretically described in the scope of a Floquet theory for MEs [22].

The positivity of the EP, a statement of the second law, ensures the limitation of the efficiency by the Carnot bound in (46) and in (51). However, it is also a necessary condition for Markovian dynamics, see Sec. V, thus a violation of the second law may happen for non-Markovian evolutions and that bound may be surpassed. This would happen for any gauge since the dynamics is invariant under gauge transformations.

B. Gauge and efficiency

Our previous results show that all gauges of a thermal machine described by a Markovian ME are subjected to the Carnot bound, however, it remains to show how the efficiency changes according to a gauge choice. We will tackle this question for a thermodynamical-invariant thermal machine, which unexpectedly has its efficiency changed, despite the invariance.

The main point is to take into consideration that the invariance conditions in (29) do not apply for each current $\mathcal{J}_\mu$ in (15) but only for the whole $\mathcal{J}$ in (16). In other words, $\mathcal{J}_\mu' \neq \mathcal{J}_\mu$ in general, even for an invariant system where $\mathcal{J}' = \mathcal{J}$. Consequently, in general, $\mathcal{J}_{\rm c}' \neq \mathcal{J}_{\rm c}$ and $\mathcal{J}_{\rm h}' \neq \mathcal{J}_{\rm h}$, as the sum of the Lindblad operators relative to their respective reservoirs. However, the invariance of $\mathcal{J}$ and definitions Eqs. (45) and (49) ensure

$$\mathcal{J}_{\rm c}' + \mathcal{J}_{\rm h}' = \mathcal{J}_{\rm c} + \mathcal{J}_{\rm h} \iff \left(Q_\ell^{\rm h} - Q_0^{\rm h}\right) = -\left(Q_\ell^{\rm c} - Q_0^{\rm c}\right). \tag{52}$$

Using (47), one can rewrite Eq. (50) as

$$\begin{aligned}\tilde{\Sigma}' - \tilde{\Sigma} &= -\beta_{\rm h}\left(Q_\ell^{\rm h} - Q_0^{\rm h}\right) - \beta_{\rm c}\left(Q_\ell^{\rm c} - Q_0^{\rm c}\right) \\ &= (\beta_{\rm c} - \beta_{\rm h})\left(Q_\ell^{\rm h} - Q_0^{\rm h}\right),\end{aligned} \tag{53}$$

which is the integral formulation of Eq. (39); the second equality is obtained using the relation (52). The last equality in (53) is symmetric concerning the paths ℓ and ℓ_0, reflecting that both paths are equally possible gauges of the same evolution. It asserts that, if the entropy production (considered positive) is bigger in one gauge, the positive heat will be greater than in the other. The machine efficiency will change accordingly due to the thermodynamical invariance. Since $\mathcal{P} = \mathcal{P}'$, thus $|W_\ell| = |W_{\ell_0}|$, which gives $\eta' = |W_\ell|/Q_\ell^{\rm h} = |W_{\ell_0}|/Q_\ell^{\rm h}$, and the machine efficiency increases for a reduction of the entropy production and *vice versa*.

For a noninvariant system, the work performed and heat absorbed both changes with gauges, and generically nothing more can be said besides the limitation of the efficiency by the Carnot bound, as stated in (51).

C. Example: The three-level maser

The quantum thermal engine introduced in Ref. [1] considers a three-level atom coupled to two thermal baths and to a radiation field, as depicted in Fig. 2.

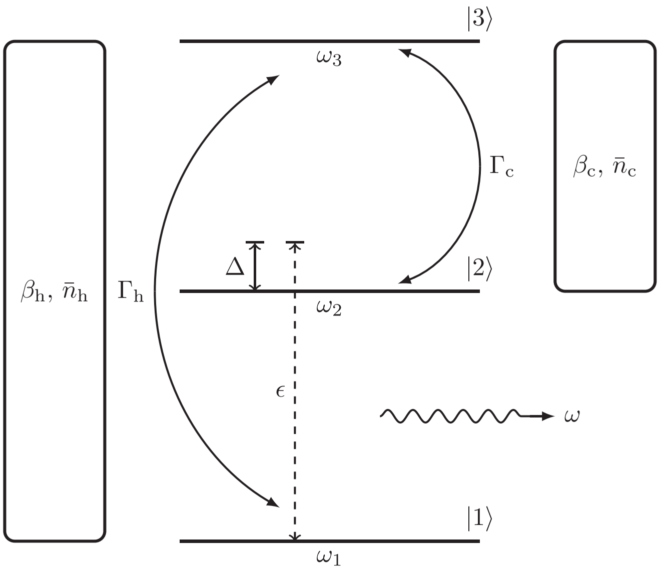

FIG. 2. Scheme of a three-level quantum thermal machine for a system with energies $\hbar\omega_m$ for $m = 1, 2, 3$. Bath α with population $\bar{n}_\alpha = \bar{n}_\alpha := (e^{\beta_\alpha \hbar\omega_\alpha} - 1)^{-1}$ and inverse temperature β_α induces transitions with rate Γ_α for $\alpha \in \{c, h\}$ with $\omega_h = \omega_3 - \omega_1$ and $\omega_c = \omega_3 - \omega_2$. Levels 1 and 2 are connected by an external classical field $\hat{V}(t)$ and, at the end of the cycle, a photon is emitted with frequency ω. This figure is largely inspired by Fig. 1 of Ref. [34].

The Hamiltonian of this system is $\hat{H} = \hat{H}_0 + \hat{V}(t)$ as in Ref. [34], with

$$\hat{H}_0 = \sum_{m=1}^{3} \hbar\omega_m |m\rangle\langle m|,$$
$$\hat{V}(t) = \hbar\epsilon(e^{i\omega t}|1\rangle\langle 2| + e^{-i\omega t}|2\rangle\langle 1|),$$

where $\hat{H}_0$ governs the dynamics of the atomic levels with $\omega_1 < \omega_2 < \omega_3$, and the atom-field interaction potential $\hat{V}(t)$ has coupling constant ϵ, while ω is the field angular frequency.

Each thermal reservoir is described by two Lindblad operators, corresponding to thermal transitions between the energy levels:

$$\hat{A}_{h,1} = \sqrt{\hbar\Gamma_h\bar{n}_h}|3\rangle\langle 1|, \quad \hat{A}_{h,2} = \sqrt{\hbar\Gamma_h(\bar{n}_h + 1)}|1\rangle\langle 3|,$$

for the hotter at "inverse temperature" β_h, while

$$\hat{A}_{c,1} = \sqrt{\hbar\Gamma_c\bar{n}_c}|3\rangle\langle 2|, \quad \hat{A}_{c,2} = \sqrt{\hbar\Gamma_c(\bar{n}_c + 1)}|2\rangle\langle 3|,$$

are associated with the colder at temperature β_c.

The ME governing the system evolution is written as (2) with $M = 4$, $\mu \in \{(h, 1), (h, 2), (c, 1), (c, 2)\}$, and $g_{\mu\nu} = \delta_{\mu\nu}$. From now on and without loss of generality, we will use $\Gamma_h = \Gamma_c =: \Gamma$ and $\Delta = 0$.

After a transient, the system attains a limit cycle, the path ℓ_0 in (31), described by a periodic density matrix given by

$$\hat{\rho}(t) = \hat{\rho}(t + \tau) = \begin{pmatrix} \rho_{11} & \rho_{12}e^{i\omega t} & 0 \\ \rho_{12}^* e^{-i\omega t} & \rho_{22} & 0 \\ 0 & 0 & \rho_{33} \end{pmatrix},$$

where the period of the cycle is determined by $\omega = \omega_2 - \omega_1 = 2\pi/\tau$ and the elements ρ_{ij} are constants ($\rho_{jj} \in \mathbb{R}$ and $\rho_{12} \in \mathbb{C}$) given by [34]

$$\rho_{11} = [\Gamma\bar{n}_c(\bar{n}_h + 1) + \lambda(\bar{n}_c + \bar{n}_h + 2)]K^{-1},$$
$$\rho_{22} = [\Gamma(\bar{n}_c + 1)\bar{n}_h + \lambda(\bar{n}_c + \bar{n}_h + 2)]K^{-1},$$
$$\rho_{33} = 1 - \rho_{11} - \rho_{22}, \quad \rho_{12} = -i\epsilon\lambda^{-1}(\rho_{22} - \rho_{11}),$$

where

$$\lambda := 8\epsilon^2\Gamma^{-1}(\bar{n}_c + \bar{n}_h)^{-2},$$
$$K := \lambda(4 + 3\bar{n}_c + 3\bar{n}_h) + \Gamma(\bar{n}_c + \bar{n}_h + 3\bar{n}_c\bar{n}_h) > 0.$$

Despite the lengthy expressions, by now it will be helpful to note only that $\mathrm{Re}\rho_{12} \leqslant 0$ and $\mathrm{Im}\rho_{12} \leqslant 0$.

The invariance condition in Eq. (29) is promptly verified for the periodic solution, since $\langle\hat{A}_{\alpha,j}\rangle = \mathrm{Tr}[\hat{\rho}(t)\hat{A}_{\alpha,j}] = 0$ for $\alpha \in \{h, c\}$ and $j = 1, 2$. Thus, for a state in the limit cycle, $\mathcal{J}' = \mathcal{J}$, $\mathcal{P}' = \mathcal{P}$, and $\langle\hat{H}'\rangle = \langle\hat{H}\rangle$. So, heat and work are determined by (33) for any gauge. Noteworthy, in the transient, the system will be only gauge-invariant if the initial state satisfies Eq. (29).

The currents associated with the baths are $\mathcal{J}_h = \mathcal{J}_{h,1} + \mathcal{J}_{h,2}$ and $\mathcal{J}_c = \mathcal{J}_{c,1} + \mathcal{J}_{c,2}$, where each current is given by (10) with $\mu \in \{(h, 1), (h, 2), (c, 1), (c, 2)\}$. Performing the calculations for the above Hamiltonian and Lindblad operators,

$$\mathcal{J}_h = \hbar\Gamma K^{-1}(\bar{n}_h - \bar{n}_c)\lambda\omega_h \geqslant 0,$$
$$\mathcal{J}_c = -\hbar\Gamma K^{-1}(\bar{n}_h - \bar{n}_c)\lambda\omega_c \leqslant 0. \tag{54}$$

Although $\mathcal{J}$ is gauge invariant, the above currents in general are not, as we will see in a while. From Eq. (8) and the above Hamiltonian, the power becomes $\mathcal{P} = \langle\partial_t\hat{V}\rangle$ and, due to its invariance, gauge-invariant work

$$W_{\ell_0} = \int_0^\tau \langle\partial_t\hat{V}\rangle dt = 4\pi\hbar\epsilon\mathrm{Im}(\rho_{12}) \leqslant 0 \tag{55}$$

is performed by the system, see Eq. (33), while heat is absorbed from the hotter reservoir.

To compare the efficiencies (46) and (51), we will choose a closed path ℓ in (30) described by the gauge functions

$$\gamma_{h,1} = \gamma_{c,1}^* = Ce^{i\omega t/2}, \quad \gamma_{h,2} = \gamma_{c,2} = \phi = 0, \quad U_{\mu\nu} = \delta_{\mu\nu},$$

where ω is the same frequency as the state evolution. Explicitly calculating each $\mathcal{J}'_\mu$ in (15), using $\mathcal{J}_\mu$ from (10) and above gauge functions, the gauge induces the following change for the hot current:

$$\mathcal{J}'_h - \mathcal{J}_h = -\frac{1}{2}\Gamma\sqrt{\bar{n}_c\bar{n}_h}|C|^2\mathrm{Im}(\rho_{12}) > 0, \tag{56}$$

which integrated over one period gives

$$Q^h_\ell - Q^h_{\ell_0} = \tau(\mathcal{J}'_h - \mathcal{J}_h) > 0.$$

From the invariance of $\mathcal{J}$, see Eq. (52), $\mathcal{J}'_c - \mathcal{J}_c = -(\mathcal{J}'_h - \mathcal{J}_h)$ and $Q^c_\ell - Q^c_{\ell_0} = -(Q^h_\ell - Q^h_{\ell_0})$. Since $Q^h_\ell > Q^h_{\ell_0}$ and the work in (55) is invariant, from (51) and (46), the gauge transformation thus decreases the efficiency, i.e., $\eta' < \eta$, while the EP increases, see (53). Replacing $\gamma_{c,1}$ by $-\gamma_{c,1}$, while keeping all the other gauge functions, the relation (56) will become $\mathcal{J}'_h - \mathcal{J}_h < 0$. In this case, the efficiency and the EP will respectively increase and decrease.

To show explicitly that the efficiency is bounded by the Carnot limit, as stated in (48), we thus return to the gauge defined by the path ℓ_0 and use the currents in (54):

$$\frac{|\mathcal{J}_c|}{\mathcal{J}_h} = \frac{\omega_c}{\omega_h} = \frac{\beta_h}{\beta_c}\ln\left(\frac{\bar{n}_c^{-1}+1}{\bar{n}_h^{-1}+1}\right) \geqslant \frac{\beta_h}{\beta_c},$$

where we inverted the expression for the occupation number $\bar{n}_\alpha$, and the inequality is due to $\bar{n}_h \geqslant \bar{n}_c$. Using the definition in (46) with $Q_0^\alpha = \oint_{\ell_0} \mathcal{J}_\alpha dt = \tau \mathcal{J}_\alpha$, the efficiency reads

$$\eta = 1 - |\mathcal{J}_c|/\mathcal{J}_h = 1 - \omega_c/\omega_h \leqslant 1 - \beta_h/\beta_c,$$

as we want to show. Trivially, since in path ℓ the gauge transformation reduces the efficiency, this will be also bounded by the Carnot limit, agreeing with (51).

As a last comment, not all gauge transformations can change the EP and the efficiency. For instance, choosing

$$\gamma_{h,1} = \gamma_{c,1}^* = Ce^{-i\omega t}, \quad \gamma_{h,2} = \gamma_{c,2} = \phi = 0, \quad U_{\mu\nu} = \delta_{\mu\nu},$$

a very similar gauge to the previous one, we find

$$\mathcal{J}_h' - \mathcal{J}_h = -\frac{1}{2}\Gamma\sqrt{\bar{n}_c\bar{n}_h}|C|^2 \mathrm{Im}(\rho_{12}e^{3i\omega t}),$$

which integrated over one period gives $Q_\ell^h - Q_{\ell_0}^h = 0$, and thus neither the efficiency nor the EP is changed.

Finally, we remark that in ℓ_0, the Lindblad operators $\hat{A}_\mu$ with $\mu \in \{(h, 1), (h, 2), (c, 1), (c, 2)\}$ have $\mathrm{Tr}\hat{A}_\mu = 0\ \forall\ \mu$, and thus satisfy the minimal dissipation condition (iv) in Sec. IV A. The new set of Lindblad operators in ℓ is such that $\mathrm{Tr}\hat{A}_\mu = \gamma_\mu$ for $\mu \in \{(h, 1), (c, 1)\}$ and $\mathrm{Tr}\hat{A}_\mu = 0$ for $\mu \in \{(h, 2), (c, 2)\}$, according to Eq. (4), which remove the system from minimal dissipation. On another side, nonthermal energy sources can change the efficiency of a quantum machine [43,44], which is a behind physical reason explaining the gauge-induced efficiency change: The operators $\hat{A}_\mu$ in ℓ_0 describe the interaction of the system with thermal reservoirs, while in ℓ they are "displaced" by the gauge, $\hat{A}_\mu' = \hat{A}_\mu + \gamma_\mu$, representing the coupling with a nonthermal energy source.

VIII. FINAL REMARKS AND OUTLOOKS

The ME in (2) and the thermodynamical quantities in (8) provide a natural generalization of the thermodynamical paradigmatic model constituted by a system Markovianly weak-coupled to thermal baths [38], developed mainly in Refs. [3,4]. In any situation, ME gauges in (4) are ascribed to information lack owing to the trace in (1). If instead, one has access to the global system $\hat{\rho}_0 \otimes \hat{\rho}_E$ and the global Hamiltonian $\hat{H}_{SE}$, then in this case, the unitary evolution will ultimately determine the dynamics and the energetic exchanges undergone by the system without needing an ME description or gauges. Nonetheless, the debate about thermodynamical definitions is open even for global unitary evolution [9,13,16,21].

The unavoidable gauge influence on thermodynamics was already noted in previous works [10,11]. Probably the first in recognizing the problem, Ref. [10] circumvents the question restricting the thermodynamic analysis only to the Markovian weak-coupling-limit established by Davies [35], which, however, is still gauge-dependent, while the authors of Ref. [11] postulate one specific gauge for any ME, the minimal dissipation gauge in Sec. IV B, and develop the whole thermodynamical circumscribed to this choice.

The crucial point of our work is the identification of the gauge-contributions $\mathcal{J}_{\delta\hat{H}}$ and $\mathcal{C}_{\delta\hat{H}}$ in (13) and $\langle \partial_t \delta\hat{H} \rangle$ with the standard statistical interpretation of heat and work, see Sec. II D. Thanks to this agreement, even for a noninvariant system, the contributions of heat and work from the interaction could be broken unequivocally as in Eq. (32). Since $\mathcal{C}_{\delta\hat{H}}$ has no classical interpretation, see Sec. II D, our definition of heat Q_ℓ in (32) is the amount of energy exchanged due to the system E and is *a posteriori* justified in (39) as a contribution to entropy production.

We stress the need for a process-dependent interpretation linked to a gauge of the ME. Without an *a priori* physical criterion, there is no way to select one specific gauge from the system evolution, see Sec. IV, consequently, thermodynamical quantities for the same system will be ill defined. Fortunately, the mean energy of the system, despite gauge dependent, is gauge covariant and legitimizes the first law for each gauge, see Eq. (11). It is important to recall that, even without gauges, the first law needs some modifications to accomplish an interplay of terms between the generators, which in the end is a gauge transformation, see Sec. II C.

A complete thermodynamical description of MEs still lacks an EP formulation [7], see Sec. V, which would end up in an expression for the second law. However, the recent results in Ref. [11] already enabled the construction of a quantum thermal machine for systems strongly coupled to thermal baths, as well as its limitation by the Carnot bound for any gauge of the system, as we presented in Sec. VII. In the scope of MEs with fixed points, expressions for the EP and its rate are known, see Sec. V, enabling a complete thermodynamical description, which also takes into account the gauges. This is exemplified in Sec. VI with the thermodynamical description of the decoherence effect. In both cases, violations of the second law related to non-Markovianity [25,26] are discussed. These violations are independent of gauges since being Markovian or not is a property of the dynamics, which is gauge-invariant.

Although Alicki in Ref. [3] had undertaken thermodynamical definitions for the ME in (2), their interpretation is independent of the dynamics itself. For instance, the first law (7) is rewritten to emphasize the role of coherences [15–17], similar to $\mathcal{C}_{\delta\hat{H}}$ in (13). The interchange among pictures of quantum evolution (Schrödinger, Heisenberg, and Dirac) was the main motivation for another modification of the first law by the inclusion of a reminiscent work term [19], which is similar to the gauge-induced power term (17). Gauge transformations like (4) were not yet put forward for any one of the above proposals and may provide interesting results.

Another perspective for quantum thermodynamics sets aside a dynamical description by an ME and focuses on thermodynamical functions, in analogy to the Gibbs formulation of potentials in classical thermodynamics [23]. In a typical scenario, the system is pushed away from equilibrium by generalized forces, often stochastic forces, see Ref. [20] and its references. For instance, in Ref. [14] a system initially in equilibrium with a thermal reservoir is isolated from it in order to suffer a unitary evolution. At the end of this protocol, the employment of the statistical interpretation determines the EP and all relevant thermodynamical functions; see also Ref. [12], for applications to the harmonic oscillator. A similar protocol is put forward in Ref. [21] to extract or perform work from an individual quantum system as free-energy variation. On one side, these works provide strong definitions for thermodynamical functions, which are immune to gauges. On another side, the ME conjugated to Alicki's formulas is not restricted to specific protocols and environments.

Other approaches join MEs and thermodynamical functions and one effortlessly proves that the energy or entropy quantities are gauge-dependent. Defining the informational free energy [42], the authors presented the correlation heat and the system entropy which are gauge-dependent, despite the gauge-invariance of informational free energy. The consecrated thermodynamical relation between entropy, internal energy, and informational free energy is gauge-covariant, as in (19). The works [43,45] adopt the concepts of passive energy and ergotropy, both gauge-dependent energy pieces for a gauge-covariant first law. The interpretation for the gauge-induced modifications, as in Sec. II D, and their consequences should be investigated.

In the end, we comment on wider applications of the basic concept behind our approach. Those gauge symmetries are properties of the dynamics, thus functions of the system operators $\{\hat{H}, \hat{L}_\mu\}$ can be affected by gauge transformations. Consider the following examples:

(i) The efficiency of a quantum thermal machine is related to fluctuations of heat and work [7,34] and, from the perspective of thermodynamical uncertainty relations (TURs), a gauge that increases the efficiency of the machine will increase these fluctuations.

(ii) Multitime correlation functions are dynamic functions of operators related to experimentally accessible quantities [24,46], measures of the system energy will change depending on a gauge choice.

(iii) Leggett-Garg inequalities constitute tests for macrorealistic physical theories [47]. Violations or not of such inequalities, for systems described by an ME [48], can be affected by gauges if the operators involved in the inequalities were associated with functions of $\{\hat{H}, \hat{L}_\mu\}$.

Recently, the work [49] appeared in ArXiv. The authors there propose definitions of thermodynamical quantities based on the invariance of the mean energy of the system. Alicki's thermodynamical functions are replaced by Haar-averaged quantities over the unitary subgroup composed by unitary symmetries of the Hamiltonian operator, which they called gauge-emergent symmetry. Our treatment departs from an opposite direction: the noninvariance of the mean energy and the consequential effects of the gauge transformations inherent to the ME scenario. However, investigating a similar construction for our results is a question to be explored.

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[1] H. E. D. Scovil and E. O. Schulz-DuBois, Three-Level Masers as Heat Engines, Phys. Rev. Lett. **2**, 262 (1959).
[2] W. Pusz and S. L. Woronowicz, Passive states and KMS states for general quantum systems, Commun. Math. Phys. **58**, 273 (1978).
[3] R. Alicki, The quantum open system as a model of the heat engine, J. Phys. A: Math. Gen. **12**, L103 (1979); E. B. Davies and H. Spohn, Open quantum systems with time-dependent Hamiltonians and their linear response, J. Stat. Phys. **19**, 511 (1978); H. Spohn and J. L. Lebowitz, Irreversible thermodynamics for quantum systems weakly coupled to thermal reservoirs, in *Advances in Chemical Physics*, edited by S. A. Rice (John Wiley and Sons, Ltd, New York, 1978).
[4] H. Spohn, Entropy production for quantum dynamical semigroups, J. Math. Phys. **19**, 1227 (1978).
[5] R. Alicki and R. Kosloff, Introduction to quantum thermodynamics: History and prospects, in *Thermodynamics in the Quantum Regime*, Fundamental Theories of Physics (Springer, Cham, 2018).
[6] G. Lindblad, Completely positive maps and entropy inequalities, Commun. Math. Phys. **40**, 147 (1975).
[7] G. T. Landi and M. Paternostro, Irreversible entropy production, from quantum to classical, Rev. Mod. Phys. **93**, 035008 (2021).
[8] G. P. Hildred *et al.*, Thermal reservoir effects in resonance fluorescence, J. Phys. B: At. Mol. Phys. **16**, 1703 (1983).
[9] C. Elouard, D. Herrera-Martí, M. Esposito and A. Auffèves, Thermodynamics of optical Bloch equations, New J. Phys. **22**, 103039 (2020).
[10] R. Kosloff, Quantum thermodynamics: A dynamical viewpoint, Entropy **15**, 2100 (2013); Quantum thermodynamics and open systems modeling, J. Chem. Phys. **150**, 204105 (2019).
[11] A. Colla and H.-P. Breuer, Open-system approach to non equilibrium quantum thermodynamics at arbitrary coupling, Phys. Rev. A **105**, 052216 (2022).
[12] S. Deffner and E. Lutz, Nonequilibrium work distribution of a quantum harmonic oscillator, Phys. Rev. E **77**, 021128 (2008); F. Galve and E. Lutz, Nonequilibrium thermodynamic analysis of squeezing, Phys. Rev. A **79**, 055804 (2009).
[13] M. Esposito *et al.*, Entropy production as correlation between system and reservoir, New J. Phys. **12**, 013013 (2010).
[14] S. Deffner and E. Lutz, Nonequilibrium Entropy Production for Open Quantum Systems, Phys. Rev. Lett. **107**, 140404 (2011).
[15] B. L. Bernardo, Unraveling the role of coherence in the first law of quantum thermodynamics, Phys. Rev. E **102**, 062152 (2020).
[16] S. Alipour *et al.*, Correlations in quantum thermodynamics: Heat, work, and entropy production, Sci. Rep. **6**, 35568 (2016).
[17] B. Ahmadi *et al.*, On the contribution of work or heat in exchanged energy via interaction in open bipartite quantum systems, Sci. Rep. **13**, 160 (2023).

[18] A. Vallejo, A. Romanelli, and R. Donangelo, Qubit thermodynamics far from equilibrium: Two perspectives about the nature of heat and work in the quantum regime, Phys. Rev. E **103**, 042105 (2021).

[19] E. Boukobza and D. J. Tannor, Thermodynamics of bipartite systems: Application to light-matter interactions, Phys. Rev. A **74**, 063823 (2006).

[20] W. L. Ribeiro *et al.*, Quantum thermodynamics and work fluctuations with applications to magnetic resonance Am. J. Phys. **84**, 948 (2016).

[21] P. Skrzypczyk *et al.*, Work extraction and thermodynamics for individual quantum systems Nat. Commun. **5**, 4185 (2014).

[22] S. Scopa, G. T. Landi, and D. Karevski, Lindblad-Floquet description of finite-time quantum heat engines, Phys. Rev. A **97**, 062121 (2018).

[23] H. B. Callen, *Thermodynamics and an Introduction to Thermostatistics*, 2nd revised ed. (John Wiley and Sons, New York, 1985).

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

[25] H.-P. Breuer, E. M. Laine, J. Piilo, and B. Vacchini, Colloquium: Non-Markovian dynamics in open quantum systems, Rev. Mod. Phys. **88**, 021002 (2016).

[26] I. de Vega and D. Alonso, Dynamics of non-Markovian open quantum systems, Rev. Mod. Phys. **89**, 015001 (2017).

[27] M. A. Schlosshauer, *Decoherence and the Quantum-to-Classical Transition* (Springer, Berlin, 2008).

[28] G. Lindblad, On the generators of quantum dynamical semigroups, Commun. Math. Phys. **48**, 119 (1976); V. Gorini *et al.*, Completely positive dynamical semigroups of n-level systems, J. Math. Phys. **17**, 821 (1976).

[29] A. Asadian, D. Manzano, M. Tiersch, and H. J. Briegel, Heat transport through lattices of quantum harmonic oscillators in arbitrary dimensions, Phys. Rev. E **87**, 012109 (2013); F. Nicacio, A. Ferraro, A. Imparato, M. Paternostro, and F. L. Semiao, Thermal transport in out-of-equilibrium quantum harmonic chains, *ibid.* **91**, 042116 (2015); P. H. Guimarães, G. T. Landi, and M. J. de Oliveira, Nonequilibrium quantum chains under multisite Lindblad baths, *ibid.* **94**, 032139 (2016); A. Riera-Campeny, M. Mehboudi, M. Pons, and A. Sanpera, Dynamically induced heat rectification in quantum systems, *ibid.* **99**, 032126 (2019); T. F. F. Santos and M. F. Santos, Efficiency of optically pumping a quantum battery and a two-stroke heat engine Phys. Rev. A **106**, 052203 (2022).

[30] D. Maldonado-Mundo, P. Ohberg, B. W. Lovett, and E. Andersson, Investigating the generality of time-local master equations, Phys. Rev. A **86**, 042107 (2012).

[31] A. O. Caldeira and A. J. Leggett, Path integral approach to quantum Brownian motion, Physica A **121**, 587 (1983); B. L. Hu, J. P. Paz, and Y. Zhang, Quantum Brownian motion in a general environment: Exact master equation with nonlocal dissipation and colored noise, Phys. Rev. D **45**, 2843 (1992); L. Ferialdi, Exact Closed Master Equation for Gaussian Non-Markovian Dynamics, Phys. Rev. Lett. **116**, 120402 (2016); W.-M. Zhang *et al.*, General non-Markovian Dynamics of Open Quantum Systems, *ibid.* **109**, 170402 (2012); H.-P. Breuer, B. Kappler, and F. Petruccione, Stochastic wavefunction method for non-Markovian quantum master equations, Phys. Rev. A **59**, 1633 (1999); A. Smirne and B. Vacchini, Nakajima-Zwanzig versus time-convolutionless master equation for the non-Markovian dynamics of a two-level system, *ibid.* **82**, 022110 (2010).

[32] R. Alicki, On the detailed balance condition for non-Hamiltonian systems, Rep. Math. Phys. **10**, 249 (1976); R. Alicki and K. Lendi, *Quantum Dynamical Semigroups and Applications–Lecture Notes in Physics* (Springer, Berlin, 2007); E. A. Carlen and J. Maas, Gradient flow and entropy inequalities for quantum Markov semigroups with detailed balance, J. Funct. Anal. **273**, 1810 (2017).

[33] F. Toscano and F. Nicacio, Thermal equilibrium in Gaussian dynamical semigroups, Phys. Rev. A **106**, 062207 (2022).

[34] A. A. S. Kalaee, A. Wacker, and P. P. Potts, Violating the thermodynamic uncertainty relation in the three-level maser, Phys. Rev. E **104**, L012103 (2021).

[35] E. B. Davies, Markovian master equations, Commun. Math. Phys. **39**, 91 (1974).

[36] Following Ref. [26], differentiating Eq. (1) with respect to time, one can write straightforwardly $\partial_t\hat{\rho} = \dot{\Phi}_t\Phi_t^{-1}[\hat{\rho}(t)] = \mathfrak{L}(\hat{\rho})$, which is the time-local generator of the dynamics and only depends on the invertibility of Φ_t, as stated. The explicit expressions for the generator in (3) or in (2), also derived in Ref. [26], follows from $\mathfrak{L} = \dot{\Phi}_t\Phi_t^{-1}$ according to the same procedure of the seminal works on dynamical semigroups [28].

[37] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2001).

[38] The original paper [3] has dealt with more restricted conditions: "We investigate the quantum open system S weakly interacting with N independent thermal reservoirs, the initial states of which are KMS states at inverse temperatures $\{\beta_k\}$," and "we assume that these external conditions change very slowly", where the words "external conditions" refer to a time-dependent Hamiltonian. However, the extension for the generic scenario governed by Eq. (2) is natural and preserves the thermodynamical definitions (8).

[39] R. Balian, *From Microphysics to Macrophysics: Methods and Applications of Statistical Physics* (Springer, Berlin, 2007), Vol. I.

[40] N. Boulant, T. F. Havel, M. A. Pravia, and D. G. Cory, Robust method for estimating the Lindblad operators of a dissipative quantum process from measurements of the density operator at multiple time points, Phys. Rev. A **67**, 042322 (2003); M. Howard *et al.*, Quantum process tomography and Lindblad estimation of a solid-state qubit, New J. Phys. **8**, 33 (2006).

[41] A. W. Marshall, I. Olkin and B. C. Arnold, *Inequalities: Theory of Majorization and Its Applications* (Springer, New York, 2010).

[42] B. Gardas and S. Deffner Thermodynamic universality of quantum Carnot engines, Phys. Rev. E **92**, 042126 (2015).

[43] W. Niedenzu *et al.*, Quantum engine efficiency bound beyond the second law of thermodynamics, Nat. Commun. **9**, 165 (2018).

[44] J. Roßnagel, O. Abah, F. Schmidt-Kaler, K. Singer, and E. Lutz, Nanoscale Heat Engine Beyond the Carnot Limit, Phys. Rev. Lett. **112**, 030602 (2014); G. Manzano, F. Galve, R. Zambrini,

and J. M. R. Parrondo, Entropy production and thermodynamic power of the squeezed thermal reservoir, Phys. Rev. E **93**, 052120 (2016).

[45] A. E. Allahverdyan, R. Balian and T. M. Nieuwenhuizen, Maximal work extraction from finite quantum systems, Europhys. Lett. **67**, 565 (2004).

[46] S. Khan, B. K. Agarwalla, and S. Jain, Quantum regression theorem for multi-time correlators: A detailed analysis in the Heisenberg picture, Phys. Rev. A **106**, 022214 (2022).

[47] A. J. Leggett and A. Garg, Quantum Mechanics Versus Macroscopic Realism: Is the Flux There When Nobody Looks? Phys. Rev. Lett. **54**, 857 (1985).

[48] C. Emary *et al.*, Leggett–Garg inequalities, Rep. Prog. Phys. **77**, 016001 (2014); J. J. Mendoza-Arenas *et al.*, Enhancing violations of Leggett-Garg inequalities in non equilibrium correlated many-body systems by interactions and decoherence, Sci. Rep. **9**, 17772 (2019).

[49] L. C. Céleri and Ł. Rudnicki, Gauge invariant quantum thermodynamics: Consequences for the first law, arXiv:2104.10153v2.