


Irreversible entropy production: From classical to quantum

Gabriel T. Landi

Instituto de Física da Universidade de São Paulo, 05314-970 São Paulo, Brazil

Mauro Paternostro*

*Centre for Theoretical Atomic, Molecular and Optical Physics,
School of Mathematics and Physics, Queen's University Belfast,
Belfast BT7 1NN, United Kingdom*

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Entropy production is a key quantity in any finite-time thermodynamic process. It is intimately tied with the fundamental laws of thermodynamics, embodying a tool to extend thermodynamic considerations all the way to nonequilibrium processes. It is also often used in attempts to provide the quantitative characterization of logical and thermodynamic irreversibility, stemming from processes in physics, chemistry, and biology. Notwithstanding its fundamental character, a unifying theory of entropy production valid for general processes, both classical and quantum, has not yet been formulated. Developments pivoting around the frameworks of stochastic thermodynamics, open quantum systems, and quantum information theory have led to substantial progress in such endeavors. This has culminated in the unlocking of a new generation of experiments able to address stochastic thermodynamic processes and the impact of entropy production on them. This review aims to provide a compendium on the current framework for the description, assessment, and manipulation of entropy production. Formal aspects of its formulation and the implications stemming from the potential quantum nature of a given process, including a detailed survey of recent experiments, are both presented.

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CONTENTS

I. Introduction	2	D. On-off work and Spohn's separation	22
A. Irreversible thermodynamics	2	E. Pauli master equations and Schnakenberg's approach	23
II. Why Entropy Production Matters	3	F. Pauli master equation for multiple baths	24
A. Operation of heat engines	3	G. Classical phase space	25
B. Heat and particle flow	4	H. Quantum phase space	26
C. Landauer's erasure	5	VI. Resource-Theoretic Approach	29
D. Thermodynamic uncertainty relations	5	A. Thermomajorization	30
E. Fluctuation theorems	6	B. The second laws of thermodynamics	31
F. Stochastic thermodynamics	6	C. Coherence and the resource theory of asymmetry	32
G. Maxwell, Szilard, and information thermodynamics	7	D. Fluctuating work in the resource theory context	33
III. Entropy Production in Quantum Processes	7	E. Reconciliation with the stochastic approach	35
A. Global unitary dynamics for system + environment	7	VII. Applications	36
B. Thermal environments	8	A. The SWAP engine	36
C. Maps with global fixed points	9	B. Stroke-based engines	37
D. Strict energy conservation and thermal operations	9	C. Squeezed baths	38
E. Fluctuation theorems	10	D. Quantum heat	40
F. Nonequilibrium lag	12	E. Infinitesimal quenches	41
IV. Information-Theoretic Aspects	13	F. Dissipative phase transitions: Basic models	43
A. Corrections to Landauer's principle	13	G. Dissipative phase transitions: Entropy production	44
B. Conditional entropy production	15	H. Effects of non-Markovian dynamics on entropy production	46
C. Heat flow in the presence of correlations	16	VIII. Experimental Assessment of Quantum Entropy Production	48
D. Fluctuation theorem under classical and quantum correlations	17	A. Assessment at the level of quantum trajectories	48
V. Quantum Dynamics and the Classical Limit	18	B. Assessment of the effects of quantum measurements	48
A. Collisional models	18	C. Assessment of the nonequilibrium Landauer principle	50
B. The emergence of a preferred basis	19	D. Assessment of entropy production in nonequilibrium steady states	51
C. Continuous-time limit	20	IX. Conclusions	53
		Acknowledgments	54
		References	55

*m.paternostro@qub.ac.uk

I. INTRODUCTION

In every finite-time process, entropy may flow from one system to another. However, entropy does not satisfy a continuity equation, so it may also be irreversibly produced (Carnot, 1824; Clausius, 1854, 1865). Such *entropy production* (Σ) is always non-negative and zero only in the limiting case where the process is reversible. It therefore serves as the key quantity behind the second law of thermodynamics, which can be stated mathematically as

$$\Sigma \geq 0. \quad (1)$$

Albeit compact, this expression has far-reaching consequences, as it places severe restrictions on the types of transformations allowed in a physical process. At a foundational level, the statement embodied by Eq. (1) manifests the lack of time reversal in finite-time processes and stems from the existence of an *arrow of time* (Eddington, 1928; Schnakenberg, 1976; Pomeau, 1982; Luo, Van den Broeck, and Nicolis, 1984; Mackey, 1989, 1992; Qian, 2001a; Jiang, Qian, and Zhang, 2003; Maes and Netocynny, 2003; Gaspard, 2004; Costa, Goldberger, and Peng, 2005; Seifert, 2005; Porporato, Rigby, and Daly, 2007; Blythe, 2008; Parrondo, Van den Broeck, and Kawai, 2009; Batalhão *et al.*, 2015). Hence, the characterization and assessment of irreversible entropy production is one of the most important tasks in nonequilibrium physics.

The formulation of the entropy production problem, however, is not universal. It depends on the underlying physical system, as well as its governing dynamical laws. Despite this, during the last century several widely applicable frameworks have been developed, from Onsager's reciprocity theory (Onsager, 1931a; de Groot and Mazur, 1961) to the celebrated fluctuation theorems (Esposito, Harbola, and Mukamel, 2009; Campisi, Hänggi, and Talkner, 2011; Goold *et al.*, 2016; Vinjanampathy and Anders, 2016). More recently the demonstrated possibility to control elementary quantum systems has drawn attention to the potential for thermodynamic applications in the quantum domain. This is the primary drive toward a formulation of a theory of entropy production capable of encompassing both classical and quantum features.

The goal of this review is to provide an overview of the progress in this formulation. Our approach will be centered around a unified picture of the second law, described in terms of global system-environment quantum unitary interactions; see Sec. III. This allows us to establish a link with information theory and construct entropy production solely in terms of information-theoretic quantities. The result is a generalized form of the second law, valid beyond the standard paradigms of thermodynamics, but with classical results recovered in the suitable limit. This approach also has a clear operational interpretation, with irreversibility emerging from the restrictions on the allowed set of operations for a given thermodynamic process. For a broader perspective on the developments in quantum thermodynamics over the last two decades, see Binder *et al.* (2019).

The results of Sec. III are central to this review. Before arriving there, we establish the notation and jargon in Sec. I.A, then discuss in Sec. II why the entropy production problem is

relevant. We then explore the consequences and ramifications of such a unified formulation. Section IV focuses on information-theoretic corrections to Landauer principle and the role of classical and quantum correlations in heat flow. Section V embodies another essential part of the review. We use the concepts developed in Sec. III as building blocks to assess the entropy production in more general types of dynamics, constructed in terms of a collisional model. This allows us to address the classical limit as a particular case of the quantum formulation.

The link between information and thermodynamics has other far-reaching consequences, as it allows information to be cast as a resource, on equal footing with traditional thermodynamic resources such as heat and work. That is, information can be consumed, stored, or interconverted into other resources. And it can be used to fuel thermodynamic tasks, such as Maxwell's demon engines. This is the topic of Sec. VI. In the quantum domain this acquires additional significance due to the possibility of manipulating quantum coherence, as well as quantum correlations such as discord and entanglement. How these features are implemented within a quantum formulation of the entropy production problem is a central theme of this review.

Finally, we discuss applications and experiments in Secs. VII and VIII. There is an inevitable arbitrariness on the choice of papers to cover, and we have chosen to address those that we believe (i) are representative of the types of problems the community is currently interested in, and (ii) have the potential to open unexplored avenues of research. Concerning the experiments, we have also tried to focus on those contributions that specifically characterize the entropy production at the quantum level.

We finish this review in Sec. IX by taking a step back to look at the larger picture. We compare the formulation put forth in Sec. III to other approaches, both historical and modern. The main argument we make is that the second law is always formulated by starting with a basic physical principle such as those of Carnot, Clausius, and Kelvin, or statements such as "the entropy of the Universe never decreases." One then asks what the overarching consequences of this principle are and which other principles can be derived from it. This provides a measure of how general it is. The information-theoretic formulation of Sec. IX falls under this category. However, the basic principle's main advantage is that it starts by assuming full knowledge of all degrees of freedom involved, thus allowing for precise mathematical statements. Irreversibility is then constructed operationally by specifying which sources of information can, or cannot, be known in a given process. This feature greatly generalizes the breadth and scope of the second law. It not only contains classical statements as particular cases, it can also go much further, removing the constraints in the standard thermal paradigms, such as the need for macroscopically large thermal baths.

A. Irreversible thermodynamics

To clarify the basic ideas, as well as fix the notation, we start with a textbook review of entropy production in classical thermodynamics (Fermi, 1956; Callen, 1985). We consider the simplest scenario of a system S interacting with multiple

reservoirs E_1, E_2, \dots , each with a temperature T_i . The flow of entropy from S to E_i during a given process is given by the famous Clausius expression (Clausius, 1854, 1865)

$$\Phi_i = \frac{Q_{E_i}}{T_i}, \quad (2)$$

where Q_{E_i} is the heat that entered E_i (positive when energy leaves the system).¹ According to the Clausius principle, the corresponding change in the system entropy S_S will be bounded by

$$\Delta S_S \geq -\sum_i \frac{Q_{E_i}}{T_i}. \quad (3)$$

Motivated by this inequality, one then defines the entropy production as

$$\Sigma = \Delta S_S + \sum_i \frac{Q_{E_i}}{T_i} \geq 0. \quad (4)$$

The entropy of a system may either increase or decrease during a process, so ΔS_S does not have a well-defined sign. This is due to the terms Q_{E_i}/T_i , since heat can flow both ways. The only quantity that has a well-defined sign is the entropy production Σ .

In the past, the terms *entropy* and *entropy production* were often used interchangeably, but they have evolved to have entirely different meanings. Entropy refers to a property of the system whereas entropy production refers to *transformation-transformation* undergone by the system. Thus, entropy production is actually closer in meaning to the original use of the word entropy, as coined by Clausius in the 1860s (Clausius, 1854, 1865), in which *tropé* refers to the word “transformation” in ancient Greek.

The first law of thermodynamics states that the total change in internal energy of the system will be given by

$$\Delta H_S = W - \sum_i Q_{E_i}, \quad (5)$$

where W is the work performed by an external agent, with $W > 0$ indicating that work was performed on the system. Alternatively, one may also simply view W as the mismatch between the local energy changes ΔH_S and Q_{E_i} in system and baths. Focusing on the case where there is a single reservoir present, if we substitute $Q_E = W - \Delta H_S$ into Eq. (4) we may write the entropy production as

$$\Sigma = \beta(W - \Delta F_S), \quad (6)$$

where $\beta = 1/T$ ($k_B = 1$) and $\Delta F_S = \Delta H_S - T\Delta S_S$ is the change in free energy of the system. For multiple baths at

¹We always define heat in this way: as the change in energy of the environment. The reason is that, as becomes clear in Sec. III, this helps to avoid ambiguities concerning the distinction between heat and work, something that is quite delicate in the quantum domain.

different temperatures, it is in general not possible to express Σ in this way and one must use Eq. (4).

It is often useful to express the results in terms of the entropy production rate $\dot{\Sigma} = d\Sigma/dt$. In this case the second law is usually written as

$$\frac{dS_S}{dt} = \dot{\Sigma} - \dot{\Phi}, \quad \dot{\Sigma} \geq 0, \quad (7)$$

with $\dot{\Phi} = \sum_i \dot{Q}_{E_i}/T_i$ the entropy flow rate. Equation (7) is particularly suited to studying nonequilibrium steady states (NESSs) that occur when a system is coupled to two or more reservoirs kept at different temperatures. The typical scenario to have in mind is a piece of metal coupled to a hot bath at one end and a cold one at the other. In this case, after a long time has passed the system will eventually reach a steady state where $dS_S/dt = 0$. This, however, does not mean the system is in equilibrium. It simply means that $\dot{\Sigma} = \dot{\Phi}$; that is, entropy is continually being produced in the system, but all of it is being dumped into the reservoirs. A NESS is therefore characterized by a finite and constant entropy production rate $\dot{\Sigma}$. Thermal equilibrium, on the other hand, occurs only when $\dot{\Sigma} = \dot{\Phi} = 0$.

Irrespective of the definitions of entropy production and entropy production rate, the second law of thermodynamics can ultimately be summarized by the statement that both $\Sigma \geq 0$ and $\dot{\Sigma} \geq 0$ are true. Next we discuss some of the far-reaching consequences of this seemingly simple statement.

II. WHY ENTROPY PRODUCTION MATTERS

The goal of this section is to illustrate, by means of examples, why entropy production is relevant in characterizing nonequilibrium systems.

A. Operation of heat engines

Consider a system interacting continuously with two reservoirs at temperatures T_h and $T_c < T_h$, plus an external agent on which the system can perform work. The first and second laws, Eqs. (5) and (7), then become

$$\frac{dH_S}{dt} = \dot{W} - \dot{Q}_h - \dot{Q}_c, \quad (8)$$

$$\dot{\Sigma} = \frac{dS_S}{dt} + \frac{\dot{Q}_h}{T_h} + \frac{\dot{Q}_c}{T_c}. \quad (9)$$

Writing the results in terms of rates makes the analysis simpler. One may picture this, for instance, as a continuously operated machine, or it may also be a stroke-based machine, but where the strokes happen so fast that we may write all thermodynamic quantities as rates (like a car engine). Following Marcella (1992), we now show how the usual statements of the second law can all be viewed as a consequence of Eqs. (8) and (9).

If the machine is operated for a sufficiently long time, it will eventually reach a steady state (limit cycle) where $dH_S/dt = dS_S/dt = 0$. This therefore means that all quantities in Eqs. (8) and (9) balance out as follows:

$$\dot{W} = \dot{Q}_h + \dot{Q}_c, \quad (10)$$

$$\dot{\Sigma} = \frac{\dot{Q}_h}{T_h} + \frac{\dot{Q}_c}{T_c}. \quad (11)$$

The steady state is therefore characterized by a steady conversion of heat into work accompanied by a steady production of entropy.

In the standard operation of a heat engine, heat flows from the hot bath to the system ($\dot{Q}_h < 0$) and work is extracted ($\dot{W} < 0$). Using Eqs. (10) and (11) one may write the efficiency of the engine as

$$\eta = \frac{\dot{W}}{\dot{Q}_h} = 1 + \frac{\dot{Q}_c}{\dot{Q}_h} = 1 - \frac{T_c}{T_h} + \frac{T_c}{\dot{Q}_h} \dot{\Sigma}. \quad (12)$$

The first two terms on the right-hand side are simply Carnot's efficiency $\eta_C = 1 - T_c/T_h$. Since $\dot{Q}_h < 0$, the second law (1) implies that the last term in Eq. (12) will be strictly non-positive. Hence, the efficiency of an engine is always reduced from Carnot's efficiency by an amount proportional to the entropy production $\eta = \eta_C - T_c \dot{\Sigma}/|\dot{Q}_h|$. This is the Carnot statement of the second law (Carnot, 1824):

“The efficiency of any quasi-static or reversible cycle between two heat reservoirs depends only on the temperatures of the reservoirs themselves, and is the same, regardless of the working substance. An engine operated in this way is the most efficient possible heat engine using those two temperatures.”

It is also useful to cast Eq. (12) in terms of the output power ($P = -\dot{W}$), which leads to

$$\dot{\Sigma} = \frac{P}{T_c} \frac{\eta_C - \eta}{\eta}. \quad (13)$$

We therefore see that, for fixed power output, the closer we are to Carnot efficiency, the smaller the entropy production rate is. This illustrates why entropy production is often used as a quantifier of the degree of irreversibility.

Next suppose we have access to a only single bath, so $\dot{Q}_c = 0$. Equation (10) then reduces to $\dot{W} = \dot{Q}_h$ so that Eq. (11) becomes

$$\dot{\Sigma} = \frac{\dot{Q}_h}{T_h} = \frac{\dot{W}}{T_h} \geq 0. \quad (14)$$

Positive work means work is injected into the system instead of being extracted. Hence, work cannot be extracted from a single bath. This is precisely the Kelvin-Planck statement of the second law (Thomson, 1851; Planck, 1903):

“It is impossible to devise a cyclically operating device, the sole effect of which is to absorb energy in the form of heat from a single thermal reservoir and to deliver an equivalent amount of work.”

Last, suppose that there is no work involved ($\dot{W} = 0$), but instead only heat flow between the two reservoirs. Equation (10) then yields $\dot{Q}_h = -\dot{Q}_c$, which plugging into Eq. (11) leads to

$$\dot{\Sigma} = \left(\frac{1}{T_c} - \frac{1}{T_h} \right) \dot{Q}_c \geq 0. \quad (15)$$

If $T_c < T_h$, we must then necessarily have $\dot{Q}_c \geq 0$; i.e., heat flows from hot to cold. This is Clausius's statement of the second law (Clausius, 1854; Clausius, 1865):

“Heat can never pass from a colder to a warmer body without some other change, connected therewith, occurring at the same time.”

B. Heat and particle flow

Continuing with the assumption that $\dot{W} = 0$, we now assume that the environments also allow for particle flow. The first law (8) is modified to

$$\frac{dH_S}{dt} = -\dot{Q}_h - \dot{Q}_c + \mu_h \dot{N}_h + \mu_c \dot{N}_c, \quad (16)$$

where μ_i are the chemical potentials of each bath and \dot{N}_i are the corresponding particle fluxes from bath to system (i.e., $N_i > 0$ when particles enter the system). The last two terms represent chemical work.

Particle conservation implies that, in the steady state, $\dot{N}_c = -\dot{N}_h$. But this does not mean that $\dot{Q}_h = -\dot{Q}_c$. Indeed, their mismatch is precisely,

$$\dot{Q}_h = -\dot{Q}_c + (\mu_h - \mu_c) \dot{N}_h,$$

which is nonzero whenever there is a chemical potential difference. Using this to eliminate \dot{Q}_h allows us to write Eq. (9) as

$$\dot{\Sigma} = \left(\frac{1}{T_c} - \frac{1}{T_h} \right) \dot{Q}_c + \frac{\mu_h - \mu_c}{T_c} \dot{N}_h. \quad (17)$$

If we assume that $T_c = T_h$, then the second law implies that if $\mu_h > \mu_c$, one must have $\dot{N}_h > 0$; that is, a particle flows from high chemical potential to low chemical potential.

We see in Eq. (17) the appearance of both a gradient of temperature and a gradient of chemical potential. These are called thermodynamic affinities, or generalized forces, as they are responsible for driving the system out of equilibrium. Each current has a corresponding conjugated affinity; heat \dot{Q}_c is conjugated to the affinity $1/T_c - 1/T_h$, while particle current \dot{N}_h is conjugated to $(\mu_h - \mu_c)/T_c$. The entropy production in Eq. (17) is thus simply the product of currents and affinities.

For concreteness, suppose that $(T_c, \mu_c) = (T, \mu)$ and $(T_h, \mu_h) = (T + \delta T, \mu + \delta \mu)$, where δT and $\delta \mu$ are small. Equation (17) then becomes

$$\dot{\Sigma} = \frac{\delta T}{T^2} \dot{Q}_c + \frac{\delta \mu}{T} \dot{N}_h. \quad (18)$$

Intuitively, we expect the currents to be zero when the affinities are zero. Moreover, if the affinities are small, the currents should also be proportionally small. Hence, in macroscopic systems it is natural to expect a linear dependence of the form (de Groot and Mazur, 1961)

$$\begin{pmatrix} \dot{Q}_c \\ \dot{N}_h \end{pmatrix} = \frac{1}{T} \begin{pmatrix} L_{qq} & L_{qn} \\ L_{nq} & L_{nn} \end{pmatrix} \begin{pmatrix} \delta T/T \\ \delta\mu \end{pmatrix}, \quad (19)$$

where L_{ij} are called the Onsager transport coefficients (Onsager, 1931a, 1931b). This kind of relation is not a consequence of the second law (18): it is an additional assumption that relies on the underlying dynamics of the system.

The coefficient L_{qq} represents Fourier's law of heat conduction. Similarly, L_{nn} represents either Fick's law of diffusion in the case of particle transport (e.g., chemical solutions) or Ohm's law in the case of electric transport. The cross coefficients L_{qn} and L_{nq} are the Peltier and Seebeck coefficients, which are the basis for thermoelectrics. They describe the flow of heat due to a chemical potential gradient and the flow of particles due to a temperature gradient. Onsager showed that, due to the underlying time-reversal invariance of the dynamics, the cross coefficients actually coincide ($L_{qn} = L_{nq}$). As a consequence, the matrix L is symmetric.

Inserting Eq. (19) into Eq. (18), we find that in the linear response regime the entropy production will be in the following quadratic form in the vector of affinities $\mathbf{x} = (\delta T/T^2, \delta\mu/T)$:

$$\dot{\Sigma} = \mathbf{x}^T L \mathbf{x} \geq 0. \quad (20)$$

Since this must be true for all \mathbf{x} , it then follows that L must be positive semidefinite. Thus, even though the second law does not predict the linear response relations (19), it places strict restrictions on the values that the transport coefficients may take.

C. Landauer's erasure

Consider again the Clausius inequality (3), but focus on the following case of a single bath at a temperature T :

$$Q_E \geq -T\Delta S_S. \quad (21)$$

It is important to realize how this bound relates quantities from two different systems: It bounds the heat absorbed by the bath to a quantity related to the entropy change of the system. It turns out that, while initially constructed within the realm of macroscopic thermodynamics, this same inequality also holds true when the system is microscopic, with the entropy now being the system's information-theoretic entropy (either Shannon's or von Neumann's, as later defined).² In this context, Eq. (21) places restriction on the *heat cost of*

²Landauer's principle is often stated in terms of the heat cost to erase 1 bit of information, which is $Q_E \geq T \ln 2$. This is actually a particular case of Eq. (21) for dichotomic (binary) variables.

erasing information, which is called Landauer's principle (Landauer, 1961).

We say information is erased when $\Delta S_S < 0$ (Shannon and Weaver, 1949). This is a bit counterintuitive at first because large entropy means little information, so $\Delta S_S < 0$ means that the information after interacting with a bath is larger than what we initially had (it looks like information is acquired, not erased). But what is acquired is information about the final state of the system, not the initial state. Before interacting with the bath the system had some information stored in it, which the experimenter simply did not know about (hence the large entropy). The act of interacting with a bath irreversibly erases this information (Plenio and Vitelli, 2001).

Landauer's erasure therefore fits naturally within the entropy production framework since erasing information is an inherently irreversible operation. In fact, it is suggestive to interpret Landauer's principle as a direct consequence of the second law (1), written as $\Sigma = \beta Q_E + \Delta S_S \geq 0$. This connection is subtle: In the second law, S_S is the thermodynamic entropy (see Sec. IX for a more precise definition), whereas in Eq. (21) it is the information-theoretic entropy. Despite this, it turns out that Landauer's principle can be rederived using the more modern formulation of the second law, which is the subject of this review. This connection was firmly established by Esposito, Lindenberg, and Van Den Broeck (2010) and Reeb and Wolf (2014) and is one of the hallmarks of the modern formulation of quantum thermodynamics. It is reviewed in detail in Secs. III and IV.A.

D. Thermodynamic uncertainty relations

In the previous examples, all thermodynamic quantities were treated as simple numbers that could not fluctuate. In macroscopic systems this is usually a good approximation due to the large number of particles involved. But in mesoscopic and microscopic systems, fluctuations play an important role. It was recently discovered that some properties of the fluctuations are also largely bounded by the average entropy production. Consider the transport of heat from a hot to a cold system and let \dot{Q} denote the average heat rate. In addition, we define Δ_Q^2 as the time-averaged variance of the heat current. Barato and Seifert (2015) and Pietzonka, Barato, and Seifert (2016) showed that, for certain classical Markovian systems, the signal-to-noise ratio Δ_Q^2/Q^2 satisfies a thermodynamic uncertainty relation (TUR)

$$\Delta_Q^2/\dot{Q}^2 \geq 2/\dot{\Sigma}, \quad (22)$$

where $\dot{\Sigma}$ is the average entropy production rate. The TUR shows that fluctuations are bounded by the average entropy production. Albeit simple, this bound is actually counterintuitive: Since $\dot{\Sigma}$ appears in the denominator, in order to curb fluctuations (reduce the left-hand side) one must actually increase the entropy production. More irreversible processes therefore fluctuate less.

A TUR can also be adapted to autonomous engines (Pietzonka and Seifert, 2018). In this case one instead studies the average output power $P = -\dot{W}$, as well as its corresponding variance Δ_P^2 . A TUR of the same shape as Eq. (22) also

holds for P . That is, $\Delta_P^2/P^2 \geq 2/\dot{\Sigma}$. However, in this case one can go further and relate P and $\dot{\Sigma}$ using Eq. (13). Writing $P = -\eta\dot{Q}_h$ (which simply follows from the definition of efficiency as $\eta = \dot{W}/\dot{Q}_h$), one then finds that

$$\Delta_P^2 \geq 2T_c P \frac{\eta}{\eta_c - \eta}. \quad (23)$$

Hence, we see that, for the fixed average power P , as one approaches Carnot's efficiency the fluctuations in the power must diverge.³ This therefore reflects a fundamental trade-off between operation efficiency and fluctuations. In real devices, particularly at the nanoscale, fluctuations could have a deleterious effect in the engine's operation. Equation (23) therefore provides guidelines on how to curb them. For a recent overview on the latest developments in TURs, see Horowitz and Gingrich (2020).

E. Fluctuation theorems

TURs illustrate the benefits of looking at fluctuations of thermodynamic quantities. Such benefits are even more evident owing to fluctuation theorems (FTs) (Evans, Cohen, and Morriss, 1993; Gallavotti and Cohen, 1995; Jarzynski, 1997; Crooks, 1998; Esposito, Harbola, and Mukamel, 2009; Campisi, Hänggi, and Talkner, 2011), which have been a central topic of research over the last two decades. FTs address the probability distribution of thermodynamic quantities such as work (Jarzynski, 1997; Crooks, 1998) and heat (Jarzynski and Wójcik, 2004) and can be framed in a unifying language in terms of entropy production, which is thus placed at the center of investigations of the thermodynamics of microscopic systems.

The basic idea is to study the probability distribution $P_F(\sigma)$ of the entropy production in a certain process, such as work extraction or heat exchange (the subscript F stands for "forward"). This is to be compared with the corresponding time-reversed ("backward") distribution $P_B(\sigma)$. FTs reflect a symmetry of these two distributions, constraining the forward and backward distributions, which usually have the form

$$\frac{P_F(\sigma)}{P_B(-\sigma)} = e^\sigma. \quad (24)$$

This is known as a detailed FT. And it immediately implies that

$$\langle e^{-\sigma} \rangle = \sum_\sigma P_F(\sigma) e^{-\sigma} = 1, \quad (25)$$

which is called an integral FT. In turn, Eq. (25), combined with Jensen's inequality, implies that

³Strictly speaking, the divergence never actually occurs since P implicitly depends on η and, in particular, is zero for a Carnot engine (since a Carnot engine must operate quasistatically and hence will have zero output power). Notwithstanding, there will in general be ranges of the engine's parameter space where one can vary η for a fixed P .

$$\langle \sigma \rangle \geq 0. \quad (26)$$

Thus, on average the entropy production is always non-negative. The idea, therefore, is that, when the entropy production is described as a fluctuating quantity, the second law is valid only on average and may eventually be violated at the stochastic level. In this sense, FTs contain the second law.

FTs were addressed in detail by Esposito, Harbola, and Mukamel (2009), Campisi, Hänggi, and Talkner (2011), Jarzynski (2011), and Seifert (2012). In Sec. III.E we focus on reviewing some more recent developments, particularly those concerned with quantum processes. We also discuss some subtleties raised by Manzano, Horowitz, and Parrondo (2018) regarding how to define the backward process.

An intuition into what Eq. (24) entails is gathered by considering the scenario of Jarzynski and Wójcik (2004), which consists of two thermal systems, prepared at temperatures T_A and T_B , which are then put into contact and allowed to exchange heat. As discussed in Sec. III.E, the entropy production in this case is given by $\sigma = \beta_A Q_A + \beta_B Q_B$; see also Eq. (11). If one assumes that there is no work involved, $Q_A = -Q_B \equiv Q$ and we may write $\sigma = \Delta\beta Q_A$, where $\Delta\beta = \beta_A - \beta_B$. Moreover, in this scenario it turns out that the forward and backward processes are actually the same (this would not be case, for instance, if an external agent were explicitly performing work). Equation (24) therefore reduces to

$$\frac{P(Q)}{P(-Q)} = e^{\Delta\beta Q}. \quad (27)$$

The FT therefore directly compares the probability of exchanging heat Q or $-Q$. Suppose that $T_B > T_A$ so that $\Delta\beta = \beta_A - \beta_B > 0$. In this case we expect heat to flow from B to A , so we expect $Q = Q_A \geq 0$. Owing to fluctuations, however, it is possible to eventually observe $Q < 0$. What Eq. (27) says is that the probability of observing negative heats is exponentially smaller than that of observing a flow in the "right" direction: $P(-Q) = e^{-\Delta\beta Q} P(Q)$. Note also that heat is an extensive quantity. Hence, for macroscopic systems, the exponent $e^{-\Delta\beta Q}$ tends to be extremely small; only in mesoscopic and nanoscopic systems, where fluctuations are significant, will $P(-Q)$ be non-negligible.

F. Stochastic thermodynamics

Consider a system interacting with one or more reservoirs and undergoing a generic thermodynamic process. At the microscopic level, the system is described by a stochastic trajectory that is different each time the dynamics of the system is considered. Hence, one may construct a probability distribution for each individual trajectory. For classical systems, the sole knowledge of such trajectories is sufficient to formulate the entropy production resulting from the stochastic dynamics (Seifert, 2005). This is a significant feature in the description of classical microscopic processes. The reason for this is that often one does not have a physical model for the global dynamics, but only an effective reduced description. Being able to express the entropy production solely through this effective description thus provides a major advantage.

This approach, called stochastic thermodynamics, has been reviewed in detail in a substantive body of literature, including Seifert (2012) and Van den Broeck and Esposito (2015); see also Secs. V.F and V.G. In contrast, a major difficulty in the formulation of entropy production for quantum processes is that, in general, the reduced description does not suffice to unambiguously determine the entropy production. In other words, the latter can be defined only with knowledge of the global system-environment interaction, whose lack might lead to inconsistencies, including the apparent violation of the second law (Levy and Kosloff, 2014). Note that a reduced description may well provide a good approximation for the dynamics, but this does not imply that it also well approximates the thermodynamics. A major theme of this review, particularly in Sec. V, is to address in detail under which conditions a reduced description suffices, as far as the second law is concerned.

G. Maxwell, Szilard, and information thermodynamics

In his famous treatise *The Theory of Heat* (Maxwell, 1888), Maxwell describes a thought experiment where a demon, capable of knowing the precise position and moment of all particles in a gas, uses that information to violate the second law. It does that by inserting a partition in a box and selectively opening a small hatch when a hot particle comes through. After a sufficient time, all hot particles will be on one side and all cold ones on the other. Szilard (1929) used the same idea to make an engine cyclically extract work from a single reservoir, thus apparently violating Carnot's statement (Sec. II.A). Recently these ideas attracted a surge of interest, with several experiments providing physical implementations of Maxwell's demon (Toyabe *et al.*, 2010; Camati *et al.*, 2016; Peterson *et al.*, 2016; Elouard, Herrera-Martí, Huard, and Auffèves, 2017; Masuyama *et al.*, 2018; Naghiloo *et al.*, 2020) and proof-of-principle demonstrations of Szilard's engine (Koski *et al.*, 2014, 2015; Paneru *et al.*, 2018).

The problem can be phrased in terms of information gain and feedback control. That is, information is acquired about the system through measurements, which is in turn used to perform some action on it (the feedback). To "exorcise" the demon (i.e., reinstate the validity of the second law), this information has to be included in a description of the entropy production. This was first done by Bennett (1973), who used Landauer's principle (Sec. II.C) to show that the heat cost associated with erasing information exactly counterbalances the work extracted by the demon.

A stochastic description of these ideas, in terms of fluctuation theorems, was first put forth in a series of seminal papers by Sagawa and Ueda (2009a, 2009b, 2010). The basic idea is that the stochastic entropy production σ must now be modified to $\sigma \rightarrow \sigma + I$, where I is an information-theoretic term accounting for how much information was gained about the system during the process. Equation (25) is then changed to $\langle e^{-\sigma-I} \rangle = 1$, which in turn implies $\langle \sigma \rangle \geq -\langle I \rangle$. For $\langle I \rangle > 0$, the average entropy production may thus be negative.

When extending these ideas to the quantum domain, the inevitable backaction caused by quantum measurements should be considered. Acquiring information about the system is no longer without consequences and may, in fact, severely

degrade the system. The recent developments in such interplay between information and thermodynamics is reviewed in Sec. IV.

III. ENTROPY PRODUCTION IN QUANTUM PROCESSES

A. Global unitary dynamics for system + environment

A unified formulation for entropy production in open quantum systems, which holds for arbitrary nonthermal environments and arbitrary dynamics, can be made by analyzing the global system-environment unitary evolution. We consider the interaction of a system S with an environment E , prepared in arbitrary states ρ_S and ρ_E , by means of a global unitary U . The final state of the composite SE system after the interaction is given by

$$\rho'_{SE} = U(\rho_S \otimes \rho_E)U^\dagger. \quad (28)$$

This map is general. All information about the types of interactions involved is encoded in U , which therefore may enable us to contemplate both weak and strong coupling, as well as time-dependent Hamiltonians and work protocols. The map also makes no assumptions about the structure of E , which does not need to be macroscopic and may well have dimensions comparable to those of S . One could therefore have S and E be two qubits or have S be a hot pan and E a large bucket of water. Both cases can be described by the same map (28) (although, admittedly, in the latter the unitary U would be a bit more complicated).

The reduced state of the system can be obtained by tracing over the environment, which leads to the quantum operation

$$\rho'_S = \mathcal{E}(\rho_S) = \text{tr}_E \rho'_{SE} = \text{tr}_E \{U(\rho_S \otimes \rho_E)U^\dagger\}. \quad (29)$$

On a conceptual level, tracing over the degrees of freedom of the environment can be pinpointed as the origin of irreversibility in this process. After all, the map (28) is unitary, and hence reversible by construction. But tracing over (discarding) the environment embodies the assumption that after the interaction one no longer has access to its degrees of freedom or is able to perform on it any local operation. Irreversibility thus emerges from discarding any information contained locally in the state of E , as well as the nonlocal information shared between S and E .

The entropy production separately quantifies these two contributions and is given by

$$\Sigma = \mathcal{I}_{\rho'_{SE}}(S:E) + S(\rho'_E || \rho_E). \quad (30)$$

To our knowledge, Eq. (30) was first put forth by Esposito, Lindenberg, and Van Den Broeck (2010). Its justification and ramifications are the central topic of this section. This culminates with a description in terms of fluctuation theorems, first discussed by Manzano, Horowitz, and Parrondo (2018), which is reviewed in Sec. III.E.

The first term in Eq. (30) is the mutual information developed between system and environment due to their interaction, where the mutual information of any bipartite system AB is defined as

$$\mathcal{I}_{\rho_{AB}}(A:B) = S(\rho_{AB}||\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \quad (31)$$

with $S(\rho) = -\text{tr}(\rho \ln \rho)$ the von Neumann entropy. $\mathcal{I}_{\rho'_{SE}}(S:E)$ thus quantifies the amount of shared information that is lost if one no longer has access to the state of E . The second term in Eq. (30), on the other hand, is the quantum relative entropy, defined as

$$S(\rho||\sigma) = \text{tr}\{\rho \ln \rho - \rho \ln \sigma\}, \quad (32)$$

which is a type of distance between two density matrices.⁴ The term $S(\rho'_E||\rho_E)$ thus quantifies how the environment was pushed away from equilibrium, a process that is irreversible since we are assuming that one can no longer perform local operations on it. In both formulas $\rho'_E = \text{tr}_S \rho'_{SE}$ is the reduced density matrix of the environment after the map (28). Combining the definitions in Eqs. (31) and (32), it is also possible to rewrite Eq. (30) as

$$\Sigma = S(\rho'_{SE}||\rho'_S \otimes \rho_E). \quad (33)$$

Notice the asymmetry in this formula: the quantity on the right is a tensor product between the final state ρ'_S of the system and the initial state ρ_E of the bath. The interpretation for this is discussed in Sec. III.E.

For a generic environment, the entropy production in Eq. (30) will no longer be given by the Clausius expression (4). Notwithstanding, it is still reasonable to define a similar splitting and write

$$\Sigma = \Delta S_S + \Phi, \quad (34)$$

where Φ is called the entropy flux from the system to the environment. Equation (34) can actually be viewed as the definition of Φ . As we later see, for thermal systems one recovers $\Phi = Q_E/T$. But in general the expression for Φ will be different.

The reason why it makes sense to call Φ a flux is as follows. Since the system and environment are initially uncorrelated, one has that $S(\rho'_{SE}) = S(\rho_S) + S(\rho_E)$. Thus, the mutual information may be expressed as

$$\mathcal{I}_{\rho'_{SE}}(S:E) = \Delta S_S + \Delta S_E, \quad (35)$$

where $\Delta S_S = S(\rho'_S) - S(\rho_S)$ and the approach is similar for ΔS_E . Equation (30) can then be written as

$$\Sigma = \Delta S_S + \text{tr}_E\{(\rho_E - \rho'_E) \ln \rho_E\}. \quad (36)$$

Comparing Eq. (36) with Eq. (34), one finds that the entropy flux is

$$\Phi = S(\rho'_E) - S(\rho_E) + S(\rho'_E||\rho_E) = \text{tr}_E\{(\rho_E - \rho'_E) \ln \rho_E\}. \quad (37)$$

⁴Strictly speaking it is not a distance, since it does not satisfy the triangle inequality. Notwithstanding, it is such that $S(\rho||\sigma) \geq 0$ and $S(\rho||\sigma) = 0$ if and only if $\rho = \sigma$.

The entropy flux thus depends solely on the local state of the environment. The entropy production is thus split into two terms: ΔS_S , which refers only to the system, and Φ , which refers only to the bath.

Equation (30) can be viewed as a general proposal for the entropy production in any system-environment interaction. It is clearly non-negative as both terms are individually non-negative. But that does not suffice for it to be considered a physically consistent definition. To do so this formula must acquire operational significance, which can be done by specializing it to specific contexts. This is our focus in Secs. III.B–III.E.

B. Thermal environments

We assume that the environment is thermal, $\rho_E = \rho_E^{\text{th}} = e^{-\beta H_E}/Z_E$. Again, we do not assume that it is necessarily macroscopic, only that it is initially in a thermal state. Inserting this into Eq. (36), but only in the logarithm, leads to

$$\Sigma = \Delta S_S + \beta Q_E, \quad (38)$$

where

$$Q_E = \text{tr}\{H_E(\rho'_E - \rho_E^{\text{th}})\} \quad (39)$$

is the total change in energy of the environment during the unitary U . Equation (38) thus coincides with the standard form of the second law [Eq. (4)]. This is noteworthy: ρ_E^{th} is the only assumption required to convert the general, and fully information-theoretic, expression [Eq. (30)] into the traditional thermodynamic expression in Eq. (38).

There is a subtlety, however. Namely, that the heat entering Eq. (38) refers to the change in energy of the environment [Eq. (39)]. This hides the fact that the process may also involve work, which is encoded in the unitary U . The heat Q_E will therefore in general not coincide with the change in system energy ΔH_S . This allows us to define work as their mismatch as follows:

$$W := \Delta H_S + Q_E. \quad (40)$$

Equation (40) is valid whether or not the Hamiltonian of the system changed during the process. For simplicity, we are assuming that it remains the same, but the results also hold if it does not. Substituting this for Q_E into Eq. (38) then leads to the second law in the form of Eq. (6); viz.,

$$\Sigma = \beta(W - \Delta F_S), \quad (41)$$

where $\Delta F = F(\rho'_S) - F(\rho_S)$ is the change in nonequilibrium free energy

$$F(\rho_S) = \text{tr}(H_S \rho_S) - TS(\rho_S) = F_{\text{eq}} + TS(\rho_S||\rho_S^{\text{th}}), \quad (42)$$

which is defined for any state ρ_S , with $\rho_S^{\text{th}} = e^{-\beta H_S}/Z_S$ referring to a thermal state of the system at the same temperature T as the bath [if the final Hamiltonian is H'_S , then $F(\rho'_S)$ should be defined with respect to H'_S]. We thus

conclude that the general proposal (30) for the structure of the entropy production reduces exactly to the expected thermal results whenever the bath is assumed to start in thermal equilibrium. Even the form (42) remains the same, provided one now works instead with the nonequilibrium free energy.

Equation (36) can also be specialized to the case where E is composed of multiple parts E_1, E_2, \dots , with $\rho_E = \rho_{E_1} \otimes \rho_{E_2} \otimes \dots$ and each part prepared in a thermal state $\rho_{E_i} = e^{-\beta_i H_{E_i}} / Z_{E_i}$ at different inverse temperatures β_i . In this case an identical calculation leads to

$$\Sigma = \Delta S_S + \sum_i \beta_i Q_{E_i}, \quad (43)$$

which is Eq. (4). Even though Eq. (43) involves only the local changes in energy of each bath, the map (28) will still generate correlations between the different E_i since they all interact with a common system. To see how these correlations affect Σ , one may start with Eq. (30) and add and subtract a term $\sum_i S(\rho_{E_i})$. This then allows us to write

$$\Sigma = \mathcal{I}_{\rho_{SE}'}(S: E_1: E_2: \dots) + \sum_i S(\rho_{E_i}' \| \rho_{E_i}), \quad (44)$$

where $\mathcal{I}_{\rho_{SE}'}(S: E_1: E_2: \dots) = S(\rho_S') + \sum_i S(\rho_{E_i}) - S(\rho_{SE}')$ is the so-called total correlation (Goold *et al.*, 2015) between the system and the individual environmental components. This quantity captures not only the correlations between S and E but also the correlations between E_i and E_j . This therefore shows that entropy is also produced due to the accumulation of multipartite correlations between the different parts of the bath as a consequence of their common interaction with the system.

C. Maps with global fixed points

Next we specialize to a different scenario. We consider once again the map in Eq. (28) and no longer assume that ρ_E is thermal. Instead, we look into those cases where the map has a global fixed point, that is, a special state ρ_S^* satisfying

$$U(\rho_S^* \otimes \rho_E)U^\dagger = \rho_S^* \otimes \rho_E. \quad (45)$$

Notice that this condition is much stronger than $\rho_S^* = \mathcal{E}(\rho_S^*)$, which would be a local fixed point (global implies local, but the converse is seldom true). An example of maps with global fixed points are the so-called thermal operations, which are reviewed in Sec. III.D.

We now focus on the entropy flux (37). Expanding the trace over E to be over $S + E$ allows us to write it as $\Phi = \text{tr}_{SE}\{(\rho_S \rho_E - \rho_{SE}') \ln \rho_E\}$ (we omit the tensor product symbol for simplicity). Next we take the logarithm on both sides of Eq. (45), which allows us to write

$$U^\dagger(\ln \rho_E)U - \ln \rho_E = -U^\dagger(\ln \rho_S^*)U + \ln \rho_S^*.$$

Plugging this into the expression for Φ and then carrying out the trace over E , one then finally finds that

$$\Phi = \text{tr}_S\{(\rho_S' - \rho_S) \ln \rho_S^*\}. \quad (46)$$

For systems with a global fixed point, the entropy flux can thus be written solely in terms of system-related quantities.

Plugging this into Eq. (36) then allows us to express the entropy production as

$$\Sigma = S(\rho_S \| \rho_S^*) - S(\rho_S' \| \rho_S^*). \quad (47)$$

Equation (47) is written solely in terms of local quantities of the system. This is possible only for systems with global fixed points; for local fixed points, the entropy production is an intrinsically nonlocal quantity.⁵

The positivity of Eq. (47) is guaranteed by its definition in Eq. (30). But from the optics of Eq. (47), positivity can also be viewed as a consequence of the data processing inequality:

$$S(\mathcal{E}(\rho) \| \mathcal{E}(\sigma)) \leq S(\rho \| \sigma), \quad (48)$$

which holds for any quantum channel \mathcal{E} . But since ρ_S^* is a fixed point of \mathcal{E} , it follows that

$$S(\rho_S' \| \rho_S^*) = S(\mathcal{E}(\rho_S) \| \mathcal{E}(\rho_S^*)) \leq S(\rho_S \| \rho_S^*), \quad (49)$$

which therefore implies $\Sigma \geq 0$. Entropy production can thus be viewed as quantifying the map's ability to process information and hence reduce the distinguishability between the initial state ρ_S and the fixed point ρ_S^* . This result emphasizes the interpretation of the entropy production (30) as a purely informational quantity, defined without any reference to the energetics of the system, such as the separation between heat and work.

D. Strict energy conservation and thermal operations

Thermal operations, first introduced by Janzing *et al.* (2000) and later popularized by Brandão *et al.* (2013, 2015) and Horodecki and Oppenheim (2013), are maps that involve a thermal environment and have a global fixed point (thus combining the results of Secs. III.B and III.C). One way to ensure that the map has a global fixed point when interacting with a thermal bath is to impose the requirement that the unitary global U in Eq. (28) should satisfy the so-called strict energy conservation condition

$$[U, H_S + H_E] = 0 \quad (50)$$

(note that in general U does not commute with H_S and H_E individually, only with their sum). This implies that

$$U e^{-\beta(H_S + H_E)} U^\dagger = e^{-\beta(H_S + H_E)}, \quad (51)$$

so ρ_S^{th} is a global fixed point of the dynamics, provided that it is defined with the same β as the environment. As a

⁵At first glance, Eq. (41) also seems to be written solely in terms of local quantities of the system. But that is not true because the work W , as defined in Eq. (40), still involves quantities pertaining to the environment.

consequence, the entropy production reduces as follows to Eq. (47):

$$\Sigma = S(\rho_S \parallel \rho_S^{\text{th}}) - S(\rho'_S \parallel \rho_S^{\text{th}}). \quad (52)$$

Naively, one may think that any map involving a thermal environment would necessarily have the thermal state $\rho_S^{\text{th}} = e^{-\beta H_S} / Z_S$ as a fixed point. This, however, is in general not true. But when strict energy conservation holds, it is. Thermal operations enjoy a wide range of good properties and have been extensively studied in the literature within the context of quantum resource theories. These are reviewed in Sec. VI.

It is important to clarify the meaning of Eq. (50). Its key implication is that all energy that leaves the system enters the environment and vice versa (nothing stays “trapped” in the interaction); viz.,

$$\Delta H_S = -\Delta H_E \equiv Q_E. \quad (53)$$

This kind of condition is seldom met in practice⁶ and should thus be viewed as an idealized scenario where drawing thermodynamic conclusions is much easier. Despite this apparent artificiality, Eq. (50) is actually incredibly similar to the weak-coupling approximation present in the vast majority of open quantum system studies [a discussion on how violations of this condition affect thermodynamics of strongly coupled systems was given by Hilt *et al.* (2011)]. Weak coupling assumes that the interaction energy is small. Equation (50) assumes that the interaction can be arbitrarily large, but nothing stays trapped in it. To a great extent, this is essentially the same thing. The major difference is that weak coupling is imposed as an approximation, whereas Eq. (50) is postulated *a priori*.

Comparing Eq. (53) with Eq. (40) also shows that in a thermal operation there is no work involved ($W = 0$). Indeed, Eq. (52) can be rewritten in terms of the nonequilibrium free energy (42) as

$$\Sigma = -\beta \Delta F. \quad (54)$$

The expenditure of work does not have to be associated with a work protocol but may simply be related to the cost of turning the system-environment interaction on and off. To elucidate this point, we suppose that the unitary U was generated by turning on an interaction V_{SE} for a certain length of time τ . Rigorously speaking, since we turn this interaction on and off the total Hamiltonian must be time dependent and has the form $H_{SE}(t) = H_S + H_E + \lambda(t)V_{SE}$, where $\lambda(t)$ is the unit-box function between $t \in [0, \tau]$. Since the composite $S + E$ system evolves unitarily, any work that is performed can be unambiguously associated with the total change in energy of $S + E$ as follows:

⁶Unitaries of the form of Eq. (50) can be generated by resonant-type interactions. For instance, if S and E are qubits with $H_i = \Omega_i \sigma_i^z / 2$ (here $i = S, E$) and if the interaction is generated by a potential $V = g(\sigma_S^+ \sigma_E^- + \sigma_S^- \sigma_E^+)$, then the unitary will be energy conserving only when $\Omega_E = \Omega_S$.

$$W = \int_{-\infty}^{\infty} dt \left\langle \frac{\partial H_{SE}(t)}{\partial t} \right\rangle = \langle V_{SE} \rangle_0 - \langle V_{SE} \rangle_{\tau}. \quad (55)$$

We therefore see that, in general, there is a work cost associated with turning the interaction on and off. But when strict energy conservation holds, $\Delta H_S = -\Delta H_E$ and hence $W = 0$.

This on-off work is usually negligible for macroscopic systems, so classical studies never really worry about it. This is because the energies H_S and H_E are proportional to the number of atoms in the bulk, whereas the interaction V_{SE} is usually proportional to the number of atoms on the surface, which is typically negligible relative to the bulk. In most of statistical mechanics, the system is therefore always assumed to be weakly coupled to a bath. But in microscopic systems this may easily break down since V_{SE} may be of the same order as H_S (even if it is still much smaller than H_E). As a consequence, the on-off work may be significant. For instance, the SWAP engine, which was analyzed by Campisi, Pekola, and Fazio (2015), operates with two qubits and is based precisely on the extraction of on-off work; see Sec. VII.A for more details.

Properly accounting for all sources and sinks of energy is an important part of thermodynamics at the quantum level. It has also been the source of significant debate. Additional methods for dealing with this are reviewed in Sec. VI.D.

E. Fluctuation theorems

The proposal of a general form of the entropy production in Eq. (30) gains solidity by analyzing it from multiple perspectives. In this sense, insight can be gained by analyzing the corresponding fluctuation theorem at the quantum trajectory level. This problem was solved by Manzano, Horowitz, and Parrondo (2018), who also showed how the two terms in Eq. (30) are related to the definition of the backward stochastic process. Shattering previous beliefs, the backward process is not unique. Different choices of backward processes lead to different expressions for the entropy production, which quantifies the information that is assumed to be lost between forward and backward protocols (Manzano, Horowitz, and Parrondo, 2018). This therefore attributes a clear operational significance to the entropy production.

We consider here the same map as in Eq. (28). No assumptions are made about either the environment or the unitary. Let $\rho_S = \sum_n p_n |n\rangle\langle n|$ and $\rho_E = \sum_{\nu} q_{\nu} |\nu\rangle\langle \nu|$ denote the eigendecompositions of the initial states of S and E . We introduce bases for the final reduced states $\rho'_S = \sum_m p'_m |\psi_m\rangle\langle \psi_m|$ and $\rho'_E = \sum_{\mu} q'_{\mu} |\phi_{\mu}\rangle\langle \phi_{\mu}|$, which will in general differ from the bases $|n\rangle$ and $|\nu\rangle$. At the stochastic level, we now consider the following protocol. We first measure both S and E in their respective eigenbasis $|n\rangle \otimes |\nu\rangle$. Next we evolve them according to a global unitary U and finally measure them in the bases $|\psi_m\rangle \otimes |\phi_{\mu}\rangle$. The last measurement is performed in the eigenbases of the reduced density matrices ρ'_S and ρ'_E . This choice ensures that the ensemble entropy of ρ'_S remains unaffected by the measurement backaction (Elouard, Herrera-Martí, Clusel, and Auffèves, 2017; Santos *et al.*, 2019), even though it kills

any quantum correlations present in ρ'_{SE} . For other choices of the final measurement scheme, see [Manzano, Horowitz, and Parrondo \(2018\)](#) and also [Park, Kim, and Vedral \(2017\)](#).

The quantum trajectory is specified by the four measurement outcomes $\gamma = \{n, \nu, m, \mu\}$, which occur with path probability

$$P_F[\gamma] = |\langle \psi_m, \phi_\mu | U | n, \nu \rangle|^2 p_n q_\nu. \quad (56)$$

To build a fluctuation theorem one must now establish the backward process, corresponding to the time-reverse evolution with unitary U^\dagger . The key observation of [Manzano, Horowitz, and Parrondo \(2018\)](#), however, is that this backward process is not unique. The arbitrariness comes from the choice of initial state $\tilde{\rho}_{SE}$ for the backward evolution; see Fig. 1. Different choices, as we now show, lead to different expressions for the entropy production. This is also intimately related to the notion of the Petz recovery map, a systematic way to build reverse processes for general quantum channels considered by [Kwon and Kim \(2019\)](#).

For the moment, we leave $\tilde{\rho}_{SE}$ unspecified. We consider a backward process where $\tilde{\rho}_{SE}$ is first measured in the basis $|\psi_m\rangle \otimes |\phi_\mu\rangle$, then allowed to evolve with U^\dagger , and finally measured one more time, now in the basis $|n\rangle \otimes |\nu\rangle$. The corresponding backward trajectory probability will thus be

$$P_B[\gamma] = |\langle n, \nu | U^\dagger | \psi_m, \phi_\mu \rangle|^2 \tilde{\rho}_{m\mu}, \quad (57)$$

where $\tilde{\rho}_{m\mu} = \langle \psi_m, \phi_\mu | \tilde{\rho}_{SE} | \psi_m, \phi_\mu \rangle$.

Armed with P_F and P_B , the entropy production is then defined as usual as ([Evans, Cohen, and Morriss, 1993](#); [Gallavotti and Cohen, 1995](#); [Crooks, 1998](#))

$$\sigma[\gamma] = \ln \frac{P_F[\gamma]}{P_B[\gamma]}. \quad (58)$$

By construction, this quantity satisfies an integral fluctuation theorem $\langle e^{-\sigma[\gamma]} \rangle = 1$. Using Eqs. (56) and (57) the dynamical terms cancel out, leaving us with only the following boundary term:

$$\sigma[\gamma] = \ln \frac{p_n q_\nu}{\tilde{\rho}_{m\mu}}. \quad (59)$$

As we now discuss, depending on the choice of $\tilde{\rho}_{SE}$, Eq. (59) will unravel differently.

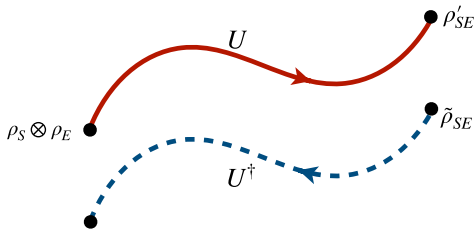


FIG. 1. General schematics for the forward and backward trajectories for the fluctuation theorems. The solid red line shows the forward trajectory, while the dashed blue curve shows the backward one.

First, suppose that we choose $\tilde{\rho}_{SE} = \rho'_S \otimes \rho_E$. This means that the system is taken at the final state (29), whereas the bath is reset to the initial state ρ_E . In this case $\tilde{\rho}_{m\mu} = p'_m q_\mu$ and Eq. (59) becomes

$$\sigma[\gamma] = \ln \frac{p_n q_\nu}{p'_m q_\mu}.$$

The average entropy production is computed as $\langle \sigma \rangle = \sum_\gamma \sigma[\gamma] P[\gamma]$. Carrying out the sum, one finds

$$\langle \sigma \rangle = \mathcal{I}_{\rho'_{SE}}(S:E) + S(\rho'_E || \rho_E) = S(\rho'_{SE} || \rho'_S \otimes \rho_E), \quad (60)$$

which is precisely the definition of Σ in Eq. (30). Notice how $\langle \sigma \rangle$ is simply the relative entropy between the final state ρ'_{SE} of the forward process and the initial state $\rho'_S \otimes \rho_E$ of the backward process. This provides a solid physical basis for Eq. (60) as being related to the act of tracing over the environment: The two terms in Eq. (60) appear because we reset E in the backward process, meaning we lost all access to both the correlations developed between S and E and the changes that were made to the state of E .

As a second choice, suppose that $\tilde{\rho}_{SE} = \rho'_S \otimes \rho'_E$. That is, S and E are initialized in the backward process at the final states of the forward process but marginalized to destroy any correlations between them. Correlations are arguably the most difficult part to access since they require global operations on $S + E$. In this case Eq. (59) becomes $\sigma[\gamma] = \ln(p_n q_\nu) / (p'_m q'_\mu)$, which upon averaging yields

$$\langle \sigma \rangle = \mathcal{I}_{\rho'_{SE}}(S:E) = \Delta S_S + \Delta S_E. \quad (61)$$

Hence, irreversibility stems solely from the SE correlations that are no longer accessible.

As a third choice, one may take the postmeasurement state

$$\begin{aligned} \tilde{\rho}_{SE} &= \Delta(\rho'_{SE}) := \sum_{m\mu} |\psi_m, \phi_\mu\rangle \langle \psi_m, \phi_\mu | \rho'_{SE} | \psi_m, \phi_\mu\rangle \langle \psi_m, \phi_\mu | \\ &= \sum_{m,\mu} \rho'_{m\mu} |\psi_m\rangle \langle \psi_m | \otimes |\phi_\mu\rangle \langle \phi_\mu |, \end{aligned} \quad (62)$$

which is obtained from the final state ρ'_{SE} after measurements in the $|\psi_m\rangle \otimes |\phi_\mu\rangle$ basis. Thus, it corresponds to the maximally dephased state in the basis $|\psi_m, \phi_\mu\rangle$ (note that, albeit dephased, this state is still classically correlated). The entropy production (59), upon averaging, reduces in this case to

$$\langle \sigma \rangle = S(\Delta(\rho'_{SE})) - S(\rho'_{SE}) = \mathcal{C}(\rho'_{SE}), \quad (63)$$

which is the relative entropy of coherence ([Streltsov, Adesso, and Plenio, 2017](#)). We thus conclude that, for this choice of backward protocol, the irreversibility stems solely from the decoherence of the measurement backaction in the final basis $|\psi_m, \phi_\mu\rangle$.

To perform a final measurement with absolutely no backaction, one would have to measure $S + E$ in the global basis diagonalizing ρ'_{SE} . In this case the entropy production would, on average, be identically zero and the process would be reversible. However, this would require assessing fully

nonlocal degrees of freedom of S and E , which would quickly become prohibitive even for small quantum systems.

As a final choice of measurement, we can assume that both system and environment are completely reset, so $\tilde{\rho}_{SE} = \rho_S \otimes \rho_E$ is exactly the initial state. Equation (59) then becomes $\sigma = \ln(p_n q_\nu) / (p_m q_\mu)$, which upon averaging becomes

$$\langle \sigma \rangle = \mathcal{I}_{\rho'_{SE}}(S:E) + S(\rho'_S || \rho_S) + S(\rho'_E || \rho_E). \quad (64)$$

The first and last terms are exactly the same as in the original definition of Σ in Eq. (30). However, we now get the additional term $S(\rho'_S || \rho_S)$, quantifying how much the system was pushed away from equilibrium. This is a consequence of the fact that in the backward process we also reset the system to its original thermal state, thus introducing an additional degree of irreversibility.

In the case where both system and environment start in thermal states but at different temperatures $\rho_S = e^{-\beta_S H_S} / Z_S$ and $\rho_E = e^{-\beta_E H_E} / Z_E$, Eq. (64) reduces to

$$\langle \sigma \rangle = \beta_S \Delta H_S + \beta_E \Delta H_E, \quad (65)$$

where $\Delta H_{S(E)}$ are the changes in energy in the system and environment, respectively. This choice of $\tilde{\rho}_{SE}$ therefore corresponds to the famous exchange fluctuation theorem (Jarzynski and Wójcik, 2004). If in addition the unitary satisfies strict energy conservation [Eq. (50)], then we may define $Q_E := \Delta H_E = -\Delta H_S$, in which case the entropy production reduces to

$$\langle \sigma \rangle = (\beta_E - \beta_S) Q_E, \quad (66)$$

which is the expression used by Jarzynski and Wójcik (2004).

A summary of these results is presented in Table I. The main message of this section is that the definition of entropy production is actually not unique but depends on the assumptions about which aspects of the system-environment dynamics become inaccessible or irretrievable. The definition (30), which we have focused on in most of this section, enables us to contemplate the most general scenario in which everything pertaining to the environment is assumed to be lost after the interaction. If the environment is macroscopic, highly chaotic, etc. (as in a bucket of water), this will inevitably be the case, so Eq. (30) will become the only relevant definition of entropy

TABLE I. Different choices for the initial state $\tilde{\rho}_{SE}$ of the backward process and the corresponding formula for the average entropy production $\langle \sigma \rangle$.

$\tilde{\rho}_{SE}$	$\langle \sigma \rangle$
$\rho'_S \otimes \rho_E$ (bath reset)	$\mathcal{I}_{\rho'_{SE}}(S:E) + S(\rho'_E \rho_E) \equiv \Sigma$ [Eq. (30)]
$\rho'_S \otimes \rho'_E$ (correlations destroyed)	$\mathcal{I}_{\rho'_{SE}}(S:E)$ $(= \Delta S_S + \Delta S_E)$
$\Delta(\rho'_{SE})$ (postmeasurement state)	$C(\rho'_{SE})$ (relative entropy of coherence)
$\rho_S \otimes \rho_E$ (both reset)	$\mathcal{I}_{\rho'_{SE}}(S:E) + S(\rho'_S \rho_S) + S(\rho'_E \rho_E)$ $= (\beta_S - \beta_E) Q_E$ (Jarzynski and Wójcik, 2004)

production. But in the quantum domain comparing the different definitions may be relevant.

One may also attempt to compare the relative importance of each term in these expressions. We assume that the bath is much larger than the system so that the process only pushes it slightly away from equilibrium, that is, such that $\rho'_E = \rho_E + \mathcal{O}(\epsilon)$ for some small parameter ϵ . Using standard perturbation theory one then finds that $\Delta S_E \propto \epsilon$ while $S(\rho'_E || \rho_E) \propto \epsilon^2$ (Rodrigues *et al.*, 2019). Thus, it becomes irrelevant whether or not to include the relative entropy term since the mutual information tends to dominate. This, however, is not always the case, as recently elucidated by Ptaszynski and Esposito (2019). As they discussed, the mutual information is actually bounded by the Araki-Lieb inequality as follows:

$$\mathcal{I}_{\rho'_{SE}}(S:E) \leq 2 \min\{S(\rho'_S), S(\rho'_E)\}.$$

For small S and large E , \mathcal{I} will be essentially capped by $S(\rho'_S)$. On the other hand, the relative entropy $S(\rho'_E || \rho_E)$ is unbounded and can thus increase indefinitely over time. This will be the case, for instance, in nonequilibrium steady states of systems connected to multiple baths.

This discussion can also be extended to multiple measurements. One way to accomplish this is through a collisional model approach, as discussed in Sec. V.A. This will simply lead to a composition of the results presented in this section. Alternatively, one may also analyze it from the perspective of stochastic master equations describing continuously measured systems. This was done by Horowitz and Parrondo (2013) and Horowitz and Sagawa (2014) and yields the entropy production as a function of the entire trajectory of quantum jumps. The exploration of different choices for the reverse trajectory, however, is not discussed as the framework is based solely on the reduced description of the system in terms of a master equation. However, at the ensemble level they obtained an entropy production consistent with Eq. (52) that should thus correspond to the bath reset choice (the first line in Table I).

F. Nonequilibrium lag

A scenario that is deeply related to the previous one, and that has been the subject of considerable research, is the nonequilibrium lag that occurs when an isolated quantum system undergoes a work protocol. This was covered in detail by Campisi, Hänggi, and Talkner (2011). Here we focus only on the most recent developments.

We consider a system S that was initially prepared in the equilibrium state $\rho_i^{\text{th}} = e^{-\beta H_i} / Z_i$ at temperature β and Hamiltonian H_i . The system is then driven by a work protocol $\lambda(t)$ that changes the Hamiltonian from $H_i = H(\lambda(0))$ to $H_f = H(\lambda(\tau))$, where τ is the duration of the protocol. The drive causes the system to evolve unitarily to a nonequilibrium state $\rho' = V \rho_i^{\text{th}} V^\dagger$, where V is the time-evolution operator generated by $H[\lambda(t)]$. After the protocol is applied, the system is placed in contact with a bath and allowed to fully thermalize toward a new equilibrium state $\rho_f^{\text{th}} = e^{-\beta H_f} / Z_f$; see Fig. 2.

The unitary drive produces no entropy since the dynamics is closed. Irreversibility stems solely from the thermalization step. The entropy production for this relaxation process will be

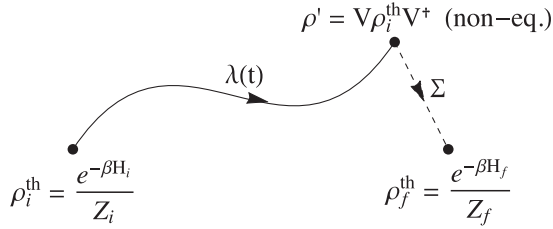


FIG. 2. Typical nonequilibrium lag scenario. A system initially prepared in a thermal state ρ_i^{th} is driven unitarily by a work protocol to a nonequilibrium state ρ' . After the protocol, the system is allowed to thermalize from ρ' to ρ_f .

given, in the simplest scenario, by Eq. (52). Since the thermalization is total, the second term vanishes, leaving us with

$$\Sigma = S(\rho' \parallel \rho_f^{\text{th}}). \quad (67)$$

Despite being associated with the thermalization process, it turns out that Eq. (67) is also of significance to the unitary evolution in itself. In fact, this is usually defined without even mentioning the thermalization. The reason for this is that Eq. (67) is also directly associated with the irreversible work produced by the unitary V :

$$\Sigma \equiv \beta W_{\text{irr}} = \beta(\langle W \rangle - \Delta F), \quad (68)$$

where $\langle W \rangle = \text{tr}(H_f \rho') - \text{tr}(H_i \rho_i^{\text{th}})$ is the average work and $\Delta F = -T \ln Z_f / Z_i$ is the change in equilibrium free energy. For this reason, Eq. (67) is also called the *nonequilibrium lag*. For all intents and purposes, nonequilibrium lag can be taken as a synonym of entropy production. The reason to introduce this terminology is simply to emphasize that it refers to the unitary protocol, for which no entropy is produced. In recent years, significant attention has been given to the nonequilibrium lag, particularly in the context of quantum phase transitions. These are reviewed in Sec. VII.E.

The nonequilibrium lag can also be studied from a stochastic perspective using the two-point measurement scheme: the first measurement is done in the eigenbasis $|n_i\rangle$ of H_i , and the second in the eigenbasis $|m_f\rangle$ of H_f . The stochastic entropy production associated with this process is then (Campisi, Hänggi, and Talkner, 2011)

$$\sigma[n_i, m_f] = \ln p_{n_i}^{\text{th}} / p_{m_f}^{\text{th}} = \beta(E_{m_f}^f - E_{n_i}^i - \Delta F), \quad (69)$$

where $E^{i(f)}$ are the energies of $H_{i(f)}$ and $\Delta F = F_f - F_i = -T \ln Z_f / Z_i$ is the change in nonequilibrium free energy. Moreover, $p_{n_i}^{\text{th}} = e^{-\beta E_{n_i}^i} / Z_i$ is the initial thermal probability and $p_{m_f}^{\text{th}} = e^{-\beta E_{m_f}^f} / Z_f$ is the thermal probability associated with the final Hamiltonian H_f . The probability distribution of σ is thus

$$P(\sigma) = \sum_{n_i, m_f} p(m_f | n_i) p_{n_i} \delta(\sigma - \sigma[n_i, m_f]), \quad (70)$$

where $p(m_f | n_i) = |\langle m_f | V | n_i \rangle|^2$ is the transition probability from $|n_i\rangle \rightarrow |m_f\rangle$. By construction, this is such that $\langle \sigma \rangle = \Sigma$ [Eq. (67)].

It is convenient to study the cumulant generating function $K(\lambda) = \ln \langle e^{-\lambda \sigma} \rangle$, which can be conveniently written as (Talkner, Lutz, and Hänggi, 2007; Esposito, Harbola, and Mukamel, 2009)

$$K(\lambda) = \ln \text{tr} \{ V^\dagger e^{-\beta \lambda (H_f - F_f)} V e^{\beta \lambda (H_i - F_i)} \rho_i^{\text{th}} \}. \quad (71)$$

The cumulants may be computed from $K(\lambda)$ through

$$\kappa_n(\sigma) = (-1)^n \left. \frac{\partial^n K}{\partial \lambda^n} \right|_{\lambda=0}. \quad (72)$$

The first cumulant is the average and is given by Eq. (67). Similarly, the second cumulant is the variance and can be written as

$$\text{var}(\sigma) = \text{tr} \{ \rho' (\ln \rho' - \ln \rho_f^{\text{th}})^2 \} - S(\rho' \parallel \rho_f^{\text{th}})^2, \quad (73)$$

which is sometimes called the relative entropy variance.

The cumulant generating function (CGF) (71) can also be expressed in terms of the so-called Rényi divergences, which are further discussed in Sec. VI and are defined as

$$S_\lambda(\rho \parallel \sigma) = \frac{1}{\lambda - 1} \ln \text{tr} \{ \rho^\lambda \sigma^{1-\lambda} \}. \quad (74)$$

Equation (74) corresponds to a generalization of the relative entropy (32) that is recovered from $S_\lambda(\rho \parallel \sigma)$ in the limit $\lambda \rightarrow 1$. Comparing Eq. (74) to Eq. (71) one then sees that (Guarnieri, Landi *et al.*, 2019)⁷

$$K(\lambda) = (\lambda - 1) S_\lambda(\rho_f^{\text{th}} \parallel \rho'), \quad (75)$$

Equation (75) was used in several recent studies. Following Guarnieri, Ng *et al.* (2019), we review in Sec. VI.E how Eq. (75) can be used as a connection to the resource-theoretic formulation of thermodynamics, which is the subject of Sec. VI. In Sec. VII.E we review the work of Miller *et al.* (2019) and Scandi *et al.* (2020), which use Eq. (75) as a tool to extract the contribution from quantum coherence in slow processes.

IV. INFORMATION-THEORETIC ASPECTS

A. Corrections to Landauer's principle

Landauer's principle was introduced in Sec. II.C and is based on the idea that information erasure is an irreversible process, with a fundamental heat cost associated with it. This is synthesized by Eq. (21), representing a lower bound on the heat Q_E dissipated to the environment in terms of the change in entropy ΔS_S of the system. Being a lower bound, one can then conclude that changes in entropy must be accompanied by a fundamental heat cost.

⁷This can be equivalently written as $K(\lambda) = -\lambda S_{1-\lambda}(\rho' \parallel \rho_f^{\text{th}})$.

In Sec. II.C we hinted at the subtle nature of Landauer's principle: in classical thermodynamics, Eq. (21) is a direct consequence of the second law, but with S_S as the thermodynamic entropy of the system. Landauer's original bound, on the other hand, concerns the information-theoretic entropy. The framework put forth in Sec. III, however, unifies both views, as it reformulates the second law in terms of the system's von Neumann entropy. Indeed, Eqs. (30) and (38) imply that

$$\Sigma = \mathcal{I}_{\rho'_{SE}}(S:E) + S(\rho'_E \parallel \rho_E) = \Delta S_S + \beta Q_E. \quad (76)$$

The second law $\Sigma \geq 0$ then yields $Q_E \geq -T\Delta S_S$, which is precisely Landauer's bound (21). Equality is achieved when $\Sigma = 0$, i.e., for reversible processes. These results were already presented by Esposito, Lindenberg, and Van Den Broeck (2010), but the link with Landauer's principle was strengthened by Reeb and Wolf (2014), who greatly popularized this subject.

Equation (21) is important because it is universal. The only hypothesis is that the bath is initially thermal (and uncorrelated from the system). Other than that, the bath may have an arbitrary dimension and arbitrary Hamiltonian, the system may be prepared in any initial state, and the interaction U can be any unitary whatsoever.

This universality, however, has a downside in that the bound is in general loose. Tighter bounds can be obtained by assuming additional information about the environment and/or the process. We now discuss several such formulations, taking care to properly state which additional pieces of information are assumed in each case. First, we consider the case where the only additional piece of information one has is that the environment is finite dimensional, with a Hilbert space dimension d_E . In this case, when $\Delta S_S < 0$, the following correction to Eq. (21) holds (Reeb and Wolf, 2014):

$$Q_E \geq -T\Delta S_S + \frac{2T(\Delta S_S)^2}{4 + \ln^2(d_E - 1)}. \quad (77)$$

Equation (77) shows that finite dimensions impose more strict constraints on heat dissipation. The correction vanishes when $d_E \rightarrow \infty$; however, notice that the dependence is logarithmic and therefore extremely slow. Additional finite-size bounds were also presented by Reeb and Wolf (2014), although they depend on more complicated functions.

The original bound (21) or its finite-size correction (77) becomes trivial in the limit $T \rightarrow 0$. This is unsatisfactory: can erasure really be performed with zero dissipation when $T \rightarrow 0$? The bound trivializes in this case due to the term $S(\rho'_E \parallel \rho_E)$ in Eq. (76), which diverges when $T \rightarrow 0$. To bypass this difficulty, Timpanaro, Santos, and Landi (2020) showed how to derive a tighter bound starting only with the mutual information term $\mathcal{I}_{\rho'_{SE}}(S:E)$. The bound in this case acquires the form

$$Q_E \geq \mathcal{Q}(S^{-1}(-\Delta S_S)), \quad (78)$$

where the functions $\mathcal{Q}(T')$ and $\mathcal{S}(T')$ are defined as

$$\mathcal{Q}(T') = \int_T^{T'} C_E(\tau) d\tau, \quad \mathcal{S}(T') = \int_T^{T'} \frac{C_E(\tau)}{\tau} d\tau, \quad (79)$$

with $C_E(T)$ the equilibrium heat capacity of the environment. In Eqs. (79) T is the actual initial temperature of the environment, whereas T' is merely the argument of the functions. This bound requires only one additional piece of information, namely, the environment's heat capacity $C_E(T)$. This is to be compared with Eq. (21), which requires only a single number T , or with Eq. (77), which requires two numbers T and d_E . Knowing an entire function $C_E(T)$ is definitely more difficult, although the heat capacity is in general an easy quantity to measure experimentally, even at extremely low temperatures. However, one can also show that the bound is always tighter than both Eqs. (21) and (77). To provide an example, if we have $C_E = aT$ for some constant a , Eq. (78) becomes

$$Q_E \geq -T\Delta S_S + \Delta S_S^2/2a. \quad (80)$$

As in Eq. (77), the correction also involves a term proportional to ΔS_S^2 , but with a coefficient that is temperature independent. Thus, in the limit $T \rightarrow 0$ the last term still survives, showing that a fundamental heat cost exists even when $T = 0$.

Tighter bounds can also be derived when information about the SE unitary U and the system initial state ρ_S are available (Goold, Paternostro, and Modi, 2015; Lorenzo *et al.*, 2015; Guarnieri *et al.*, 2017). Here we review the approach of Goold, Paternostro, and Modi (2015), which derives a bound using the fluctuating properties of heat. The key idea is to interpret the global map (28) as a quantum channel for the environment, instead of the system, as described by the Kraus map

$$\rho'_E = \text{Tr}_S[U(\rho_S \otimes \rho_E)U^\dagger] = \sum_l A_l \rho_E A_l^\dagger, \quad (81)$$

where $A_{l=jk} = \sqrt{\lambda_j} \langle s_k | U | s_j \rangle$, with $\{\lambda_j\}$ and $\{|s_j\rangle\}$ the eigenvalues and eigenstates of ρ_S . Trace preservation implies $\sum_l A_l^\dagger A_l = \mathbb{1}_E$. Letting E_n and $|r_n\rangle$ denote the eigenvalues and eigenvectors of H_E , the heat distribution of the environment (via a two-point measurement) can then be written as (Talkner, Campisi, and Hänggi, 2009)

$$P(Q_E) = \sum_{l,m,n} \langle r_n | A_l | r_m \rangle (\rho_E)_{mm} \langle r_m | A_l^\dagger | r_n \rangle \delta(Q_E - (E_n - E_m)), \quad (82)$$

with $(\rho_E)_{nm} = \langle r_n | \rho_E | r_m \rangle$. From this one may then show that $\langle e^{-\beta Q} \rangle = \text{Tr}[\mathbf{M}\rho_S]$, where $\mathbf{M} = \text{Tr}_E[U^\dagger(\mathbb{1}_S \otimes \rho_E)U]$. Using Jensen's inequality then leads to

$$\langle Q_E \rangle \geq -T \ln(\text{Tr}[\mathbf{M}\rho_S]). \quad (83)$$

This result establishes a bound on $\langle Q_E \rangle$ that depends on both the state of the system and the unitary U . It therefore also encompasses a dependence on the size of E , which is in line with Eq. (77).

Using the formalism of full counting statistics (Esposito, Harbola, and Mukamel, 2009), one can also extend these

results to obtain an entire single-parameter family of bounds (Guarnieri *et al.*, 2017). We first introduce the following cumulant generating function of $P(Q_E)$:

$$\Theta(\eta, \beta) \equiv \ln \langle e^{-\eta Q_E} \rangle = \ln \int P(Q_E) e^{-\eta Q_E} dQ_E. \quad (84)$$

Hölder's inequality then implies that, for $\eta > 0$,

$$\beta \langle Q_E \rangle \geq -\frac{\beta}{\eta} \Theta(\eta, \beta) \quad (\eta > 0), \quad (85)$$

which contains Eq. (83) as a particular case. Conversely, for $\eta < 0$ we obtain the upper bounds $\beta \langle Q_E \rangle \leq \beta \Theta(\eta, \beta) / |\eta|$. In the limit $|\eta| \rightarrow 0$ both bounds coincide with $\beta \langle Q_E \rangle$.

B. Conditional entropy production

We consider once again the general map (28) of Sec. III. But now we suppose that after the map we measure the environment, or at least part of it. Funo, Watanabe, and Ueda (2013) studied how the information acquired from this measurement affects the entropy production. Since it is only the bath that is measured, there can be no backaction to the system, as this would violate no signaling. As a consequence, one would expect that learning the outcomes of the measurements would always make the process more reversible; that is, part of the ignorance captured by the entropy production should be resolved.

To formalize this idea, we consider a generalized measurement on E described by Kraus operators $\{M_k\}$ and labeled with a set of outcomes k . We denote the local states of S and E after the map, conditioned on an outcome k , by

$$\rho'_{E|k} = \frac{M_k \rho'_E M_k^\dagger}{p_k}, \quad \rho'_{S|k} = \frac{1}{p_k} \text{tr}_E(M_k \rho'_{SE} M_k^\dagger), \quad (86)$$

where $p_k = \text{tr}(M_k \rho'_E M_k^\dagger)$ is the probability of outcome k (as before primed quantities always refer to states after the map). One may also verify that $\sum_k p_k \rho'_{S|k} = \rho'_S$, thus confirming that the measurement in E causes no backaction in S . But there may be a backaction in E , so $\tilde{\rho}_E := \sum_k p_k \rho'_{E|k} \neq \rho'_E$.

We now ask how to construct the entropy production conditioned on a given outcome. The goal is to define, in analogy with Eq. (34), a conditional entropy production Σ_k and a conditional flux Φ_k , which are related by

$$\Sigma_k = S(\rho'_{S|k}) - S(\rho_S) + \Phi_k. \quad (87)$$

Equation (87) is still merely a definition and will acquire meaning only once Σ_k and Φ_k are defined. Averaging over all outcomes k then yields the following relation between the conditional average entropy production and flux:

$$\Sigma_c = \sum_k p_k S(\rho'_{S|k}) - S(\rho_S) + \Phi_c, \quad (88)$$

where $\Sigma_c = \sum_k p_k \Sigma_k$ and we follow a similar approach for Φ_c . The entropy difference on the first two terms of the

right-hand side is known as the Ozawa–Groenewold quantum-classical information (Groenewold, 1971; Ozawa, 1986; Funo, Ueda, and Sagawa, 2018). Notice also that Σ_k and Φ_k are not necessarily linear functions of ρ'_{SE} , so in general their averages Σ_c and Φ_c do not have to coincide with the unconditional quantities Σ and Φ .

Equation (87) is merely a definition of Σ_k and Φ_k . The relevant question is how to properly define these quantities in a way that is physically consistent. We first analyze the flux. An examination of Eq. (37) shows that a natural generalization to the case of conditional states is $\Phi_k = S(\rho'_{E|k}) - S(\rho_E) + S(\rho'_{E|k} \parallel \rho_E)$, which therefore simply amounts to replacing ρ'_E with $\rho'_{E|k}$. Averaging over all p_k and using the second line in Eq. (37), one then finds that

$$\Phi_c := \sum_k p_k \Phi_k = \text{tr}\{(\rho_E - \tilde{\rho}_E) \ln \rho_E\}, \quad (89)$$

where $\tilde{\rho}_E = \sum_k p_k \rho'_{E|k}$. If the measurement is performed on the initial eigenbasis of ρ_E , it then follows that $\Phi_c = \Phi$ (even though $\tilde{\rho}_E \neq \rho'_E$). This result has a clear physical interpretation: the entropy flux refers only to the flow of information to the environment. It should therefore be independent of whether we place a condition on any measurement outcomes. The flux should therefore only change if there is backaction from the measurement. In other words, the difference $\Phi_c - \Phi$ has nothing to do with the system or the SE interaction, but rather only with the backaction caused by the measurement. For this reason, we henceforth assume that the measurement is such that $\Phi_c = \Phi$. This assumption was also used implicitly by Breuer (2003), who defined entropy production from the perspective of quantum jump trajectories.

Using $\Phi_c = \Phi$ in Eq. (88) and comparing it to Eq. (34) allows one to conclude that

$$\Sigma_c = \Sigma - \chi_M(\rho'_S), \quad (90)$$

where

$$\chi_M(\rho'_S) = S(\rho'_S) - \sum_k p_k S(\rho'_{S|k}) = \sum_k p_k S(\rho'_{S|k} \parallel \rho'_S) \quad (91)$$

is the Holevo quantity (Nielsen and Chuang, 2000), which is always non-negative. Equation (90) illustrates the idea of reducing irreversibility through measurement: Conditioning on the measurement outcomes reduces, on average, the entropy production by an amount proportional to the Holevo quantity, an object with numerous applications in information theory.

The Holevo quantity χ_M is a basis-dependent version of the classical information used in quantum discord theory (Modi *et al.*, 2012). It thus follows that, for any choice of measurement operators $\{M_k\}$, one should have $\chi_M(\rho'_S) \leq I_{\rho'_S}(S:E)$. Comparing this to the definition of Σ in Eq. (30), one then concludes from Eq. (90) that

$$\Sigma_c = I_{\rho'_S}(S:E) + S(\rho'_E \parallel \rho_E) - \chi(\rho'_S) \geq S(\rho'_E \parallel \rho_E).$$

Hence, even though $\Sigma_c \leq \Sigma$ it is nonetheless still strictly non-negative. This occurs because the interaction irreversibly

pushes the bath away from equilibrium, so that, even if all possible information were to be acquired, the dynamics would still be irreversible.

C. Heat flow in the presence of correlations

Another key manifestation of information in thermodynamics is the influence of initial correlations in the heat flow between two bodies. According to the second law, if we put into contact two systems A and B , initially prepared in equilibrium at different temperatures, heat will always flow from hot to cold [Eq. (15)]. This assumes, however, that the two bodies are initially uncorrelated. If that is not true, heat may eventually flow from cold to hot. This problem was first considered in the quantum scenario of [Partovi \(2008\)](#), who discussed only the case where the global state of AB is pure. This was then generalized by [Jennings and Rudolph \(2010\)](#) and [Bera et al. \(2017\)](#), who also addressed some of the information-theoretic aspects of the problem. An experimental demonstration of this effect was recently performed in a nuclear magnetic resonance setup ([Micadei et al., 2019](#)). In a broader sense, these ideas are ultimately related to the use of mutual information to reduce entropy, as first discussed in the seminal paper by [Lloyd \(1989\)](#).

We consider two systems with Hamiltonians H_A and H_B , prepared in a global (generally correlated) state ρ_{AB} . We assume, however, that the reduced density matrices of A and B are still thermal, $\rho_A = \text{tr}_B \rho_{AB} = e^{-\beta_A H_A} / Z_A$ and $\rho_B = e^{-\beta_B H_B} / Z_B$ at different temperatures β_A and β_B . The two systems are then made to interact with a unitary U satisfying strict energy conservation $[U, H_A + H_B] = 0$; see Eq. (50). The state after the interaction is thus $\rho'_{AB} = U \rho_{AB} U^\dagger$, from which one can compute the corresponding marginals ρ'_A and ρ'_B .

The correlations between A and B are characterized by the mutual information $\mathcal{I}_{\rho_{AB}}(A:B)$ defined in Eq. (31). Since the dynamics is unitary it follows that $S(\rho'_{AB}) = S(\rho_{AB})$, which allows one to show that

$$\Delta I(A:B) = \Delta S_A + \Delta S_B, \quad (92)$$

where $\Delta I(A:B) = I_{\rho'_{AB}}(A:B) - I_{\rho_{AB}}(A:B)$ is the change in mutual information between A and B .

Next consider the quantity

$$\mathcal{S} = S(\rho'_A || \rho_A) + S(\rho'_B || \rho_B) \geq 0, \quad (93)$$

which is non-negative because the relative entropies are non-negative. This quantity is a part of the entropy production when cast in terms of the Jarzynski-Wójcik scenario; see Eq. (64). What is important for our purposes is that this quantity is purely local, depending only on the reduced density matrices of A and B before and after the interaction. Substituting the initial thermal forms of ρ_A and ρ_B , together with Eq. (92), then leads to ([Jennings and Rudolph, 2010](#))

$$\mathcal{S} = \beta_A \Delta H_A + \beta_B \Delta H_B - \Delta I(A:B) \geq 0. \quad (94)$$

We assume that $T_A > T_B$. Because of strict energy conservation, the average heat exchanged is simply defined as

$$Q_B = \Delta H_B = \text{tr}\{H_B(U \rho_{AB} U^\dagger - \rho_{AB})\} = -\Delta H_A, \quad (95)$$

so Eq. (94) becomes

$$(\beta_B - \beta_A) Q_B \geq \Delta I(A:B). \quad (96)$$

Equation (96) can be viewed as a generalization of the bound (15) to take into account initial correlations.

If A and B are initially uncorrelated then $\Delta I(A:B) = I_{\rho'_{AB}}(A:B) \geq 0$, which implies that Q_B must have the same sign as $\beta_B - \beta_A$ (i.e., heat flows from hot to cold). But if they are initially correlated and the process is such that this correlation is consumed [$\Delta I(A:B) < 0$], then it is possible for heat to flow from cold to hot. This is thus an example of a situation where an information-theoretic resource is being consumed to perform a thermodynamic task that would not naturally occur. This is akin to refrigerators, where heat also flows from cold to hot, but the resource being used is work from the electrical plug. The result can also be formulated in the language of Maxwell's demons. A demon, in this context, has access to additional information in the form of global correlations shared between A and B . These correlations can then be consumed as a thermodynamic resource.

Correlations will not always make heat flow from cold to hot. They may well have the opposite effect, accelerating the heat from hot to cold. An illustrative example is the problem studied experimentally by [Micadei et al. \(2019\)](#). Consider two qubits with $H_i = \Omega |e\rangle\langle e|_i$ ($i = A, B$) and initially prepared in a correlated state of the form

$$\rho_{AB} = \rho_A^{\text{th}} \otimes \rho_B^{\text{th}} + \chi, \quad (97)$$

where $\rho_i^{\text{th}} = (1 - f_i) |g\rangle\langle g| + f_i |e\rangle\langle e|$, with $f_i = (e^{\Omega/T_i} + 1)^{-1}$, are the local thermal states of each qubit and $\chi = \alpha e^{i\theta} |g, e\rangle\langle e, g| + \alpha e^{-i\theta} |e, g\rangle\langle g, e|$ represents the correlations, with α and θ real parameters. The two qubits are then made to interact with an energy-preserving unitary $U = \exp\{-igt(e^{i\phi} |g, e\rangle\langle e, g| + e^{-i\phi} |e, g\rangle\langle g, e|)\}$, where ϕ is an arbitrary phase and g is the interaction strength. The heat $Q_B = \Delta H_B$ that enters system B at time t is given by

$$Q_B(t) = \Omega \sin(gt) [(f_A - f_B) \sin(gt) - 2\alpha \sin(\theta - \phi) \cos(gt)]. \quad (98)$$

We again assume that $T_A > T_B$ for concreteness. Since f_i is monotonically increasing with T_i , when $\alpha = 0$ we always get $Q_B \propto (f_A - f_B) > 0$ so that heat will flow from hot to cold. But when $\alpha \neq 0$, the direction of the heat flow will actually depend on a fine interplay between the phases θ and ϕ appearing in χ and U , respectively. These phases may combine either constructively, reversing the heat flow, or destructively, accelerating the already natural flow direction.

D. Fluctuation theorem under classical and quantum correlations

The problem treated in Sec. IV.C can also be analyzed from a quantum trajectory perspective, which will serve to highlight the nontrivial role of quantum versus classical correlations. We begin by considering the case of two-point measurements (TPM), where both A and B are measured at the beginning and the end of the process. Jevtic *et al.* (2015) discussed the implications of measuring in the local energy bases $|n_A\rangle$ and $|n_B\rangle$ of the Hamiltonians H_A and H_B . A quantum trajectory will be specified by four quantum numbers $\gamma = (n_A, n_B, m_A, m_B)$ and occurs with the probability

$$\mathcal{P}[\gamma] = |\langle m_A m_B | U | n_A n_B \rangle|^2 p_{n_A n_B}, \quad (99)$$

where $p_{n_A n_B} = \langle n_A n_B | \rho_{AB} | n_A n_B \rangle$. Since ρ_{AB} is not a product state, in general $p_{n_A n_B} \neq p_{n_A} p_{n_B}$.

The probability that a heat $q_B[\gamma] = E_{m_B} - E_{n_B}$ enters the system B will then be given by $P(q_B) = \sum_{\gamma} \delta(q_B - q_B[\gamma]) \mathcal{P}[\gamma]$. Using this to compute the average heat $\langle q_B \rangle$, we find that

$$\langle q_B \rangle = \text{tr}\{H_B[U\Delta(\rho_{AB})U^\dagger - \Delta(\rho_{AB})]\}, \quad (100)$$

where $\Delta(\rho_{AB}) = \sum_{n_A n_B} |n_A n_B\rangle \langle n_A n_B | \rho_{AB} | n_A n_B \rangle \langle n_A n_B |$ is the operation of fully dephasing ρ_{AB} in the basis $|n_A n_B\rangle$.

The important point to realize now is that Eq. (100) is in general different from the average heat in Eq. (95). The difference is due to the presence of the dephasing operator Δ and is thus a consequence of the measurement backaction, which dephases ρ_{AB} . The two quantities will coincide only when ρ_{AB} is already diagonal in $|n_A n_B\rangle$. Stated differently, when ρ_{AB} is not diagonal, the TPM scheme used here will fundamentally change the amount of heat exchanged between the two systems, producing an entirely different dynamics when compared with the bare unitary evolution. The entropy production is thus extrinsic, that is, dependent not only on the systems A and B but also on the details of how one performs the experiment.

This highlights the fundamental difference between correlations present in the populations (i.e., those that are diagonal in $|n_A n_B\rangle$) and correlations that are present in the coherences (off diagonals). The latter can be viewed as a basis-dependent quantum discord, i.e., as the amount of discord present in the energy basis (the energy basis appears as a preferred basis due to the energy-conserving nature of the unitary U , as reviewed in Sec. V.B).

Returning to Eq. (99), we introduce the reverse process, where A and B start at the same state but one applies the unitary U^\dagger instead (this is the Jarzynski-Wójcik scenario of Sec. III.E). The probability for the backward trajectory $\gamma^* = (m_A, m_B, n_A, n_B)$ is given by $\mathcal{P}[\gamma^*] = |\langle n_A n_B | U^\dagger | m_A m_B \rangle|^2 p_{m_A m_B}$. The ratio of the two processes reduces to $\mathcal{P}[\gamma]/\mathcal{P}[\gamma^*] = p_{n_A n_B}/p_{m_A m_B}$ since the dynamical term cancels out (as usual). To make the physics of this ratio more evident, we introduce the stochastic mutual information $I_{n_A n_B} = \ln p_{n_A n_B}/p_{n_A} p_{n_B}$, where $p_{n_A} = \sum_{n_B} p_{n_A n_B}$ (and likewise for p_{n_B}) are the marginal distributions of the initial state,

which we chose to be thermal ($p_{n_A} = e^{-\beta_A E_{n_A}}/Z_A$). The average of $I_{n_A n_B}$ over $p_{n_A n_B}$ yields the mutual information of the dephased state

$$\langle I_{n_A n_B} \rangle = \sum_{n_A n_B} p_{n_A n_B} \ln \frac{p_{n_A n_B}}{p_{n_A} p_{n_B}} = \mathcal{I}_{\Delta(\rho_{AB})}(A:B), \quad (101)$$

where $\mathcal{I}_\rho(A:B)$ is as defined in Eq. (31).

Writing $p_{n_A n_B} = p_{n_A} p_{n_B} e^{I_{n_A n_B}}$ allows us to express $\mathcal{P}[\gamma]/\mathcal{P}[\gamma^*] = (p_{n_A} p_{n_B}/p_{m_A} p_{m_B}) e^{-\Delta I[\gamma]}$, where $\Delta I[\gamma] = I_{m_A m_B} - I_{n_A n_B}$. But since the reduced states are thermal ($p_{n_\alpha}/p_{m_\alpha} = e^{\beta_\alpha(E_{m_\alpha} - E_{n_\alpha})}$), we may finally write

$$\mathcal{P}[\gamma]/\mathcal{P}[\gamma^*] = e^{(\beta_B - \beta_A)q_B[\gamma] - \Delta I[\gamma]}, \quad (102)$$

where we also used the fact that $E_{m_A} - E_{n_A} = -(E_{m_B} - E_{n_B})$.

Equation (102) represents a modified exchange fluctuation theorem generalizing the results of Jarzynski and Wójcik (2004) to the case where A and B have initial correlations. Equation (102) implies a nonequilibrium equality $\langle e^{(\beta_B - \beta_A)q_B[\gamma] - \Delta I[\gamma]} \rangle = 1$, which yields the bound

$$(\beta_B - \beta_A)\langle q_B[\gamma] \rangle \geq \langle \Delta I[\gamma] \rangle. \quad (103)$$

This is structurally similar to Eq. (96). However, as previously discussed they cannot be directly compared since they pertain to different processes due to the dephasing action of the first measurement.

These results show that, when constructing fluctuation theorems, quantum correlations are fundamentally hampered by the backaction of the two-point measurement scheme. A way to circumvent this is to use the notion of augmented trajectories, first discussed by Dirac (1945) and used more recently by Park, Kim, and Vedral (2017) and Micadei, Landi, and Lutz (2020). We decompose the initial (correlated) state of AB as $\rho_{AB} = \sum_s p_s |s\rangle \langle s|$, where $|s\rangle$ are eigenvectors living on the composite Hilbert space of AB . Before the dynamics, we perform instead a measurement in the basis $|s\rangle$. The second measurement can be in the energy basis, as in Sec. IV.D, since it does not matter whether we destroy the correlations after the end of the protocol.

The quantum trajectory will therefore be described in this case by the quantum numbers $\gamma = (s, m_A, m_B)$ and the corresponding path probability will be given, instead of by Eq. (99), by $\mathcal{P}[\gamma] = |\langle m_A m_B | U | s \rangle|^2 p_s$. Knowing the outcome s of the first measurement, however, does not uniquely specify which energy eigenstates $|n_A n_B\rangle$ the two systems were initially in. To account for this, we augment the trajectories by considering the conditional probability $p_{n_A n_B|s} = |\langle n_A n_B | s \rangle|^2$ that AB are found in $|n_A n_B\rangle$ given that globally they are in $|s\rangle$. The augmented trajectory $\tilde{\gamma} = (s, n_A, n_B, m_A, m_B)$ will then have a path probability

$$\tilde{\mathcal{P}}[\tilde{\gamma}] = |\langle m_A m_B | U | s \rangle|^2 p_s p_{n_A n_B|s}. \quad (104)$$

This formulation addresses the issues that arise from the backaction of the first measurement. For instance, as Micadei,

Landi, and Lutz (2020) showed, it leads to the full identity (96) and not its dephased version (103).

Equation (104) also well illustrates a recurring problem in extending thermodynamics to the quantum regime. Thermodynamics deals not with states but with processes, i.e., with transformations between states. Assessing these transformations therefore touches on the inevitable measurement backaction. Equation (104) circumvents this by constructing a distribution free from any backaction. This distribution, however, has to be constructed using full state tomography. An alternative approach put forth by Levy and Lostaglio (2019) formulates the problem by instead using the notion of quasiprobabilities, that is, probabilities that can take on negative values. As they showed, these negativities are directly related to the notion of contextuality.

V. QUANTUM DYNAMICS AND THE CLASSICAL LIMIT

The global unitary map (29) is extremely general and represents the basic structure behind most open-system dynamics (the only assumption in it is that S and E are initially uncorrelated). To make it practical, however, this map has to be specialized to specific paradigms. The usual paradigm in open quantum systems (Gardiner and Zoller, 2004; Breuer and Petruccione, 2007; Rivas and Huelga, 2012) is to assume that the environment is macroscopically large and the unitary is left turned on for an arbitrary time. Equation (28) is then naturally reinterpreted as the continuous-time map

$$\rho_S(t) = \mathcal{E}_t(\rho_S(0)) = \text{tr}_E\{U(t)[\rho_S(0) \otimes \rho_E]U^\dagger(t)\}. \quad (105)$$

Common questions in the theory of open quantum systems, such as whether the map will be divisible, are all contained in the properties of ρ_E and $U(t)$.

All results derived in Sec. III for the entropy production remain valid in this case, although it becomes more natural to study the entropy production rate $\dot{\Sigma} = d\Sigma/dt$. An important observation is that even though $\Sigma \geq 0$ by construction, this is not in general guaranteed for $\dot{\Sigma}$. This is expected to happen for macroscopic environments but has to be analyzed on a case-by-case basis. In fact, temporary negativities in $\dot{\Sigma}(t)$ can be used as a measure of non-Markovianity (Breuer *et al.*, 2016; de Vega and Alonso, 2017), as they represent instances of time where information backflows to the system (which fits well with the interpretation of $\dot{\Sigma}$ as a measure of irreversibility). This is reviewed in Sec. VII.H.

More serious difficulties arise, however, when one is interested in quantum master equations derived from the map (105). The problem is that master equations use several approximations to describe the dynamics solely from the optics of the reduced state of the system. They therefore have no information about the global $S + E$ state, which is paramount for quantifying entropy production. Thus, while these approximations may be reasonable for describing the dynamics, they can be disastrous for the thermodynamics. For instance, Levy and Kosloff (2014) showed how local master equations seem to violate the second law (such as by allowing heat to flow from cold to hot). If one also has access to the global dynamics, this would never happen by construction.

This was used by De Chiara *et al.* (2018) to reconcile local master equations with thermodynamics.

The thermodynamics of quantum master equations has to be analyzed on a case-by-case basis. Instead, we focus in this review on an alternative paradigm of the open system called collisional models (also referred to as “repeated interactions”). These models, which are detailed later, have been used for a long time in different contexts (Rau, 1963; Englert and Morigi, 2002; Scarani *et al.*, 2002). However, they recently gained a surge in popularity (Karevski and Platini, 2009; Giovannetti and Palma, 2012; Landi *et al.*, 2014; McCloskey and Paternostro, 2014; Barra, 2015; Lorenzo *et al.*, 2015; Pezzutto, Paternostro, and Omar, 2016; Cusumano *et al.*, 2018), largely because they allow full control over the approximations employed. We review here the thermodynamics of collisional models, which were laid out on firm ground by Strasberg *et al.* (2017) and then connected with master equations by Barra (2015) and De Chiara *et al.* (2018). We later show how some of the results for the thermodynamics of master equations can actually be derived as limiting cases of such models. This includes the result by Spohn (1978), as well as the formulation of continuous measurements given by Horowitz and Parrondo (2013). We also show how collisional models can be used to see the emergence of a classical limit and the classical rules of stochastic thermodynamics (Cwiklinski *et al.*, 2015).

A. Collisional models

Collisional models have drawn inspiration from Boltzmann’s original *Stosszahlansatz* (molecular chaos hypothesis). The open-system dynamics is envisioned as a series of sequential interactions, where in each time interval the system interacts with only a small fraction of the environment (which we henceforth refer to as an *ancilla*). After this interaction the ancilla is discarded and a fresh new one is introduced, again prepared in a thermal state. This is what happens in classical Brownian motion: at each moment the particle interacts with only a small number of molecules. Moreover, after they interact, the molecules return to the bath and never interact with the system again.

The collisions may be assumed to happen at random times or be sequential. We focus on the latter for concreteness and assume that each event lasts for a time τ . If we let ρ_{A_n} denote the density matrix of the n th ancilla, then the collisional model can be described by the map

$$\rho_S^{n+1} = \text{tr}_{A_n}\{U_{SA_n}(\rho_S^n \otimes \rho_{A_n})U_{SA_n}^\dagger\} := \mathcal{E}_n(\rho_S^n), \quad (106)$$

where $\rho_S^n = \rho_S(n\tau)$ is the state of the system before interacting with the n th ancilla. As can be seen, this map is simply a composition of the original map (29). Hence, all thermodynamic properties derived in Sec. III also hold for each stroke of the collisional model. Moreover, since the ancillas are assumed to be independent, it is trivial to compose the properties of multiple strokes. From a thermodynamic perspective, this offers a monumental advantage.

We can also increment the collisional model with the additional assumption that in between each SA stroke, the system also undergoes a unitary evolution; see Fig. 3(a). The map (106) is then updated to

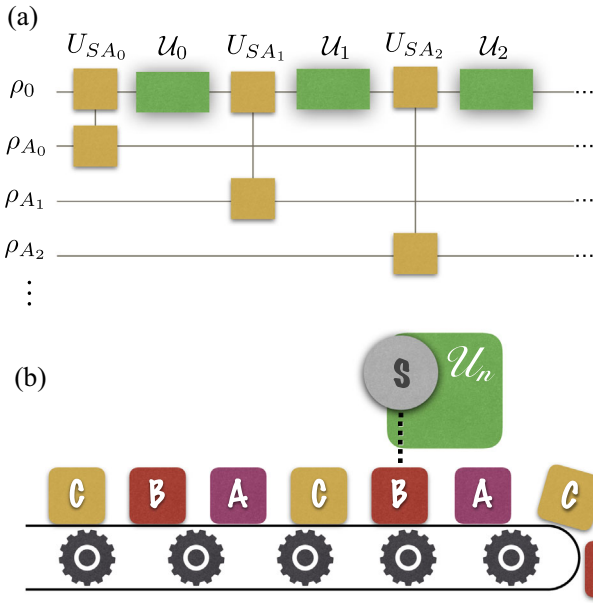


FIG. 3. (a) Diagrammatic illustration of the collisional model in Eq. (107). (b) Scheme for studying NESSs obtained when a system is coupled to multiple reservoirs. In this case the ancilla cycle through an alphabet of states $\rho_A, \rho_B, \rho_C, \rho_A, \rho_B, \dots$, so the system never reaches equilibrium, even when $\mathcal{U}_n = 1$ (no unitary strokes).

$$\rho_S^{n+1} = \mathcal{U}_n(\mathcal{E}_n(\rho_S^n)) \quad (107)$$

where $\mathcal{U}_n(\rho_S) = U_n \rho_S U_n^\dagger$ is a unitary stroke described by an arbitrary unitary U_n acting only on S . The situation where the system is always close to equilibrium was recently analyzed by Scandi *et al.* (2020). Since the unitary strokes \mathcal{U}_n involve no heat by construction, this kind of map composition is a useful way of separating heat and work, a quantum generalization of the type of splitting used by Crooks (1998). As discussed in Sec. III.D, the ancilla strokes \mathcal{E}_n may also contain a contribution due to work, depending on whether $U_{S A_n}$ satisfies strict energy conservation [Eq. (50)].

The states of the ancillas in the collisional model (107) do not have to be identical. This can be used to implement nontrivial limit cycles. The basic idea is illustrated in Fig. 3(b). It consists of setting the ancillas to cycle through an alphabet of m states, such as $\rho_A, \rho_B, \rho_C, \rho_A, \rho_B, \rho_C, \dots$ in the example of the figure. If the composite map

$$\Phi(\rho_S) = \mathcal{U}_m \circ \mathcal{E}_m \circ \dots \circ \mathcal{U}_1 \circ \mathcal{E}_1(\rho_S) \quad (108)$$

is applied for a sufficiently long time, any transients related to the system's initial conditions will vanish and the system will reach a limit cycle, characterized by $\rho_S^* = \Phi(\rho_S^*)$. Because the ancillas are always changing, however, this limit cycle will not be a fixed point of the individual maps (107), only of the composite map (108). As a consequence, the system will never reach a steady state but will instead keep bouncing back and forth within the limit cycle. This can be used to generate a diverse set of rich dynamics describing enginelike behavior.

For concreteness, we assume that within the system-ancilla strokes the system Hamiltonian remains fixed at H_S^n . During

the subsequent unitary stroke, on the other hand, it changes from H_S^n to H_S^{n+1} . The precise way through which this change takes place is encoded in the unitary \mathcal{U}_n . Heat is then defined, as in Sec. III, as the change in energy of the ancillas [see Eq. (39)], i.e., $Q_{A_n} := \text{tr}\{H_{A_n}(\rho'_{A_n} - \rho_{A_n})\}$. This is to be compared with the total change in energy of the system,

$$\Delta H_S^n = \text{tr}(H_S^{n+1} \rho_S^{n+1} - H_S^n \rho_S^n). \quad (109)$$

The mismatch between Q_{A_n} and ΔH_S^n is then attributed entirely to work. This work, however, may have a contribution from the on-off work of the system-ancilla interaction and the following contribution from the unitary U_n :

$$W_n^{\text{on-off}} = \text{tr}\{H_S^n[\mathcal{E}_n(\rho_S^n) - \rho_S^n]\} + Q_{A_n}, \quad (110)$$

$$W_n^u = \text{tr}\{H_S^{n+1} \rho_S^{n+1} - H_S^n \mathcal{E}_n(\rho_S^n)\}. \quad (111)$$

The first law therefore decomposes as

$$\Delta U_S^n = W_n^u + W_n^{\text{on-off}} + Q_{A_n}. \quad (112)$$

Notice how ΔH_S^n in Eq. (109) is a function of state, whereas Q_{A_n} and W_n are not.

As for the second law, based on the results of Sec. III we have the following three tiers of possible expressions for the entropy production:

$$\Sigma_n = \mathcal{I}_{\rho'_{S A_n}}(S:A_n) + S(\rho'_{A_n} \parallel \rho_{A_n}) \quad (113)$$

$$= \Delta S_S^n + \beta_n Q_{A_n} \quad (114)$$

$$= S(\rho_S^n \parallel \rho_S^{n,\text{th}}) - S(\rho_S^{n+1} \parallel \rho_S^{n,\text{th}}), \quad (115)$$

where $\Delta S_S^n = S(\rho_S^{n+1}) - S(\rho_S^n)$ is the change in the entropy of the system in the map (107). The first line is the general definition (30) and holds for any ancillary state. The second line is true only if the ancillas are thermal, although not necessarily at the same temperature [Eq. (38)]. Finally, the third line is true only for thermal operations [i.e., if the ancillas are thermal and the unitary satisfies the strict energy conservation condition (52)]. If the ancillas are identical, some of the indices n may be dropped and the expressions simplify a bit.

B. The emergence of a preferred basis

The classical limit is usually associated with the emergence of a preferred basis in which coherence among the basis elements tend to be suppressed. In the so-called einselection paradigm (Zurek, 1981), this basis emerges due to the contact with a heat bath. Thermal operations (Sec. III.D) provide an illustration of this principle and also highlight some of the subtle issues that arise in the classical limit.

We consider here the collisional model in Eq. (107) and assume that the ancillary stroke (106) is a thermal operation (Sec. III.D). During the unitary stroke, the Hamiltonian is assumed to change from $H_S^n = H_S(\lambda_n)$ to $H_S^{n+1} = H_S(\lambda_{n+1})$, where λ represents a generic work parameter. For simplicity,

however, we assume that this change is much faster than the system-ancilla stroke so that we may set $\mathcal{U}_n \simeq 1$.

Let $H_S^n = \sum_i E_i^n |i_n\rangle\langle i_n|$ denote the spectral decomposition of H_S^n in terms of the eigenvalues E_i^n and the corresponding eigenstates $|i_n\rangle$ at each given time n . We assume that the eigenvalues E_i^n are nondegenerate. As shown by [Cwiklinski et al. \(2015\)](#), if the map (106) is a thermal operation, the populations $\langle i_n | \rho_S^n | i_n \rangle$ at the instantaneous eigenstates will evolve according to the classical Markov chain

$$\langle i_n | \rho_S^{n+1} | i_n \rangle = \sum_j M_n(i|j) \langle j_n | \rho_S^n | j_n \rangle, \quad (116)$$

where $M_n(i|j) = \sum_{\mu,\nu} q_\nu^n |\langle i_n \mu_n | U_{SA_n} | j_n \nu_n \rangle|^2$, with q_ν^n and $|\nu_n\rangle$, $|\mu_n\rangle$ the initial populations and eigenstates of ancilla A_n , i.e., $\rho_{A_n} = e^{-\beta H_{A_n}} / Z_{A_n} = \sum_\nu q_\nu^n |\nu_n\rangle\langle \nu_n|$. We call attention to the fact that, in order to make sure that each step is a thermal operation, the states of the ancillas and the unitaries U_{SA_n} have to change to adjust to the strict energy conservation condition (50); this makes Eq. (116) difficult to realize exactly, although it is realizable approximately, as we now discuss.

Notice how the left-hand side of Eq. (116) contains $\langle i_n | \rho_S^{n+1} | i_n \rangle$, which differs in general from $\langle i_{n+1} | \rho_S^{n+1} | i_{n+1} \rangle$. This highlights a unique property of quantum dynamics, namely, that the action of the work agent may not only change the populations E_i^n of the system but also rotate the eigenbasis $|i_n\rangle$. The notion of ‘‘population and coherences’’ in Eqs. (116) and (119) should thus be interpreted with care, as they change with each step. As a consequence, even slow dynamics, which is usually somewhat dull for classical systems, may present interesting and highly nontrivial effects that are of a genuine quantum nature. This was recently explored by [Miller et al. \(2019\)](#) and [Scandi et al. \(2020\)](#) and is reviewed in Sec. VII.E.

In the remainder of this section, we focus on the case where $[H_S^n, H_S^m] = 0$ for all n and m . This means that during the work strokes the energy levels of the system may change, but the orientation of the eigenbasis $|i\rangle$ remains fixed. One may then define the populations $p_i^n = \langle i | \rho_S^n | i \rangle$ so that Eq. (116) is converted into the classical Markov chain

$$p_i^{n+1} = \sum_j M_n(i|j) p_j^n. \quad (117)$$

$M_n(i|j)$ are simply transition probabilities (their time dependence comes from the fact that the Hamiltonian may be changing in time). Moreover, as the ancillas are thermal, they satisfy the detailed balance condition

$$M_n(i|j) = M_n(j|i) e^{-\beta(E_i^n - E_j^n)}. \quad (118)$$

Thus, by all standards, the populations evolve according to an entirely classical evolution. Notably, the evolutions of populations and coherences are completely decoupled. Indeed, the latter are found to evolve according to

$$\langle i | \rho_S^{n+1} | j \rangle = \mathcal{R}_{ij}^n \langle i | \rho_S^n | j \rangle, \quad (119)$$

where $\mathcal{R}_{ij}^n = \sum_{\mu,\nu} q_\nu^n \langle i \nu_n | U_{SA_n} | \mu_n \rangle \langle j \nu_n | U_{SA_n}^\dagger | \mu_n \rangle$. One may verify that $|\mathcal{R}_{ij}^n| < 1$ ([Cwiklinski et al., 2015](#)), so the off

diagonals are suppressed further and further with each collision, until eventually vanishing.

This example shows the emergence of a preferred basis. Because of the strict energy conservation property of thermal operations, the energy basis of the system is selected as a preferred basis by the environment, a process called ‘‘environment-induced’’ selection, or einselection. This effect is clearly manifested in the entropy production. The entropy produced at each stroke will be given by Eq. (115), with $\rho_S^{n,\text{th}} = e^{-\beta H_S^n} / Z_S^n$. We may now split the relative entropy as

$$S(\rho_S^n \| \rho_S^{n,\text{th}}) = S(\mathbf{p}^n \| \mathbf{p}^{n,\text{th}}) + C(\rho_S^n), \quad (120)$$

where $S(\mathbf{p}^n \| \mathbf{p}^{n,\text{th}})$ is the classical relative entropy between the probability distributions p_i^n and $p_i^{n,\text{th}} = e^{-\beta E_i^n} / Z_S^n$; the classical relative entropy is defined as

$$S(\mathbf{p} \| \mathbf{q}) = \sum_i p_i \ln p_i / q_i. \quad (121)$$

The second term in Eq. (120), on the other hand, is the relative entropy of coherence in the energy eigenbasis $|i\rangle$: $C(\rho_S^n) = S(\mathbf{p}^n) - S(\rho_S^n)$. Plugging this into Eq. (115) allows us to split the entropy production of each step into the following two parts ([Santos et al., 2019](#); [Mohammady, Aufféves, and Anders, 2020](#)):

$$\Sigma_n = \Sigma_n^{\text{cl}} + \Sigma_n^{\text{qu}}, \quad (122)$$

where

$$\Sigma_n^{\text{cl}} = S(\mathbf{p}^n \| \mathbf{p}^{n,\text{th}}) - S(\mathbf{p}^{n+1} \| \mathbf{p}^{n,\text{th}}), \quad (123)$$

$$\Sigma_n^{\text{qu}} = C(\rho_S^n) - C(\rho_S^{n+1}). \quad (124)$$

The term Σ_n^{cl} is a purely classical contribution and coincides with the formulation used in classical stochastic processes ([Schnakenberg, 1976](#)). It describes the irreversibility associated with the system having to adapt its populations to those imposed by the environment. In addition to the formulation, however, we have an extra term Σ_n^{qu} describing the irreversibility due to the way the environment process quantum coherences. This thus represents a genuinely quantum contribution to the entropy production. Both terms are also individually non-negative ([Santos et al., 2019](#)).

C. Continuous-time limit

When the interaction time τ of each collision is small, the stroboscopic dynamics in Eq. (107) can usually be converted into a continuous-time master equation for the system ([Englert and Morigi, 2002](#); [Strasberg et al., 2017](#)). In view of the importance of quantum master equations, we review the basic procedure here. The idea is to construct a generator \mathcal{L} according to

$$\frac{d\rho_S}{dt} := \lim_{\tau \rightarrow 0} \frac{\rho_S^{n+1} - \rho_S^n}{\tau} = \mathcal{L}(\rho_S), \quad (125)$$

where ρ_S^{n+1} and ρ_S^n are separated by the collision time τ . The limit process in Eq. (125), however, has to be interpreted with care: Strictly speaking, one cannot take $\tau \rightarrow 0$, as this would imply no interaction at all. Instead, this is to be interpreted as a leading order contribution to a series expansion. In a nutshell, the main idea is to take τ sufficiently small to ensure that $d\rho_S/dt$ becomes a smooth function. Ultimately, this is a coarse-graining argument, which is actually ubiquitous in stochastic processes. It also arises, for instance, in the classical Langevin equation describing Brownian motion; see [Cresser and Facer \(2017\)](#) for a critical assessment of the coarse-graining approach.

We focus here on two distinct scenarios. We first assume that the Hamiltonian is time independent but that the collisions are not energy preserving. We then consider the case where the Hamiltonian is time dependent and the collisions are thermal operations (which is the same scenario as that discussed in Sec. VB). The starting point for both cases is actually the same. We thus remain general here and specialize the results in Sec. VD.

We focus on a single system-ancilla collision, where the Hamiltonian is given by $H = H_S + H_A + V$ and the initial states are ρ_S and ρ_A for system and ancilla (all indices n are omitted for now). The evolution of the system in this single collision is given by

$$\rho'_S = \text{tr}_A \{ e^{-i\tau H} (\rho_S \otimes \rho_A) e^{i\tau H} \}.$$

Expanding the exponentials in a power series and dividing by τ on both sides leads to

$$\frac{\rho'_S - \rho_S}{\tau} = -i[H_S + \text{tr}_A(V\rho_A), \rho_S] - \frac{\tau}{2} \text{tr}_A[V, [V, \rho_S \otimes \rho_A]]. \quad (126)$$

Equation (126) illustrates the physical meaning of the limit (125). If we naively take $\tau \rightarrow 0$, only the first term survives. But this term contains only the original system Hamiltonian plus a unitary contribution (Lamb shift) $\text{tr}_A(V\rho_A)$. Moreover, this Lamb shift is often zero for most choices of ancilla states and interactions; see [Rivas and Huelga \(2012\)](#) for more details and [Rodrigues et al. \(2019\)](#) for a counterexample. Indeed, we henceforth assume that $\text{tr}_A(V\rho_A) = 0$.

The actual dissipative contribution, which is what we are interested in, corresponds to the second term in Eq. (126). But this is still of the order of τ and hence would vanish if $\tau \rightarrow 0$. The limit (125) should therefore correspond to a limit where $(\rho'_S - \rho_S)/\tau$ is sufficiently smooth to be interpreted as a derivative, but the last term is nonetheless not vanishingly small. A more systematic way of implementing this is to introduce a fictitious scaling of the potential by changing $V \rightarrow V/\sqrt{\tau}$. This means that, while we take the interaction time to be short, we also take it to be strong in the same proportions. This scaling is not physical but helps us to identify the terms to neglect in the series expansion. An identical situation also appears in classical Brownian motion: the white noise entering the Langevin equation can be seen as resulting from a sequence of independent kicks, each

occurring for an infinitesimal time Δt and for whom the magnitude scales as $1/\sqrt{\Delta t}$.

With such rescaling Eq. (126) becomes

$$\rho_S^{n+1} = \rho_S^n - i\tau[H_S^n, \rho_S^n] + \tau\mathcal{D}_n(\rho_S^n), \quad (127)$$

where we have already reintroduced all indices n . We also defined

$$\mathcal{D}_n(\rho_S) = -\frac{1}{2} \text{tr}_{A_n} [V_n, [V_n, \rho_S \otimes \rho_{A_n}]]. \quad (128)$$

Taking the limit $\tau \rightarrow 0$ then finally leads to

$$\frac{d\rho_S}{dt} = -i[H_S(t), \rho_S] + \mathcal{D}_t(\rho_S), \quad (129)$$

where $H_S(t = n\tau) = H_S^n$, and likewise for \mathcal{D}_t .

Equation (128) can always be put in Lindblad form ([Breuer and Petruccione, 2007](#)) by decomposing the interaction as $V_n = \sum_k M_k F_k = \sum_k F_k^\dagger M_k^\dagger$, where M_k and F_k are Hermitian operators of the system and ancilla, respectively. This leads to

$$\mathcal{D}(\rho_S) = \sum_{k,q} \langle F_q^\dagger F_k \rangle_n [M_k \rho_S M_q^\dagger - \frac{1}{2} \{M_q^\dagger M_k, \rho_S\}], \quad (130)$$

where $\langle F_q^\dagger F_k \rangle_n = \text{tr}(F_q^\dagger F_k \rho_{A_n})$ is, by construction, positive semidefinite. The evolution is thus Markovian and can always be put in canonical form.

To provide another example, we consider an interaction appearing often in the literature, i.e.,

$$V = \sum_k g_k (L_k^\dagger A_k + L_k A_k^\dagger), \quad (131)$$

where L_k and A_k are operators for the system and ancilla, respectively. We assume that $\langle A_k A_q \rangle = 0$, $\langle A_k^\dagger A_q \rangle = \delta_{k,q} \langle A_k^\dagger A_k \rangle$. Equation (128) then acquires the familiar form

$$\mathcal{D}(\rho_S) = \sum_k \{ \gamma_k^+ D[L_k] + \gamma_k^- D[L_k^\dagger] \}, \quad (132)$$

where $D[L] = L\rho_S L^\dagger - (1/2)\{L^\dagger L, \rho_S\}$ and $\gamma_k^+ = g_k^2 \langle A_k A_k^\dagger \rangle$, $\gamma_k^- = g_k^2 \langle A_k^\dagger A_k \rangle$.

A further specialization is to the case where the A_k are eigenoperators of the ancilla Hamiltonian. That is, they satisfy $[H_A, A_k] = -\omega_k A_k$ for some set of Bohr (transition) frequencies ω_k . If the state of the ancillas is a thermal state $\rho_A^{\text{th}} = e^{-\beta H_A} / Z_A$, then this property will ensure that the coefficients γ_k^\pm satisfy the detailed balance

$$\gamma_k^- / \gamma_k^+ = e^{-\beta \omega_k}. \quad (133)$$

When one considers the Fermi-Dirac distribution with $f_k := \langle A_k^\dagger A_k \rangle = (e^{\beta \omega_k} + 1)^{-1} = 1 - \langle A_k A_k^\dagger \rangle$, Eq. (132) becomes $\mathcal{D}(\rho_S) = \sum_k g_k^2 \{ (1 - f_k) D[L_k] + f_k D[L_k^\dagger] \}$. We might instead take the Bose-Einstein distribution with $n_k := \langle A_k^\dagger A_k \rangle = (e^{\beta \omega_k} - 1)^{-1} = \langle A_k A_k^\dagger \rangle - 1$ to get

$\mathcal{D}(\rho_S) = \sum_k g_k^2 \{(n_k + 1)D[L_k] + n_k D[L_k^\dagger]\}$. The entropy production in this case must be computed using Eq. (114) since the reservoirs are assumed to be thermal, but V is not necessarily a thermal operation. Since we are interested in the continuous-time limit, we instead compute the entropy production rate

$$\dot{\Sigma} = \lim_{\tau \rightarrow 0} \frac{\Delta S_S^n}{\tau} + \beta Q_{A_n}. \quad (134)$$

The first term tends to $dS(\rho_S)/dt$, the rate of change of the system's von Neumann entropy. But the last term still involves a quantity related to the ancillas. We now discuss under which conditions Eq. (134) can be recast solely in terms of quantities related to the system.

D. On-off work and Spohn's separation

Equation (134) highlights the need for addressing under which conditions the entropy production can be written solely in terms of system-related quantities. This was already broadly discussed in Sec. III. However, here it acquires additional significance since master equations are often used as phenomenological models of open-system dynamics without knowledge of the baths and system-bath interactions.

To gain insight into this nontrivial question, first consider the case where the system Hamiltonian is time independent ($H_S^n = H_S$) and the ancillas are identically prepared ($\rho_{A_n} = \rho_A$). The change in energy of the system and ancilla in one collision can be determined as follows from Eq. (127) and the corresponding analogous equation for the evolution of ρ_{A_n} :

$$\Delta H_S^n = -\frac{\tau}{2} \text{tr}\{[V, [V, H_S]]\rho_S^n \otimes \rho_A\}, \quad (135)$$

$$\Delta H_{A_n} = -\frac{\tau}{2} \text{tr}\{[V, [V, H_A]]\rho_S^n \otimes \rho_A\} \equiv Q_{A_n}, \quad (136)$$

where Q_{A_n} is precisely the quantity appearing in Eq. (134). In general, the violation of strict energy conservation $[V, H_S + H_A] \neq 0$ implies that $\Delta H_S^n \neq -Q_{A_n}$, and hence there will be a finite amount of on-off work (Sec. III.D).

This is where the difficulties in dealing with the thermodynamics of master equations start. If one has access only to Eq. (129), it is not clear how to split ΔH_S^n into heat and work. According to Eq. (129), one should have

$$\frac{d\langle H_S \rangle}{dt} = \text{tr}_S\{H_S \mathcal{D}(\rho_S)\}, \quad (137)$$

and it is not at all obvious which part of this expression is heat and which part is work (something that is evident from the global dynamics). The problem is that in general Q_{A_n} simply cannot be written in terms of quantities pertaining solely to the system.

There is, however, an important case where this turns out to be possible, namely, when the violation of strict energy conservation is caused by an operator of the system, not the ancilla. That is, in this case it is possible to decompose the system Hamiltonian as $H_S = H_{S,0} + H_{S,1}$ such that

$$[V, H_{S,0} + H_A] = 0 \quad \text{but} \quad [V, H_{S,1}] \neq 0. \quad (138)$$

If this is true, then we may substitute $[V, H_A] = -[V, H_{S,0}]$ into Eq. (136), leading to

$$Q_{A_n} = \frac{\tau}{2} \text{tr}\{[V, [V, H_{S,0}]]\rho_S^n \otimes \rho_A\}. \quad (139)$$

As a consequence, we can now split Eq. (142) as

$$\frac{d\langle H_S \rangle}{dt} = \text{tr}_S\{H_{S,0} \mathcal{D}(\rho_S)\} + \text{tr}_S\{H_{S,1} \mathcal{D}(\rho_S)\} \quad (140)$$

$$= -\dot{Q}_A + \dot{W}, \quad (141)$$

hence allowing us to unambiguously identify the first term as heat and the second as on-off work. In this case, Eq. (132) may therefore be written as

$$\dot{\Sigma} = \frac{dS_S}{dt} - \dot{Q}_A = \frac{dS_S}{dt} + \text{tr}_S\{H_{S,0} \mathcal{D}(\rho_S)\}, \quad (142)$$

which is thus expressed solely in terms of quantities of the system. Note that these results also hold if the ancillas are not prepared in thermal states. This was used by Rényi (1960) to study collisional models with weakly coherent ancillas. We also mention that the approach taken here starts with a discrete model and eventually reaches a coarse-grained, continuous-time limit for the entropy production rate. The opposite route can also be taken. That is, the entropy production rate of a continuous process can also be discretized in small time steps, which will then be depicted by a collisional model. This was used by Monsel, Elouard, and Auffèves (2018) to construct a method for measuring the entropy production of a driven autonomous system.

The previously described situation often happens when the system is composed of multiple interacting parts, but with only one of the parts coupled to the ancillas (Barra, 2015; De Chiara *et al.*, 2018; Pereira, 2018). For instance, suppose that the system is composed of two subsystems S_1 and S_2 with a total Hamiltonian $H_S = H_{S_1} + H_{S_2} + V_{S_1, S_2}$, where V_{S_1, S_2} is the interaction between them. Moreover, suppose that there is only one bath and it is coupled only to S_1 . The interaction V_{A, S_1} between S_1 and the ancillas A_n is assumed to be locally energy preserving ($[V_{A, S_1}, H_{S_1} + H_A] = 0$). Notwithstanding, in general $[V_{A, S_1}, V_{S_1, S_2}] \neq 0$. Thus, albeit locally energy preserving the collision may not be globally energy preserving due to the interaction between S_1 and S_2 . The term V_{S_1, S_2} will therefore play the role of $H_{S,1}$ in Eq. (140) and will be responsible for the on-off work.

To provide a concrete example, consider a minimal model consisting of two qubits, with $H_S = \omega_1 \sigma_z^1 + \omega_2 \sigma_z^2 + \lambda(\sigma_+^1 \sigma_-^2 + \sigma_-^1 \sigma_+^2)$ (Barra, 2015). For simplicity, we assume that only qubit 1 is coupled to a bath. The extension to two baths, one coupled to each qubit, is straightforward. We also take the bath to be described by a collisional model, where the ancillas are made of thermal qubits with frequency ω_1 (i.e., resonant with qubit 1). The system will then evolve according to

$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S] + g^2(1-f)D[\sigma_-^1] + g^2fD[\sigma_+^1]. \quad (143)$$

[see the discussion following Eq. (133)]. Equation (138) will be satisfied in this case, with $H_{S,0} \rightarrow \omega_1\sigma_z^1 + \omega_2\sigma_z^2$ and $H_{S,1} = \lambda(\sigma_+^1\sigma_-^2 + \sigma_-^1\sigma_+^2)$. As a consequence, there will be work involved. The heat exchanged with the ancillas is going to be $-Q_A = \omega_1\text{tr}_S[\sigma_z^1\mathcal{D}(\rho_S)]$, while the work will be $W = \lambda\text{tr}[(\sigma_+^1\sigma_-^2 + \sigma_-^1\sigma_+^2)\mathcal{D}(\rho_S)]$. It is the heat Q_A that should enter Eq. (142). If this is done, then one is guaranteed to find $\dot{\Sigma} \geq 0$ at all times. Conversely, if one instead uses $\text{tr}[H_S\mathcal{D}(\rho_S)]$ as a definition of heat, this will lead to violations of the second law, as discussed by [Levy and Kosloff \(2014\)](#).

We now change the scenario and consider Eq. (129) when $H_S(t)$ is explicitly time dependent, but with the interactions engineered to be thermal operations. This means there is no on-off work involved, and $[V_n, H_{A_n}] = -[V_n, H_S^n]$. As a consequence, the heat exchanged to the ancillas [Eq. (136)] becomes

$$Q_{A_n} = \frac{\tau}{2}\text{tr}\{[V_n, [V_n, H_S^n]]\rho_S^n \otimes \rho_{A_n}\}, \quad (144)$$

which is written solely in terms of system-related quantities. From the master equation (129) we now find the energy balance

$$\frac{d\langle H_S \rangle}{dt} = \text{tr}\left\{\frac{\partial H_S}{\partial t}\rho_S\right\} + \text{tr}\{H_S(t)\mathcal{D}_t(\rho_S)\}. \quad (145)$$

Comparing Eqs. (144) and (145) then leads to the celebrated Spohn separation of work and heat ([Spohn, 1978](#))

$$\dot{Q}_A = -\text{tr}\{H_S(t)\mathcal{D}_t(\rho_S)\}, \quad \dot{W} = \text{tr}\{\dot{H}_S(t)\rho_S\}. \quad (146)$$

Spohn's separation is usually employed phenomenologically: it is used when one has access to a master equation of the form of Eq. (129) and wants to split the changes in energy into heat and work. Equation (146) shows that this separation is not at all universal. Quite the contrary: notice that for it to hold we had to assume that, even though the Hamiltonian is changing at each time step, the system-ancilla interaction and the state of the ancilla were adjusted to guarantee that the map was always a thermal operation. This would require considerable fine-tuning and is difficult to realize in practice.

E. Pauli master equations and Schnakenberg's approach

The Markov chain (116) can be viewed as the classical dynamics emerging from the quantum collisional model (107) in the case of thermal operations. Similarly, one may also consider the classical limit of the continuous-time master equation (129). All issues discussed in Sec. V.B also remain in this case, in particular, the nontrivial distinction between population and coherences in the case where the eigenbasis of $H_S(t)$ is time dependent.

To simplify the problem, we thus consider the scenario where only the eigenvalues of $H_S(t)$ are allowed to depend on time: $H_S(t) = \sum_i E_i(t)|i\rangle\langle i|$. The populations will then evolve according to Eq. (117). To obtain the short-time limit,

we assume that $U_{S A_n} = \exp\{-i\tau(H_S^n + H_{A_n} + V_n/\sqrt{\tau})\}$ and expand it in a power series in τ . This leads to

$$M_n(i|j) = \delta_{ij} + \tau\left(W_{ij} - \delta_{ij}\sum_k W_{kj}\right), \quad (147)$$

where we have introduced the transition probabilities $W_{ij}(t) = \sum_{\mu,\nu} q_\nu^n |\langle i, \mu | V_n | j, \nu \rangle|^2$ and its time dependence will be omitted for clarity when possible. Plugging this into Eq. (117) and taking $\tau \rightarrow 0$ then leads to the classical Pauli master equation ([Breuer and Petruccione, 2007](#))

$$\frac{dp_i}{dt} = \sum_j \{W_{ij}p_j(t) - W_{ji}p_i(t)\}. \quad (148)$$

This procedure shows how, under specific conditions, one can recover the classical master equation evolution from the underlying quantum dynamics.

We now proceed to study the entropy production solely from the perspective of the Pauli master equation (148). We review the framework put forth by [Schnakenberg \(1976\)](#). This approach is interesting because it also contemplates scenarios beyond the standard thermal-bath interaction. Master equations of the form of Eq. (148) also find a plethora of applications, from biomolecular processes to financial markets. And Schnakenberg's approach allows one to construct the entropy production rate and an entropy flux rate, irrespective of what physical system the master equation represents. The physical interpretation of $\dot{\Sigma}$ and $\dot{\Phi}$ is not necessarily evident in general. Notwithstanding, it reproduces the thermal results as a particular case, as one would expect. This is an advantage of classical systems that cannot be extended to the quantum case.

The starting point is to consider the evolution of the Shannon entropy

$$S(\mathbf{p}) = -\sum_i p_i \ln p_i. \quad (149)$$

Differentiating with respect to time and inserting Eq. (148) yields

$$\frac{dS}{dt} = \frac{1}{2}\sum_{i,j} (W_{ij}p_j - W_{ji}p_i) \ln p_j/p_i. \quad (150)$$

Schnakenberg then proposed that the following quantity be associated with an entropy production:

$$\dot{\Sigma}(t) = \frac{1}{2}\sum_{i,j} (W_{ij}p_j - W_{ji}p_i) \ln \frac{W_{ij}p_j}{W_{ji}p_i}. \quad (151)$$

Equation (151) is always non-negative as it has the form $(x-y)\ln(x/y) \geq 0$. That is in principle not enough to label a quantity as the entropy production. To scrutinize the correctness of this formula, one must analyze it from different perspectives.

The difference between $\dot{\Sigma}$ and dS/dt is associated with an entropy flux rate $\dot{\Phi}$ according to Eq. (7). Using Eqs. (150) and (151) one then arrives at

$$\dot{\Phi}(t) = \frac{1}{2} \sum_{i,j} (W_{ij}p_j - W_{ji}p_i) \ln \left(\frac{W_{ij}}{W_{ji}} \right). \quad (152)$$

The entropy flux is thus seen to be linear in the probabilities p_i .

Additional justification for Eqs. (151) and (152) can be given if we assume that the dynamics satisfies the detailed balance (van Kampen, 2007; Gardiner, 2010; Tomé and de Oliveira, 2014), viz.,

$$W_{ij}p_j^* = W_{ji}p_i^*, \quad (153)$$

where p_i^* is the steady-state distribution of Eq. (148) (not necessarily a thermal state). In this case, Eq. (151) may be rewritten in terms of the classical Kullback-Leibler divergence (121) as

$$\dot{\Sigma} = - \frac{dS(\mathbf{p}||\mathbf{p}^*)}{dt}, \quad (154)$$

which is the continuous-time and classical analog of Eq. (47). The entropy flux (152), on the other hand, can be rearranged as

$$\dot{\Phi} = \sum_i \frac{dp_i}{dt} \ln p_i^*. \quad (155)$$

In the case where the steady-state distribution is also the thermal equilibrium state ($p_i^* = e^{-\beta E_i}/Z$), this becomes

$$\dot{\Phi} = -\beta \sum_i E_i \frac{dp_i}{dt} = -\beta \dot{Q} \quad (156)$$

so that we recover the well-known thermodynamic result (7).

Returning to the general expression (151), it is also interesting to define the probability current

$$J_{ij} = W_{ij}p_j - W_{ji}p_i, \quad (157)$$

which represents the current of probability flowing from j to i . If we then define the following so-called conjugated force:

$$X_{ij} = \ln \frac{W_{ij}p_j}{W_{ji}p_i}, \quad (158)$$

then the entropy production can be cast as

$$\dot{\Sigma} = \frac{1}{2} \sum_{ij} J_{ij} X_{ij}, \quad (159)$$

which is a stochastic version of Onsager's form (18); i.e., the entropy production is a product of fluxes times forces. The difference is that here these are not macroscopic fluxes (like

the flow of energy), but rather microscopic currents of probability.

F. Pauli master equation for multiple baths

When extending the Pauli master equation (148) to multiple baths, one usually assumes that the transition rates W_{ij} from different reservoirs contribute additively (Maguire, Iles-Smith, and Nazir, 2019; McConnell and Nazir, 2019). That is, they can be split as

$$W_{ij} = \sum_{\alpha} W_{ij}^{\alpha}, \quad (160)$$

where α represents the different reservoirs present in the problem. Thus, for instance, if each reservoir is thermal, at temperature T_{α} each rate in Eq. (160) would individually satisfy the detailed balance

$$W_{ij}^{\alpha}/W_{ji}^{\alpha} = e^{-\beta_{\alpha}(E_i-E_j)}. \quad (161)$$

This assumption is known to describe a broad range of mesoscopic systems well, from biological engines to nano-scale junctions (Van den Broeck and Esposito, 2015). However, when viewed as a limiting case of quantum processes it is extremely strong. First and foremost, the Liouvillian of the master equation will, itself, not be separable in general. But even if it is (such as in the case of local master equations), this does not mean that the corresponding Pauli equation will have additive rates, since the preferred basis of one bath may not coincide with the preferred basis of the other. As a consequence, understanding under which conditions Eq. (160) can be viewed as the limiting case of a quantum process is not trivial and, to our knowledge, is still an open problem.

Notwithstanding these difficulties, Eq. (160) provides an interesting platform for characterizing entropy production. Starting with Eq. (150) and plugging it into Eq. (160) leads to

$$\frac{dS}{dt} = \frac{1}{2} \sum_{i,j,\alpha} (W_{ij}^{\alpha}p_j - W_{ji}^{\alpha}p_i) \ln p_j/p_i. \quad (162)$$

Following Esposito and Van Den Broeck (2010) the correct way of identifying the entropy production is to add and subtract $\ln W_{ij}^{\alpha}/W_{ji}^{\alpha}$ in each term of the sum. The entropy production rate is then identified as

$$\dot{\Sigma} = \frac{1}{2} \sum_{i,j,\alpha} (W_{ij}^{\alpha}p_j - W_{ji}^{\alpha}p_i) \ln \frac{W_{ij}^{\alpha}p_j}{W_{ji}^{\alpha}p_i}. \quad (163)$$

Notice that Eq. (163) is not equivalent to Eq. (151), which we would have obtained if we had added and subtracted $\ln W_{ij}/W_{ji}$ instead. Equation (163) is the correct expression, as it yields proper thermodynamic expressions for the fluxes. Indeed, as shown by Esposito and Van Den Broeck (2010), if this identification is not properly made one will in general be underestimating the entropy produced. More details on the formulation of entropy production in this scenario were given by Van den Broeck and Esposito (2015). An extension to

account for information flows was done by Horowitz and Esposito (2014).

G. Classical phase space

Stochastic thermodynamics can also be formulated for systems described by continuous degrees of freedom (such as position and momenta). In this case Eq. (148) is replaced by a Fokker-Planck equation. The formulation of the second law for such systems was recently reviewed in detail by Seifert (2012). Here, with Sec. V.H in mind we focus on two illustrative examples.

The first is the so-called colloidal particle (Seifert, 2012), which is described by a single random variable x evolving according to the Langevin equation

$$\dot{x} = f(x) + B\dot{\xi}(t), \quad (164)$$

where $f(x) = -\partial_x V(x)$ is a conservative force stemming from a potential $V(x)$, B is a constant, and $\xi(t)$ is a standard Wiener (i.e., Gaussian) process. One may equivalently describe the dynamics in terms of a Fokker-Planck equation for the probability density $P_t(x)$, which in this case reads

$$\frac{\partial P_t(x)}{\partial t} = -\frac{\partial J}{\partial x} = -\frac{\partial}{\partial x} \left[f(x)P_t(x) - D_c \frac{\partial P_t(x)}{\partial x} \right], \quad (165)$$

where $D_c = B^2/2$ is the diffusion constant. The Fokker-Planck equation can be viewed as a continuity equation for $P(x)$, with $J(x) = f(x)P_t(x) - D_c \partial_x P_t(x)$ representing a probability current. The noise in Eq. (164) is ascribed to a thermal bath at a temperature T . As a consequence, one may verify that, in order for the system to properly thermalize, one must choose $D_c \propto T$. In this case, the unique steady state of Eq. (165) will be the thermal state $P_{\text{th}} = e^{-\beta V(x)}/Z$, where Z is the partition function.

The definition of the entropy production associated with the Fokker-Planck equation (165), including its stochastic formulation and the associated fluctuation theorems, was discussed extensively by Seifert (2012). Extensions to more general Fokker-Planck equations were discussed by Qian (2001b) and Tomé and de Oliveira (2010), and a more robust framework based on path integrals was given by Spinney and Ford (2012). Here we point out a complementary approach, namely, that with Eq. (154) in mind one may propose to define the entropy production as

$$\dot{\Sigma} = -\frac{d}{dt} S(P_t \| P_{\text{th}}), \quad (166)$$

where $S(P_t \| P_{\text{th}}) = \int dx P_t(x) \ln P_t(x)/P_{\text{th}}(x)$ is the continuous analog of Eq. (121). Inserting Eq. (165) into Eq. (166), one finds

$$\dot{\Sigma} = \int dx \frac{\partial J}{\partial x} \ln P_t(x)/P_{\text{th}}. \quad (167)$$

Next we integrate by parts. Boundary terms are assumed to vanish as $P_t(x) \rightarrow 0$ for $x \rightarrow \pm\infty$. Moreover, using the

definition of $J(x)$ together with the fact that $P_{\text{th}} \propto e^{-\beta V(x)}$, one may verify that

$$\frac{\partial}{\partial x} \ln P_t(x)/P_{\text{th}} = -\frac{J(x)}{D_c P_t(x)}. \quad (168)$$

Therefore Eq. (166) becomes

$$\dot{\Sigma} = \frac{1}{D_c} \int dx \frac{J(x)^2}{P_t(x)}, \quad (169)$$

which is the same result as given by Seifert (2012). This has a clear physical interpretation: the quantity $v(x) = J(x)/P(x)$ can be interpreted as a velocity in phase space. The entropy production (169) is thus seen to be associated with a mean-squared velocity. Thus, by construction it is always non-negative and null if and only if the current itself vanishes. A method for estimating $\dot{\Sigma}$ using machine learning on the stochastic trajectory $x(t)$ was recently put forth by Seif, Hafezi, and Jarzynski (2021).

Finally, it is worth mentioning that this approach, where Eq. (166) is taken as the starting point for defining the entropy production, is not always possible, in particular, when the system is connected to multiple baths. We chose to present it here nonetheless because it attributes a clear information-theoretic meaning to the entropy production, specially in light of the discussion in Sec. III.

Next we consider a generalization of Eq. (164) to the case of multiple modes so that $x = (x_1, \dots, x_n)$ is now a vector of random variables. This could indicate, for instance, a collection of position and momenta. The vector x continues to be described by a Langevin equation of the form of Eq. (164). However, now $f(x)$ is an n -dimensional vector and $\xi(t)$ is an m -dimensional vector of independent Wiener processes. As a consequence, B is taken to be an $n \times m$ matrix. We assume that B is independent of x , thus making this a problem with additive noise [multiplicative noise introduces significant mathematical complications (Spinney and Ford, 2012)].

We now focus on the special case of linear forces $f(x) = -Ax$, where A is an $n \times n$ matrix. We no longer assume that $f(x)$ is a conservative force, but it may well contain damping terms. We do assume, though, that its eigenvalues have positive real parts, thus guaranteeing the stability of the problem. Linear systems of Langevin equations of this form often appear in quantum optical experiments as a semiclassical description of fluctuations in optical fields.

For such systems, it is more convenient to recast the dynamical equation in terms of the first moments \bar{x} and the covariance matrix (CM), defined as $\Theta = \langle x x^T \rangle - \langle x \rangle \langle x^T \rangle$. One may verify that Θ evolves according to a Lyapunov equation

$$\dot{\Theta} = -(A\Theta + \Theta A^T) + 2D, \quad (170)$$

where we have introduced the diffusion matrix $D = BB^T/2 \geq 0$. The equilibrium solution of Eq. (170) satisfies the condition $A\Theta + \Theta A^T = 2D$. Continuous-time Lyapunov equations of this form have found significant applications in the fields of linear systems, control theory,

and quantum optics (Brogan, 1991). The formulation of the entropy production for this kind of problem can be constructed by introducing the distinction between even or odd functions under time reversal. Intuitive instances of even variables include the positioning of mechanical systems and voltages in circuits, with their odd counterparts being velocities and currents.

It is then possible to identify the reversible parts of Eq. (170), that is, the part that is even under time reversal, from the irreversible one that changes sign upon inversion of the sign of time. We call A^{irr} the irreversible part of A such that $A = A^{\text{rev}} + A^{\text{irr}}$. Convenient expressions for the entropy production and flux rates [see Eq. (7)] were derived for this scenario by Landi, Tomé, and de Oliveira (2013) and Brunelli *et al.* (2018) under the assumption of Gaussian states and dynamics. As mentioned, this is often the case in many quantum optical experiments. Indeed, such expressions have been instrumental to the interpretation of the experiments reported on by Brunelli *et al.* (2018), which are reviewed in Sec. VIII.D.

H. Quantum phase space

Many aspects of the transition from quantum to classical can be neatly visualized by moving to quantum phase space. The role of quantum effects in the entropy production is one of them. In this section, we consider semiclassical formulations of the entropy production problem based on quantum phase space. The idea is to replace the von Neumann entropy with a generalized entropy function associated with the distribution in phase space. This yields a semiclassical formulation that coincides with standard thermodynamics at high temperatures but leads to valuable new insights otherwise. The approach, as we show, can also be naturally extended to nonequilibrium reservoirs, such as dephasing and squeezed baths (which are also reviewed in Sec. VII.C).

We consider a system of n in general interacting harmonic oscillators (bosonic modes) whose positions and momenta (quadratures) we label as q_i and p_i , respectively ($i = 1, \dots, n$). We arrange them in the $2n$ -dimensional vector $X^T = (q_1, p_1, q_2, p_2, \dots, q_n, p_n)$. We also define the corresponding annihilation operators as $a_i = (q_i + ip_i)/\sqrt{2}$. Moreover, in this section we assume for simplicity units such that $\hbar = k_B = 1$.

We discuss here two of the most widely used approaches for quantum phase space: the Wigner and the Husimi function (Lee, 1995). Given a density matrix ρ , the former is defined as

$$\mathcal{W}(\mathbf{x}) = \frac{1}{\pi^{2n}} \int d^{2n}\lambda e^{-\sum_i (\lambda_i \alpha_i^* - \lambda_i^* \alpha_i)} \text{tr} \{ \rho e^{\sum_i (\lambda_i a_i^\dagger - \lambda_i^* a_i)} \}, \quad (171)$$

where the integral is over the entire complex plane of each λ_i , i.e., $d^{2n}\lambda = \prod_i d\text{Re}(\lambda_i) d\text{Im}(\lambda_i)$. Moreover, the argument \mathbf{x} of the Wigner function stands for a $2n$ -dimensional vector with entries $x_{2i-1} = (\alpha_i + \alpha_i^*)/\sqrt{2}$ and $x_{2i} = i(\alpha_i^* - \alpha_i)/\sqrt{2}$. One could equivalently interpret \mathcal{W} to be a function of the $2n$ complex variables (α_i, α_i^*) . We use the two representations interchangeably in what follows.

An alternative, equivalent formulation is in terms of the Husimi- \mathcal{Q} function, which is defined as

$$\mathcal{Q}(\alpha) = \frac{1}{\pi^n} \langle \alpha | \rho | \alpha \rangle, \quad (172)$$

where $|\alpha\rangle = \otimes_{i=1}^n |\alpha_i\rangle$ and each $|\alpha_i\rangle$ is a coherent state of mode i , i.e., $a_i |\alpha_i\rangle = \alpha_i |\alpha_i\rangle$. The Husimi function is interpreted as the probability distribution for the outcome of a homodyne measurement; that is, simultaneous (but noisy) measurements of both position and momentum (Arthurs, 1965; Braunstein, Caves, and Milburn, 1991).

While \mathcal{W} can be negative for certain states, \mathcal{Q} is always strictly non-negative. The relation between the Wigner and Husimi functions is via a Gaussian convolution

$$\mathcal{Q}(\alpha) = \frac{2^n}{\pi^n} \int d^{2n}\lambda \mathcal{W}(\lambda) e^{-2 \sum_i |\alpha_i - \lambda_i|^2}. \quad (173)$$

This therefore shows how \mathcal{Q} can be viewed as a type of coarse-grained version of the Wigner function, which has often been used to explore the classical-quantum boundary (Takahashi and Saitô, 1985). This coarse graining is just enough to make $\mathcal{Q} \geq 0$ for all ρ . The Wigner function is in one-to-one correspondence with the state ρ . Despite this coarse graining, the same is also true of \mathcal{Q} . This is a consequence of the overcompleteness of the coherent state basis.

A particularly important class of states in the context of quantum phase space involves those that are Gaussian (Ferraro, Olivares, and Paris, 2005). Gaussian states are completely characterized by their first moments $\bar{x}_i = \langle X_i \rangle$ and CM, whose elements we rewrite for convenience as

$$\Theta_{ij} = \frac{1}{2} \langle \{X_i, X_j\} \rangle - \langle X_i \rangle \langle X_j \rangle. \quad (174)$$

Thus, for Gaussian states the correspondence between ρ and the Wigner or Husimi function is extended to the first moments and the covariance matrix, which now fully characterize the properties of the system. The Wigner function for Gaussian states has the form of a multivariate normal

$$\mathcal{W}(x) = \frac{e^{-(1/2)(x-\bar{x})^T \Theta^{-1} (x-\bar{x})}}{\sqrt{(2\pi)^n \det(\Theta)}}, \quad \mathcal{Q}(x) = \frac{e^{-(1/2)(x-\bar{x})^T \Theta_Q^{-1} (x-\bar{x})}}{\sqrt{(2\pi)^n \det(\Theta_Q)}}, \quad (175)$$

where $\Theta_Q = \Theta + \mathbb{I}/2$ is the original CM, incremented by vacuum fluctuations. This is directly associated with the coarse-grained nature of \mathcal{Q} , which causes the CM associated with \mathcal{Q} to be larger by a factor of $1/2$.

Gaussian states are useful for systems undergoing Gaussian processes, that is, processes that preserve the Gaussian character of a given input state. This in turn implies that the operation is linear in the phase-space variables, and thus generated by a Hamiltonian that is a bilinear form of position and momentum. Such a class of states and operations is particularly useful for illustrating the general context that we aim to address. It plays a crucial role in quantum optics and quantum information processing as an important resource for quantum communication protocols (Braunstein and van

Loock, 2005; Cerf, Leuchs, and Polzik, 2007; Serafini, 2017) and a representation for the ground or thermal equilibrium states of linear systems. Gaussian states are also routinely prepared in many experimental settings, from linear optics to platforms exploiting general light-matter interactions (Cerf, Leuchs, and Polzik, 2007; Serafini, 2017). The formulation of entropy production in terms of quantum phase space is greatly simplified for Gaussian states and operations; the formalism, however, is not restricted to this case, and we later discuss the Gaussian and non-Gaussian processes in parallel.

Given the interpretation of \mathcal{W} and \mathcal{Q} as quasiprobability distributions in phase space, one may now naturally contemplate the possibility of using their associated Shannon entropies as quantifiers of information. The following Shannon entropy of $\mathcal{W}(\mathbf{x})$ is called the Wigner entropy:

$$\mathcal{S}_W = - \int d^{2n} \mathbf{x} \mathcal{W}(\mathbf{x}) \ln \mathcal{W}(\mathbf{x}). \quad (176)$$

An operational interpretation for \mathcal{S}_W was given by Bužek, Keitel, and Knight (1995), who showed that it can be viewed as a sampling entropy via homodyne measurements. For general non-Gaussian states, \mathcal{W} may be negative so that the integral in Eq. (176) delivers a complex-valued entropy, which is not suitable as a measure of information. For Gaussian states, however, \mathcal{S}_W acquires a good interpretation. First, an explicit calculation using $\mathcal{W}(x)$ in Eq. (175) leads to (Bužek, Keitel, and Knight, 1995; Adesso, Girolami, and Serafini, 2012; Landi, Tomé, and de Oliveira, 2013)

$$\mathcal{S}_W = \frac{1}{2} \ln \det(\Theta) + \frac{n}{2} \log(2\pi e). \quad (177)$$

Equation (177) shows that the entropy is determined solely by the determinant of the CM, therefore providing an extremely efficient way of evaluating the entropy of the system. It is notable that, for Gaussian states, \mathcal{S}_W is directly connected to the Rényi-2 entropy. Recalling the definition $S_\alpha = (1 - \alpha)^{-1} \ln \text{tr} \rho^\alpha$ of the Rényi- α entropy, it was shown by Adesso, Girolami, and Serafini (2012) that $S_2 = (1/2) \ln \det(\Theta)$, hence

$$\mathcal{S}_W = S_2 + \text{const.} \quad (178)$$

Equation (178) links the Wigner entropy to S_2 , an important information-theoretic quantity (Rényi, 1960) of strong thermodynamic relevance (Baez, 2011).

For states whose Wigner functions are not necessarily positive, one may alternatively study the following Shannon entropy of the Husimi function:

$$\mathcal{S}_Q = - \int d^{2n} \alpha \mathcal{Q} \ln \mathcal{Q}, \quad (179)$$

known as *Wehrl's entropy* (Wehrl, 1978; Wehrl, 1979). Since $\mathcal{Q} \geq 0$, Wehrl's entropy is always well defined and real. It can also be given an operational interpretation as a coarse graining of the von Neumann entropy, stemming from a convolution of the system's state with Gaussian noise induced by a heterodyne measurement (Wódkiewicz, 1984; Bužek, Keitel, and

Knight, 1995). As a consequence, \mathcal{S}_Q upper bounds the von Neumann entropy [$\mathcal{S}_Q \geq S(\rho)$] (Lieb, 1978). Another advantage of the Husimi function and the Wehrl entropy is that they can be extended to spin systems in terms of spin-coherent states. This is further discussed later.

We are now in the position to introduce the formulation of entropy production within the context of the Wigner and Wehrl entropies. The main advantage of moving to quantum phase space is that any master equation can be mapped into a quantum Fokker-Planck equation for \mathcal{W} or \mathcal{Q} . Tools of classical stochastic processes can then be employed in order to obtain simple expressions for the entropy production rate and flux. This can be done for a wide variety of environments interacting with the system of interest (Santos, Landi, and Paternostro, 2017), including nonequilibrium baths. In what follows, we present an account of possible approaches toward the derivation of explicit expressions for such quantities.

For illustration, we begin by considering a single bosonic mode described by a standard Lindblad master equation of the form

$$\partial_t \rho = -i[H, \rho] + \mathcal{D}(\rho), \quad (180)$$

where $H = \omega(a^\dagger a + 1/2)$ and

$$\mathcal{D}(\rho) = \gamma(\bar{n} + 1)D[a] + \gamma\bar{n}D[a^\dagger], \quad (181)$$

where $D[L] = L\rho L^\dagger - (1/2)\{L^\dagger L, \rho\}$, γ is the damping rate, and $\bar{n} = (e^{\beta\omega} - 1)^{-1}$ is the Bose-Einstein distribution. Using standard correspondence tables (Gardiner and Zoller, 2004) one can convert Eq. (180) into a quantum Fokker-Planck equation for either \mathcal{W} or \mathcal{Q} . In the case of the Wigner function, this becomes

$$\partial_t \mathcal{W} = \mathcal{U}(\mathcal{W}) + \partial_\alpha J(\mathcal{W}) + \partial_{\alpha^*} J^*(\mathcal{W}), \quad (182)$$

where $\mathcal{U}(\mathcal{W}) = i\omega[\partial_\alpha(\alpha\mathcal{W}) - \partial_{\alpha^*}(\alpha^*\mathcal{W})]$ is a differential operator associated with the unitary part of Eq. (180) and

$$J(\mathcal{W}) = \frac{\gamma}{2}[\alpha\mathcal{W} + (\bar{n} + 1/2)\partial_{\alpha^*}\mathcal{W}] \quad (183)$$

is a complex-valued phase-space current associated with the irreversible part of the dynamics. Equation (182) can be viewed as a continuity equation in quantum phase space, where the changes in \mathcal{W} stem from gradients of unitary and irreversible currents. In particular, the current J vanishes if and only if \mathcal{W} is a thermal state with occupation \bar{n} , that is, for $\mathcal{W}_{\text{eq}} = e^{-|\alpha|^2/(\bar{n}+1/2)}/[\pi(\bar{n} + 1/2)]$. While Eq. (182) vanishes for such a thermal state, the fact that the individual currents vanish is a stronger statement, which in classical systems is usually attributed to detailed balance. It also provides an alternative interpretation for the thermal equilibrium state as the unique state for which no quasiprobability currents flow.

The problem can be equivalently expressed as a Fokker-Planck equation for the Husimi function. The equation will have the same form as Eq. (182), with small modifications. For the choice of Hamiltonian in Eq. (180), the unitary part

turns out to be same, with \mathcal{W} replaced by \mathcal{Q} . But this is a coincidence of this simple Hamiltonian, as the unitary parts in general may differ significantly. The shape of the irreversible currents $J(\mathcal{Q})$ will look exactly like Eq. (183) except that $\bar{n} + 1/2$ is replaced by $\bar{n} + 1$. This reflects the additional vacuum fluctuations that naturally appear in the Husimi function, which are similar to what was found in Eq. (175).

The formalism for the calculation of the entropy production rate set forth in Sec. III, in particular, Eq. (47), suggests that a meaningful definition for the Wigner entropy production could be [see Eq. (154)]

$$\dot{\Sigma}_W(t) = -\frac{d}{dt} S_W(\mathcal{W}(t) \| \mathcal{W}_{\text{eq}}). \quad (184)$$

Here $S_W(\mathcal{W}_1 \| \mathcal{W}_2) = \int d^2\alpha \mathcal{W}_1 \ln \mathcal{W}_1 / \mathcal{W}_2$ is the Wigner analog of the Kullback-Leibler divergence. As [Adesso, Girolami, and Serafini \(2012\)](#) showed, for Gaussian states this coincides with the Rényi-2 mutual information. By using the rhs of Eq. (182) in the definition of $\dot{\Sigma}_W$ and integrating by parts over the phase space, we get ([Santos, Landi, and Paternostro, 2017](#))

$$\dot{\Sigma}_W(t) = \frac{4}{\gamma(\bar{n} + 1/2)} \int d^2\alpha \frac{|J(\mathcal{W})|^2}{\mathcal{W}}. \quad (185)$$

Equation (185) has several good properties and a clear physical interpretation. First, $\dot{\Sigma}_W \geq 0$, as expected for any second law. Second, $\dot{\Sigma}_W = 0$ if and only if the currents vanish, which happens if and only if $\mathcal{W} = \mathcal{W}_{\text{eq}}$. Thus, the entropy production is zero only when the system is in thermal equilibrium with the bath. Third, Eq. (185) directly links entropy production with the existence of irreversible currents in phase space. In particular, one can derive a phase-space velocity $J(\mathcal{W})/\mathcal{W}$ ([Seifert, 2012](#)) so that $\dot{\Sigma}_W$ is interpreted as the mean-squared phase-space velocity.

Next we turn to the entropy flux, which can be computed from $\dot{\Phi}_W = \dot{\Sigma}_W - dS_W/dt$; see Eq. (7). Using the explicit form of $J(\mathcal{W})$ in Eq. (183) together with Eq. (185), one finds that

$$\dot{\Phi}_W = \frac{\gamma}{\bar{n} + 1/2} (\langle a^\dagger a \rangle - \bar{n}). \quad (186)$$

The interpretation of Eq. (186) is straightforward as well. Starting with Eq. (180), one may compute the energy flow to the bath, which reads $\langle \dot{H} \rangle = \omega\gamma(\bar{n} - \langle a^\dagger a \rangle)$. For simplicity, we assume that this can be attributed to heat entering the bath ($\langle \dot{H} \rangle \equiv -\dot{Q}_E$; see Sec. V.D. As a consequence, comparing this with Eq. (186), one finds that

$$\dot{\Phi}_W = \frac{\dot{Q}_E}{\omega(\bar{n} + 1/2)}. \quad (187)$$

Equation (187) can be compared with the standard thermodynamic result $\dot{\Phi} = \dot{Q}_E/T$ [Eq. (2)]. We see that formulating the problem in terms of the Wigner function leads to a modification of the standard thermodynamic result, where the heat flux is now weighted by a new prefactor $\omega(\bar{n} + 1/2)$ instead of the temperature T . When $T \gg \omega$, however, a series expansion

leads to $\omega(\bar{n} + 1/2) \simeq T$. Thus, one recovers the standard thermodynamic results at high temperatures.

A particularly important special case of the previous formalism is to describe photon losses in optical cavities. The standard dissipator used to describe this $\mathcal{D}(\rho) = \gamma[apa^\dagger - (1/2)\{a^\dagger a, \rho\}]$ corresponds to a zero-temperature ($\bar{n} \rightarrow 0$) limit of Eq. (181). The problem with this is that the standard formulation of the second law breaks down in this limit since the relative entropy in Eq. (30) diverges when the environment is in a pure state. The phase-space approach, on the other hand, remains perfectly well defined in this limit, thanks to the factors of $1/2$ in Eqs. (185) and (187). The reason, therefore, is because the phase-space approach also takes into account vacuum fluctuations, which persist even at zero temperature.

Equations (185) and (187) provide solid physical grounds for the choice of Eq. (184) as a basic definition of entropy production in the context of quantum phase space. ([Santos, Landi, and Paternostro \(2017\)](#)) put forth two additional approaches to the derivation these results, one of them based on the complex-plane averaging of stochastic trajectories. The fact that all approaches agree corroborates the correctness of the framework. We mention, however, that Eq. (184) is not expected to hold for all types of phase-space open dynamics. It fails, for instance, in the case of a linear lattice connected to multiple baths ([Malouf et al., 2019](#)). Hence, the previous construction should ultimately be performed on a case-by-case basis.

We also mention that these results remain valid if one instead uses the Husimi function. The only difference is that all factors of $\bar{n} + 1/2$ should be replaced by $\bar{n} + 1$. This apparent similarity between the two approaches, however, is deceiving, as it only happens for the simple models considered here. In more complicated scenarios, the two approaches may differ significantly. A good example is the case of two-photon losses described by a Lindblad dissipator $a^2\rho a^{\dagger 2} - (1/2)\{a^{\dagger 2}a^2, \rho\}$ (a highly non-Gaussian process). The Fokker-Planck equation associated with this dissipator is completely different if one employs either the Wigner or the Husimi function, as a direct calculation shows. The same is also true for more complicated unitary contributions. In fact, due to the coarse-grained nature of the Husimi function, unitary terms may contribute for the evolution of \mathcal{S}_Q . These terms may be particularly important in systems undergoing dissipative phase transitions ([Goes, Fiore, and Landi, 2020](#)), which are reviewed in Sec. VII.F. But they also persist even in completely isolated systems undergoing unitary dynamics, which were studied by [Goes et al. \(2020\)](#).

The previously presented approach can also be flexibly extended to master equations describing nonequilibrium reservoirs. We consider two examples. The first is a squeezed thermal bath that, in addition to the thermal occupation \bar{n} , is also described by a squeezing parameter $z = re^{i\theta}$. The full form of the dissipator in this case is presented in Eq. (264). The calculations in this case are analogous and amount solely to the substitution

$$J(\mathcal{W}) \rightarrow J(\mathcal{W}) \cosh r + [\gamma\alpha^*\mathcal{W} - J^*(\mathcal{W})]e^{i(\theta-2\omega,t)} \sinh r, \quad (188)$$

where ω_s is the central frequency of the broadband bath and accounts for nonresonant energy exchanges with the system. Squeezed baths are further reviewed in Sec. VII.C.

The second example we discuss is that of a dephasing bath, which describes the loss of quantum coherence without the exchange of excitations. The effects of a dephasing bath can be accounted for in Eq. (180) by using the superoperator

$$\mathcal{D}^{\text{deph}}(\rho) = -\frac{\lambda}{2}[a^\dagger a, [a^\dagger a, \rho]], \quad (189)$$

with λ the dephasing rate. A similar procedure in this case reveals that the flux is identically zero ($\dot{\Phi}_W \equiv 0$). This is in agreement with the idea that this sort of environmental effect is not associated with a flux of excitations to or from the system. As a consequence, one may identify the rate of change of the Wigner entropy of the system with the entropy production rate, which takes the form (Santos, Landi, and Paternostro, 2017)

$$\dot{\Sigma}_W^{\text{deph}}(t) = \frac{2}{\lambda} \int \frac{|J^{\text{deph}}(\mathcal{W})|^2}{|\alpha|^2 \mathcal{W}} d^2\alpha, \quad (190)$$

where we have introduced the dephasing current $J^{\text{deph}}(\mathcal{W}) = \lambda\alpha[\alpha^* \partial_{\alpha^*} \mathcal{W} - \alpha \partial_{\alpha} \mathcal{W}]/2$. We therefore see that a similar structure emerges, but one now associated with the irreversible currents generated by the dephasing bath. There is also an additional factor of $|\alpha|^2$ in the numerator, which tends to favor currents near the origin of the complex plane.

Santos *et al.* (2018) extended the formalism of phase-space approaches to entropy production to the case of spinlike systems, making use of the useful spin-coherent state representation (Radcliffe, 1971; Takahashi and Saitô, 1985).

VI. RESOURCE-THEORETIC APPROACH

Quantum features can be exploited to provide advantages for a series of applications. Different applications, however, exploit different features. For instance, quantum communications may exploit entanglement, while metrological applications may exploit radiation squeezing. Each of these features therefore represents a resource, which can be consumed to yield a quantum advantage for certain tasks. Resource theories provide a mathematical formulation of this idea. Initially focused on entanglement (Horodecki, Horodecki, and Horodecki, 2009), they were subsequently extended to several other resources, including purity (Horodecki, Horodecki, and Oppenheim, 2003), asymmetry (Horodecki, Horodecki, and Oppenheim, 2003), and coherence (Streltsov, Adesso, and Plenio, 2017). A recent review was given by Chitambar and Gour (2019).

Thermodynamics can also be cast in this framework, known as the *resource theory of athermality*, which was first pioneered by Brandão *et al.* (2013). In this case, the resources are all quantum states that are not in thermal equilibrium. The reason is that such states can be used to extract work, which is the most fundamental task of thermodynamics, hence athermality (i.e., how “far” a system is from equilibrium) is the resource that is consumed to extract work.

Earlier works on the resource theory of athermality were reviewed by Goold *et al.* (2016). In this section we focus on some of the more recent developments, as well as on aspects that pertain specifically to entropy production.

The starting point for any resource theory is the definition of the allowed free operations, that is, operations that merely consume a resource and never create it. In the case of thermodynamics, this indicates no associated work. Moreover, the idea is to focus on operations that are physically meaningful and endowed with interesting properties. While there is no unique proposal [see Bera *et al.* (2017)], the most widely used thus far have been the thermal operations discussed in Sec. III.D.

Recall that a thermal operation (TO) is any map $\mathcal{T}(\rho)$ of the form (Brandão *et al.*, 2013)

$$\mathcal{T}(\rho_S) = \text{tr}_E\{U(\rho_S \otimes \rho_E^{\text{th}})U^\dagger\}, \quad [U, H_S + H_E] = 0, \quad (191)$$

with $\rho_E^{\text{th}} = e^{-\beta H_E}/Z_E$. That is, a TO is a map where the system interacts with a thermal environment by means of a unitary that preserves the total energy; see Eq. (50). As discussed in Sec. III.D, this kind of operation has a series of good properties. First, the fixed point of the map is the thermal state $\rho_S^{\text{th}} = e^{-\beta H_S}/Z_S$. Hence, it describes the partial (or full) thermalization of the system toward ρ_S^{th} . Second, $[U, H_S + H_E] = 0$ implies that there is no work involved in coupling S and E , so the change in energy of S coincides with the heat that flows to E . Third, the entropy production of the process can be written as follows solely in terms of system-related quantities as in Eq. (52):

$$\Sigma = S(\rho_S \|\rho_S^{\text{th}}) - S(\rho'_S \|\rho_S^{\text{th}}) = -\beta \Delta F, \quad (192)$$

where $\rho'_S = \mathcal{T}(\rho_S)$ is the state of the system after the map and $\Delta F = F(\rho'_S) - F(\rho_S)$, where $F(\rho_S) = \text{tr}(H_S \rho_S) - TS(\rho_S)$ is the nonequilibrium free energy of ρ_S .

In the resource theory of athermality, the state ρ_S^{th} is called the free state. Any state that is not ρ_S^{th} is viewed as a resource (this includes thermal states at a different temperature β'). The TOs (191) represent the free operations; they cannot create resources but instead only consume it. Moreover, they do nothing to free states. Another key feature of resource theories is the idea of a *monotone*, i.e., a c -number function $f(\rho_S)$ satisfying

$$f(\mathcal{T}(\rho_S)) \leq f(\rho_S). \quad (193)$$

A natural monotone in this case is the relative entropy $S(\rho_S \|\rho_S^{\text{th}})$. This quantity is a monotone because ρ_S^{th} is a fixed point of \mathcal{T} , so the data processing inequality implies $S(\rho'_S \|\rho_S^{\text{th}}) \leq S(\rho_S \|\rho_S^{\text{th}})$; see Eq. (49). The entropy production (192) and the second law ($\Sigma \geq 0$) therefore naturally appear as the monotones of the resource theory.

In the case of a system with a zero Hamiltonian ($H_S = 0$), the free energy simply becomes the von Neumann entropy of the system $F(\rho_S) = -TS(\rho_S)$ and one recovers the resource theory of purity (Horodecki, Horodecki, and Oppenheim, 2003).

One of the basic questions of resource theories is: Given two states ρ_S and ρ'_S , is there an operation \mathcal{T} such that $\rho'_S = \mathcal{T}(\rho_S)$? Put differently, is it possible to convert ρ_S to ρ'_S via thermal operations? This means that one has to search over all possible maps \mathcal{T} (i.e., over all possible environments and all possible energy-preserving unitaries). The question is therefore highly nontrivial. Notwithstanding, it is also extremely important, as it allows one to establish a hierarchy of resources and thus determine how much more resourceful one state is with respect to another. As we later show, it turns out that entropy production plays a fundamental role in determining state interconversion.

In the context of thermodynamics, state interconversion is directly associated with the work of Åberg (2013), or, more specifically, the notions of *work extraction* and *work of formation* (Dahlsten *et al.*, 2011; Horodecki and Oppenheim, 2013). These tasks can be accomplished, for instance, by coupling the system to an additional work qubit (Horodecki and Oppenheim, 2013) or a continuous variable system (mimicking a classical weight) (Skrzypczyk, Short, and Popescu, 2014; Chubb, Tomamichel, and Korzekwa, 2018). The maximum amount of work that can be extracted occurs when the system is taken from a state ρ_S to the thermal state ρ_S^{th} (full thermalization). Work of formation, on the other hand, refers to the reverse problem: if the system starts in a thermal state ρ_S^{th} , what is the minimum amount of energy that must be invested to take it toward a certain state ρ_S ? Extraction and formation are therefore two examples of state interconversion.

A. Thermomajorization

We now turn to the question of state interconversion in the single-shot scenario. That is, given two states ρ_1 and ρ_2 , we ask whether it is possible to convert $\rho_1 \rightarrow \rho_2$ using only thermal operations of the form of Eq. (191). This problem was first addressed by Horodecki and Oppenheim (2013) and is based on a criterion called thermomajorization (which is a variation of the idea of majorization used in probability theory). Let $H_S = \sum_i E_i |i\rangle\langle i|$. For simplicity, we focus on states that are diagonal in the basis $|i\rangle$, i.e., which are of the form $\rho_S = \sum_i p_i |i\rangle\langle i|$. The results of Horodecki and Oppenheim (2013) also hold for states that are block diagonal [see Eq. (204)], but not for states that have arbitrary off-diagonal elements. A treatment of the latter was put forth by Lostaglio, Jennings, and Rudolph (2015) and is later reviewed.

The criteria of thermomajorization can be formulated as follows. For each given state $\rho_S = \sum_i p_i |i\rangle\langle i|$, we construct the so-called thermomajorization curve of ρ_S . First, we relabel the probabilities so that

$$p_1 e^{\beta E_1} \geq p_2 e^{\beta E_2} \geq \dots \geq p_d e^{\beta E_d}, \quad (194)$$

where d is the Hilbert space dimension, which we assume to be finite. This is called β ordering. We then construct a special curve with points

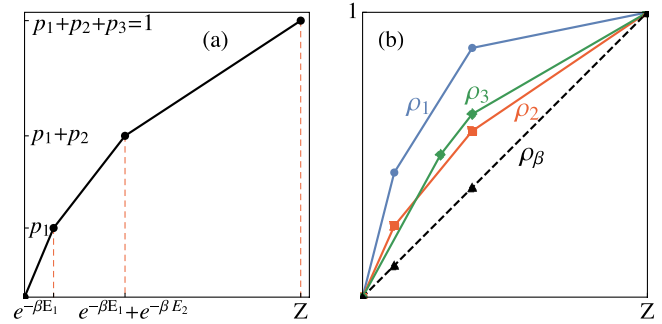


FIG. 4. Thermomajorization condition determining when two states are interconvertible using thermal operations. (a) Procedure for constructing the thermomajorization curve is given in the main text and summarized in Eq. (195). (b) This curve is then used to compare different states. The state ρ_1 thermomajorizes ρ_2 , ρ_3 , and ρ_β . Conversely, ρ_2 and ρ_3 do not thermomajorize each other. Adapted from Horodecki and Oppenheim, 2013.

$$\left\{ \sum_{i=1}^k e^{-\beta E_i}, \sum_{i=1}^k p_i \right\}, \quad k = 1, \dots, d, \quad (195)$$

as illustrated in Fig. 4(a).

This curve is used to compare different states, as we exemplify in Fig. 4(b). If the curve for a certain state ρ_1 is always above another, say, ρ_2 , we say that ρ_1 thermomajorizes ρ_2 , which is written as

$$\rho_1 \succ_{\beta} \rho_2. \quad (196)$$

In the example shown in Fig. 4(b) $\rho_1 \succ_{\beta} \rho_2$ but $\rho_2 \not\succ_{\beta} \rho_3$. By construction the thermal state ρ_{β} at temperature β is a straight line and is majorized by all other states. The majorization symbol therefore introduces a natural ordering between states. It is essential to note, however, that this ordering is made with reference to the temperature β of the bath. In particular, since any state thermomajorizes ρ_{β} , it follows that this must also be true for other thermal states with different temperatures β' , i.e., $\rho_{\beta'} \succ_{\beta'} \rho_{\beta}$ for any β' .

The main result of Horodecki and Oppenheim (2013) can now be summarized by the following theorem.

Theorem 1.—Given two block-diagonal states ρ_1 and ρ_2 , if $\rho_1 \succ_{\beta} \rho_2$ then it is possible to convert ρ_1 to ρ_2 using thermal operations.

Thermomajorization thus offers an unambiguous way of ordering states within the context of thermal operations. By analyzing which curves are above the other, we can say which states can be converted to others by means of thermal operations. The proof, as well as the intuition, behind Theorem 1 is based on the connection with majorization theory. In addition to the original reference, see Lostaglio, Jennings, and Rudolph (2015), who summarized the basic ideas, and Weilenmann *et al.* (2016), who provided a thorough discussion on the connection with majorization and the resource theory of purity.

The basic rationale goes as follows. Given two D -dimensional probability vectors γ_1 and γ_2 , we say that γ_1 majorizes γ_2 , written $\gamma_1 \succ \gamma_2$, when

$$\sum_{i=1}^k \gamma_{1i}^\downarrow \geq \sum_{i=1}^k \gamma_{2i}^\downarrow \quad (197)$$

for all $k = 1, \dots, D$. Here γ^\downarrow represents the probability γ sorted in descending order. To link majorization [Eq. (197)] to thermomajorization [Eq. (196)], consider a system with d levels and thermal distribution $p_i^{\text{th}} = e^{-\beta E_i}/Z$, where $i = 1, \dots, d$. For simplicity, we assume that the p_i^{th} are rationals; i.e., they can be written as $p_i^{\text{th}} = k_i/D$, where k_i and D are integers such that $\sum_i k_i = D$ (to ensure normalization). In practice, one can always approximate the p_i^{th} in this way, with arbitrary accuracy, by using sufficiently large integers.

Given an arbitrary probability vector $\mathbf{p} = (p_1, \dots, p_d)$, one may then define a mapping $\gamma(\mathbf{p})$ that converts the d -dimensional vector \mathbf{p} into the D -dimensional vector

$$\gamma(\mathbf{p}) = \left(\frac{p_1}{k_1}, \frac{p_1}{k_1}, \dots, \frac{p_2}{k_2}, \frac{p_2}{k_2}, \dots, \frac{p_d}{k_d}, \frac{p_d}{k_d}, \dots \right), \quad (198)$$

where each term p_i/k_i occurs k_i times. Notice that the k_i 's implicitly depend on β since they are defined from p_i^{th} .

As a particular case, we see that the map in Eq. (198) takes the thermal state p^{th} into the following uniform distribution:

$$\gamma(p^{\text{th}}) = \eta, \quad (199)$$

where $\eta_i = 1/D$ is a D -dimensional uniform distribution. This is similar in spirit to the mapping between the canonical and microcanonical ensembles in statistical mechanics, in the sense that it maps a thermal distribution in a smaller space to a uniform distribution (with all states equally likely) in a higher-dimensional space.

Thermal operations have p^{th} as a fixed point. In the larger space of dimension D , this is then converted into a map $\mathcal{R}(\gamma)$ having the uniform distribution η as the fixed point. Maps of this form are called noisy operations and play a central role in the resource theory of purity (Horodecki, Horodecki, and Oppenheim, 2003). The question posed in Theorem 1 can now be converted to, under which conditions can $\gamma(p_1)$ be converted into $\gamma(p_2)$ by means of noisy operations? As shown by Ruch, Schraner, and Seligman (1978), this is possible precisely when $\gamma(p_1) \succ \gamma(p_2)$. But because of the structure of Eq. (198), saying that $\gamma(p_1) \succ \gamma(p_2)$ is equivalent to saying that $p_1 \succ_\beta p_2$. Hence, Theorem 1 follows.

This analysis also serves to emphasize the deep connection between athermality and purity. All results for majorization are recovered from thermomajorization by setting $H_S = 0$; β ordering in Eq. (194) simply becomes descending ordering, etc. Thermomajorization is thus the generalization of majorization theory for “nonzero Hamiltonians.” This acquires a deeper significance starting in Sec. VI.B, when we discuss monotones for athermality. In the resource theory of purity, all that matters are probabilities, so the von Neumann entropy appears as the natural monotone. For athermality, however, energy also plays a role. And, as a consequence, the natural monotones will instead be related to the free energy $F = U - TS$, which is precisely a combination of energy and entropy.

B. The second laws of thermodynamics

The second law (52) says that a transition from ρ_S to ρ'_S is possible only if the corresponding entropy production is non-negative. This, however, is only a necessary condition. There may in principle exist states that cannot be interconverted into one another despite leading to a positive entropy production. For general maps, establishing sufficient and necessary conditions is unfeasible. But for the restricted class of thermal operations this turns out to be possible, as first shown by Brandão *et al.* (2015) using the idea of catalytic thermal operations.

The scenario is the same as before. However, in addition to the system S , one introduces an ancillary system, called the catalyst, with Hamiltonian H_C and prepared in an arbitrary state ρ_C . The joint SC system then undergoes a thermal operation (conserving the total energy $H_S + H_C + H_E$). The thermal operation is necessarily chosen such that the catalyst is brought back to its original state ρ_C after the process; see Fig. 5. Given this setting, one then asks whether it is possible to convert a state ρ_S into another state ρ'_S .

The usual second law, written in the form of Eq. (52), states that this is possible when $S(\rho_S \parallel \rho_S^{\text{th}}) \geq S(\rho'_S \parallel \rho_S^{\text{th}})$, a condition that is necessary but not sufficient. Instead, as shown by Brandão *et al.* (2015) a necessary and sufficient condition is provided using the following theorem.

Theorem 2.—A state ρ_S , block diagonal in the energy basis, can be converted into ρ'_S by means of catalytic thermal operations if

$$\Sigma_\alpha := S_\alpha(\rho_S \parallel \rho_S^{\text{th}}) - S_\alpha(\rho'_S \parallel \rho_S^{\text{th}}) \geq 0 \quad \forall \alpha \geq 0, \quad (200)$$

where

$$S_\alpha(\rho_S \parallel \rho_S^{\text{th}}) = \frac{1}{\alpha - 1} \ln \sum_i p_i^\alpha (p_i^{\text{th}})^{1-\alpha} \quad (201)$$

is the Rényi- α divergence.

This result thus establishes a family of second laws ($\Sigma_\alpha \geq 0$) parametrized by the continuous parameter

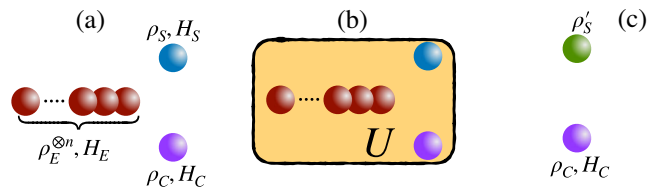


FIG. 5. Illustration of the cyclic protocol based on catalytic thermal operations used by Brandão *et al.* (2015) to generalize the second law of thermodynamics to the microscopic quantum domain. (a) System S , catalyst C , and reservoir E , each endowed with their respective Hamiltonians [H_j ($j = S, C, E$)], are prepared in an uncorrelated state. The initial state of the reservoir consists of the tensor product of n copies of the same thermal state $\rho_{\text{th},E}$. (b) Parties involved in the protocol evolve jointly via the catalytic thermal operation U such that $[U, \sum_j H_j] = 0$. (c) The process is such that, at the end of the evolution, the catalyst is brought back to its initial state, while the system S ends up in a state ρ'_S .

$\alpha \in [0, \infty)$. The usual second law in Eq. (52) is a particular case corresponding to $\alpha \rightarrow 1$.

Alternatively, one may cast the second laws in terms of Rényi- α free energies defined as

$$F_\alpha(\rho_S) = F_{\text{th}} + TS_\alpha(\rho_S || \rho_S^{\text{th}}), \quad (202)$$

where $F_{\text{th}} = -T \ln Z_S$. This represents the Rényi generalization of the nonequilibrium free energy (42). Equation (200) then becomes

$$F_\alpha(\rho_S) \geq F_\alpha(\rho'_S) \quad \forall \alpha \geq 0. \quad (203)$$

Recall from Eq. (41) that in the absence of work, $\Sigma = -\beta \Delta F$. Thus, the statement $\Sigma \geq 0$ is tantamount to saying, “In order for a process to be possible, the free energy must go down.” But, again, this is only a necessary condition. Conversely, for quantum systems and thermal operations the appropriate statement is, “All free energies must go down.”

As in Sec. VI.A, a macroscopic limit can be defined in which (i) the system’s dimensions d are large and (ii) the state of the system has an energy distribution sharply peaked around $\langle H_S \rangle$. In this case it can be shown that all second laws stated in Eq. (200) converge to the usual one [Eq. (52)].

C. Coherence and the resource theory of asymmetry

All results in Sec. VI.B hold only for states ρ_S that are block diagonal in the energy basis, that is, states of the form

$$\rho_S = \sum_{i,j} \delta(E_i = E_j) \rho_{ij} |i\rangle\langle j|, \quad (204)$$

where $\delta(a = b)$ is the Kronecker delta and $\{|i\rangle\}$ and $\{E_i\}$ are the eigenstates and eigenvalues of H_S . Coherences of this form are called nonenergetic and play a much smaller role than coherences between different energy states (energetic coherences) due to the special role that energy plays in the dynamics and because, with the exception of accidental degeneracies, different energy states are usually associated with different macroscopic configurations.

In the context of thermodynamics, it was shown by Lostaglio, Jennings, and Rudolph (2015) and Lostaglio *et al.* (2015) that energetic coherences place constraints on the allowed transformations on top of the second laws (200). This connection was made by showing that a resource theory of thermodynamics is actually composed of two parts: athermality and asymmetry.

The resource theory of asymmetry (also called quantum reference frames) concerns arbitrary transformations under a certain group (Gour and Spekkens, 2008). Let G denote a Lie group and let V_g denote a unitary corresponding to a representation $g \in G$ of the group. A state ρ is called a free state if $V_g \rho V_g^\dagger = \rho$. That is, free states are invariant under G . Similarly, an arbitrary quantum channel $\mathcal{E}(\rho)$ is called a free operation if

$$\mathcal{E}(V_g \rho V_g^\dagger) = V_g \mathcal{E}(\rho) V_g^\dagger \quad \forall \rho, g \in G. \quad (205)$$

Such channels are also called covariant.

Thermal operations [see Eq. (191)] are covariant under the group generated by time translations, i.e., where $V_t = e^{-iH_S t}$, with H_S the generator of the group. This follows from the fact that $[U, H_S + H_E] = 0$ and $e^{-iH_E t} \rho_E^{\text{th}} e^{iH_E t} = \rho_E^{\text{th}}$. After straightforward manipulations, one has

$$e^{-iH_S t} \mathcal{T}(\rho_S) e^{iH_S t} = \mathcal{T}(e^{-iH_S t} \rho_S e^{iH_S t}).$$

Thermal operations are thus also free operations with respect to asymmetry. The standpoint of this approach is therefore that, by inducing the emergence of a directional arrow of time, thermodynamic irreversibility prevents time-translational invariance in general thermodynamic processes. On the other hand, the free states will be those that are block diagonal in the basis of H_S since these are the ones that satisfy $e^{-iH_S t} \rho_S e^{iH_S t} = \rho_S$. The free states are therefore those with no energetic coherences.

A monotone for coherence can be given by the following relative entropy of coherence (Baumgratz, Cramer, and Plenio, 2014):

$$C(\rho_S) = S(\rho_S || \Delta_{H_S}(\rho_S)) = S(\Delta_{H_S}(\rho_S)) - S(\rho_S), \quad (206)$$

where $\Delta_{H_S}(\rho_S)$ is the operation that fully dephases all entries of ρ_S that are not block diagonal in the energy basis of H_S ; see the discussion in Sec. V.B. Notice, therefore, that $\Delta_{H_S}(\rho_S)$ will be a free state from the perspective of asymmetry for any ρ_S . Equation (206) therefore measures the entropic distance between the state ρ_S and its incoherent version, which is time translation invariant, hence it provides a measure of the breakdown of time-translation invariance (Rodríguez-Rosario, Frauenheim, and Aspuru-Guzik, 2013).

Moreover, since thermal operations are free operations, they can reduce only the amount of coherence in a state so that

$$C(\rho_S) \geq C(\rho'_S), \quad (207)$$

where $\rho'_S = \mathcal{T}(\rho_S)$. This statement therefore implies that thermal operations cannot generate additional time-translation asymmetry in a system. Further, it characterizes the depletion of coherence and the tendency of the system to equilibrate onto time-translation invariant states, thus elevating coherence to the role of a second important resource in thermodynamics complementing athermality.

One may now draw a parallel here with the distinction made in Sec. VI.B between the second law and the second laws: Eq. (207) is only a necessary criteria for ρ_S to be interconvertible into ρ'_S . Instead, Lostaglio, Jennings, and Rudolph (2015) proved the following stronger result.

Theorem 3.—The set of thermal operations on a quantum system is a subset of the set of time-translation invariant operations. Moreover, for all $\alpha > 0$ any thermal operation results in

$$S_\alpha(\rho_S \|\Delta_{H_S}(\rho_S)) \geq S_\alpha(\rho'_S \|\Delta_{H_S}(\rho'_S)) \geq 0 \quad \forall \alpha \geq 0. \quad (208)$$

These conditions are independent of the second laws (200) and therefore represent additional constraints that must be satisfied in systems having coherence. It is also important to note that Theorems 2 and 3 cannot be combined into a single family of inequalities. For $\alpha = 1$, as discussed in Sec. V.B, one may split

$$S(\rho_S \|\rho_S^{\text{th}}) = S(\Delta_{H_S}(\rho_S) \|\rho_S^{\text{th}}) + C(\rho_S). \quad (209)$$

The first term represents the quantity entering Eq. (200), that is, the block-diagonal part of the state. The second term, on the other hand, is the quantity appearing in Eq. (208). Hence, the case of $\alpha = 1$ can be combined into the following single statement:

$$S(\rho_S \|\rho_S^{\text{th}}) \geq S(\rho'_S \|\rho_S^{\text{th}}), \quad (210)$$

which is simply the data processing inequality. Theorems 2 and 3, however, require that the inequalities be satisfied for all $\alpha \geq 0$. For $\alpha \neq 1$, there is no simple way of combining Eqs. (200) and (208).

D. Fluctuating work in the resource theory context

The concept of work is not easily defined within a resource theory context. The reason for this is that one of the main paradigms in resource theories is to completely account for all processes. For instance, the notion of an external agent, which changes the system Hamiltonian through a work protocol, must be internalized within the description of the process, as this is the only way to guarantee that all changes in energy are accounted for. The same difficulties arise for the storage of work. The goal is therefore twofold: First, to allow for the Hamiltonian of the system to change during the process, starting at H_S and ending at H'_S and, second, to provide a physical mechanism to store the work extracted from the process (the battery). These two problems were addressed by *Alhambra et al.* (2016). The former is solved using the notion of a switch X and the latter is solved using a continuous variable work storage ancilla, called a weight W .

The thermodynamic processes in question therefore involves four parts: the system (S), weight (W), switch (X), and environment (E). The allowed operations are unitaries on $SWXE$ satisfying, as before, the strong energy conservation

$$[U_{SWXE}, H_{SWXE}] = 0, \quad (211)$$

where H_{SWXE} is the total Hamiltonian (which is specified later). We now discuss how the switch and weight have to be constructed in order to yield consistent thermodynamic results.

We begin with the switch. It is chosen as a qubit with computational basis $\{|0\rangle, |1\rangle\}$ and initially prepared in $|0\rangle\langle 0|$. We assume that the total Hamiltonian of $SWXE$ has the special form

$$H_{SWXE} = H_S \otimes |0\rangle\langle 0|_X + H'_S \otimes |1\rangle\langle 1|_X + H_W + H_E, \quad (212)$$

where H_S and H'_S are the initial and final Hamiltonians of the system and H_W and H_E are the Hamiltonians of the weight and environment, respectively. In addition, one also assumes that all unitaries U_{SWXE} have the following form of controlled operations on the switch:

$$U_{SWXE} = U_{SWE} \otimes |1\rangle\langle 0|_X + U_{SWE}^\dagger \otimes |0\rangle\langle 1|_X, \quad (213)$$

where U_{SWE} is a unitary acting only on SWE .

Given an arbitrary initial state ρ_{SWE} of SWE , this will therefore produce the map

$$U_{SWXE}(\rho_{SWE} \otimes |0\rangle\langle 0|_X)U_{SWXE}^\dagger = \rho'_{SWE} \otimes |1\rangle\langle 1|_X, \quad (214)$$

where

$$\rho'_{SWE} = U_{SWE} \rho_{SWE} U_{SWE}^\dagger. \quad (215)$$

The switch therefore internalizes the idea of a changing Hamiltonian. In particular, it solves the issue of how to express strong conservation in the case in which H_S changes during the process: namely, at the level of $SWXE$, the condition remains in the usual form (211). Conversely, at the level of SWE , plugging Eqs. (212) and (213) into Eq. (211) leads to

$$U_{SWE}(H_S + H_W + H_E) = (H'_S + H_W + H_E)U_{SWE}, \quad (216)$$

which can be viewed as a statement of strong energy conservation for the case where the system Hamiltonian changes. In the particular case where $H'_S = H_S$, we recover the usual condition $[U_{SWE}, H_S + H_W + H_E] = 0$.

As the changes in the switch are trivial [see Eq. (214)], one may henceforth focus only on SWE and its corresponding map. That is, the switch is in practice no longer necessary. We therefore now turn to the battery W . Instead of using a discrete battery, *Alhambra et al.* (2016) discussed the use of a continuous degree of freedom. That is, the battery is assumed to be described by an operator \hat{x}_W having continuous spectra (exactly like the position operator) $\hat{x}_W = \int dx x |x\rangle\langle x|_W$. This is intended to mimic a classical weight, which can be pulled up and down continuously. A similar approach is used in the resource theory of coherence (*Åberg, 2014*). The Hamiltonian of the system is then taken to be $H_W = \epsilon \hat{x}$, where ϵ is simply a scaling factor. For simplicity, we henceforth set $\epsilon = 1$, thus making \hat{x}_W have units of energy instead of position.

An immediate critique for such a Hamiltonian is that its spectrum is not lower bounded. This, however, is usually not an issue: while most of the time the ground-state energy is not involved, when it is one can always consider a regularized version of H_W . For instance, one can instead picture H_W as a displaced harmonic oscillator, but with a large mass and small frequency. The large mass makes inertial effects irrelevant and the small frequency represents a loose trap, which has virtually no influence in the system. The spectrum of a displaced oscillator, however, is always lower bounded.

Since the weight of the Hamiltonian is proportional to \hat{x}_W , displacements of the weight are generated by the corresponding conjugated momentum \hat{p}_W (defined such that

$[\hat{x}_W, \hat{p}_W] = i$). Based on this, [Alhambra et al. \(2016\)](#) postulated that, in addition to Eq. (216), the unitary U_{SWE} should also be constrained to satisfy

$$[U_{SWE}, \hat{p}_W] = 0. \quad (217)$$

Physically, this implies translation invariance for the weight: Pulling the weight before the process does not affect the dynamics. Under the constraints in Eqs. (216) and (217), the family of unitaries U_{SWE} is drastically simplified, as shown in the following lemma ([Åberg, 2014](#); [Alhambra et al., 2016](#)).

Lemma 4.—A unitary U_{SWE} satisfying Eqs. (216) and (217) can always be parametrized as

$$U_{SWE} = e^{i(H'_S + H_E)\hat{p}_W} V_{SE} e^{-i(H_S + H_E)\hat{p}_W}, \quad (218)$$

where V_{SE} is an arbitrary unitary acting only on SE .

It is important to note that the remaining unitary V_{SE} is now completely arbitrary; that is, it does not have to comply with any energy conservation requirements. In other words, V_{SE} may perform an arbitrary amount of work on SE because now this is appropriately stored in the weight W . This therefore represents a significant improvement in flexibility.

Using the representation $\hat{p}_W = \int dp p |p\rangle \langle p|_W$, we can also write

$$U_{SWE} = \int dp A_{SE}(p) |p\rangle \langle p|_W, \quad (219)$$

where

$$A_{SE}(p) = e^{i(H'_S + H_E)p} V_{SE} e^{-i(H_S + H_E)p} \quad (220)$$

are a family of unitaries parametrized by p (note how both H_S and H'_S appear in this expression). We now assume that the initial state of SWE is of the form $\rho_{SE} \otimes \rho_W$. We also assume for concreteness that $\rho_W = |\psi\rangle \langle \psi|_W$ is pure. Plugging Eq. (219) into Eq. (215) and tracing over W lead to the map

$$\rho'_{SE} = \int dp A_{SE}(p) \rho_{SE} A_{SE}^\dagger(p) |\langle p|\psi\rangle|^2. \quad (221)$$

At the level of SE , the dynamics is therefore given by a mixture of unitaries, weighted by probabilities $|\langle p|\psi\rangle|^2$ ([Masanes and Oppenheim, 2017](#)). Channels of this type are called unital. A special property of unital maps is that they always increase the entropy of SE . The presence of the weight W therefore causes the dynamics of SE to be unital instead of unitary, introducing additional noise on SE .

To proceed, we consider a slightly simpler scenario. First, note that, since V_{SE} is arbitrary, the distinction between S and E becomes somewhat arbitrary. One may therefore label SE as a new system. Or, put differently, Eq. (221) also holds when there is no environment present, in which case it can be written more explicitly as

$$\rho'_S = \int dp e^{iH'_S p} V_S e^{-iH_S p} \rho_S e^{iH_S p} V_S^\dagger e^{-iH'_S p} |\langle p|\psi\rangle|^2, \quad (222)$$

where we used Eq. (220). This is now the exact usual Jarzynski-Crooks scenario: a system S , prepared in ρ_S ,

undergoes a work protocol characterized by a unitary V_S and a change in the system Hamiltonian from H_S to H'_S . To make this connection even stronger, we also assume that $\rho_S = e^{-\beta H_S} / Z_S$. Equation (222) then simplifies further to

$$\rho'_S = \int dp e^{iH'_S p} V_S \rho_S V_S^\dagger e^{-iH'_S p} |\langle p|\psi\rangle|^2. \quad (223)$$

We now introduce the eigendecompositions $H_S = \sum_n E_n |n\rangle \langle n|$ and $H'_S = \sum_m E'_m |m\rangle \langle m|$, where in general the bases $\{|n\rangle\}$ and $\{|m\rangle\}$ need not be the same. The evolution of the diagonal entries $p'_m = \langle m|\rho'_S|m\rangle$ is then found to be

$$p'_m = \sum_n |\langle m|V_S|n\rangle|^2 p_n, \quad (224)$$

where $p_n = \langle n|\rho_S|n\rangle = e^{-\beta E_n} / Z$. This is thus independent of the weight and also exactly as one would intuitively hope. For the off diagonals, however, one finds that

$$\langle m_1|\rho'_S|m_2\rangle = \langle m_1|V_S \rho_S V_S^\dagger|m_2\rangle \int dp e^{i(E_{m_1} - E_{m_2})p} |\langle p|\psi\rangle|^2. \quad (225)$$

The “pure” evolution $V_S \rho_S V_S^\dagger$ is thus dephased by an amount that depends on the initial state $|\psi\rangle$ of the weight and the energy differences $E'_{m_1} - E'_{m_2}$.

For concreteness, we take as an example a Gaussian wave function $|\psi\rangle = \int dx \psi(x) |x\rangle$, with

$$\psi(x) = e^{-x^2/4\delta^2} / (2\pi\delta^2)^{1/4}, \quad (226)$$

where δ measures how localized $\psi(x)$ is in position space. The integral in Eq. (225) can be carried out exactly, leading to

$$\langle m_1|\rho'_S|m_2\rangle = \langle m_1|V_S \rho_S V_S^\dagger|m_2\rangle e^{-(E'_{m_1} - E'_{m_2})^2/8\delta^2}. \quad (227)$$

If $\delta \rightarrow 0$, the exponential makes all terms in the right-hand side vanish, except those where $E'_{m_1} = E'_{m_2}$. As a consequence, the dynamics takes ρ_S to $\Delta_{H'_S}(V_S \rho_S V_S^\dagger)$, where $\Delta_{H'_S}$ is the full dephasing operator in the eigenbasis of H'_S , i.e., the operator that makes $V_S \rho_S V_S^\dagger$ block diagonal. It is also important to bear in mind that $\delta \rightarrow 0$ corresponds to an ideal weight since this is the scenario where the “pointer” of the weight is perfectly localized at $x = 0$.

Conversely, when $\delta \rightarrow \infty$ the exponential in Eq. (227) vanishes, leading to $\rho'_S = V_S \rho_S V_S^\dagger$. In this limit the evolution of the system is therefore completely unaffected by the weight. However, the weight itself is now useless since it is initially spread around all positions x , so there is no way of knowing how much work was extracted. This type of scenario appears in voltage-biased Josephson junctions ([Lörch et al., 2018](#)).

It is therefore interesting to note that, as far as the diagonal entries are concerned, the initial state of the weight has no effect on the dynamics. Conversely, for the coherences there is a trade-off between dephasing and the precision with which one can use the weight to extract work. This is ultimately a consequence of the fact that the weight is performing a von

Neumann measurement on the system and therefore decoheres it in a preferred basis (Zurek, 1981).

Finally, if the initial state ρ_S of the system is not diagonal, similar conclusions also hold. In this case Eq. (222) becomes, componentwise,

$$\begin{aligned} \langle m_1 | \rho'_S | m_2 \rangle &= \sum_{n_1, n_2} \langle m_1 | V_S | n_1 \rangle \langle n_1 | \rho_S | n_2 \rangle \langle n_2 | V_S^\dagger | m_2 \rangle \\ &\times e^{-(E'_{m_1} - E'_{m_2} - E_{n_1} + E_{n_2})^2 / 8\delta^2}. \end{aligned} \quad (228)$$

The effect of the weight will be invisible only to those states for which $E'_{m_1} - E'_{m_2} = E_{n_1} - E_{n_2}$.

E. Reconciliation with the stochastic approach

We are now in the position to use the framework of Sec. VI.D to define work at the stochastic level. This will serve to reconcile the resource theory approach with the usual work statistics in the Jarzynski-Crooks scenario. We discuss this reconciliation using two complementary approaches, one based on the distribution of work (Alhambra *et al.*, 2016) and the other on the cumulant generating function (Guarnieri, Ng *et al.*, 2019).

The scenario is still the same as in Sec. VI.D. We take ρ_S to initially be thermal and consider a two-point measurement scheme. The system is first measured in the basis $|n\rangle$ and the weight is prepared in $|\psi\rangle$. One then applies the unitary $U_{SW} = e^{iH'_S \hat{p}_W} V_S e^{-iH_S \hat{p}_W}$ [Eq. (218)] and, finally, measures the system in the new energy basis $|m\rangle$ and the weight in the position basis $|x\rangle$. The reason for measuring W in $|x\rangle$ is because the weight of the Hamiltonian is $H_W = \hat{x}_W$. The position x therefore directly determines the work stored in the weight. The conditional probability of obtaining (m, x) given that initially the system was in n is then

$$P(m, x|n) = |\langle m, x | U_{SW} | n, \psi \rangle|^2. \quad (229)$$

This is also conditional on $|\psi\rangle$, but we do not write this explicitly, since $|\psi\rangle$ is fixed. Equation (229) can be simplified further using $U_{SW} = e^{iH'_S \hat{p}_W} V_S e^{-iH_S \hat{p}_W}$. In terms of $q(x) = |\psi(x)|^2$, it becomes

$$P(m, x|n) = |\langle m | V_S | n \rangle|^2 q(x + E'_m - E_n). \quad (230)$$

We therefore see that the transition probability factors as a product of a standard transition pertaining only to the system and a term associated with the initial spread of the weight.

The work distribution can now be computed by multiplying Eq. (230) by the initial probability $p_n = e^{-\beta E_n} / Z_S$ and summing over n and m , giving

$$P_F(x) = \sum_{n,m} P(m, x|n) p_n,$$

where the suffix F stands for forward protocol (an identical construction can also be made for the backward case). To match the standard notation, we henceforth write w instead of x , even though in our construction of the weight the two are the same. Substituting Eq. (230) we then arrive at

$$P_F(w) = \sum_{n,m} |\langle m | V_S | n \rangle|^2 p_n q(w + E'_m - E_n). \quad (231)$$

This result can now be directly compared to the following standard expression for the work distribution in a unitary protocol (Talkner, Lutz, and Hänggi, 2007):

$$P_F^{\text{id}}(w) = \sum_{n,m} |\langle m | V_S | n \rangle|^2 p_n \delta(w + E'_m - E_n). \quad (232)$$

We see that the only difference is that the delta function is replaced by the probability distribution q of the initial state of the weight. In fact, the two distributions are related by the convolution

$$P_F(w) = \int dw' P_F^{\text{id}}(w') q(w - w'). \quad (233)$$

These results illustrate some of the fundamental limitations of thermodynamics in the quantum regime. By internalizing the work storage device, one pays the price of obtaining a noisy work distribution, where the outcomes $P_F^{\text{id}}(w)$ are convoluted with the noise $q(w)$ stemming from the initial state of the battery. Thus, while P_F^{id} satisfies a Crooks fluctuation theorem (Crooks, 1998), the same is not true for P_F .

To take an example, again consider the Gaussian wave function in Eq. (226). In this case $q(x) = e^{-x/2\delta^2} / \sqrt{2\pi\delta^2}$, which approximates a delta function when δ is small. But what enters Eq. (231) is $q(w + E'_m - E_n)$. Thus, we reach the conclusion that, in order for the weight to faithfully capture the work statistics, the value of δ must be much smaller than the typical energy spacings $E'_m - E_n$ entering the process. This makes intuitive sense: the precision of the weight must be compatible with the typical energetic transitions entering the process.

These results help us to gain intuition into the resource-theoretic formulation of the weight as an explicit part of the composite system. They also show us how to reconcile the resource theory and stochastic approaches. Note, however, that the results summarized by Eq. (221) cover a much broader set of scenarios since they encompass (i) the presence of a bath, (ii) arbitrary initial system + bath states, and (iii) arbitrary unitaries V_{SE} . This framework thus also covers joint fluctuation theorems for heat and work, as well as quantum coherent and correlated scenarios, where the two-point measurement scheme becomes invasive.

Another way of reconciling the resource-theoretic and stochastic approaches is by means of the cumulant generating function (Guarnieri, Ng *et al.*, 2019); We again consider a closed system (no bath) undergoing a work protocol. The cumulant generating function associated with the ideal work distribution (232) is defined as

$$\Phi_\eta \equiv \ln \langle e^{-\eta W} \rangle = \ln \int P_F^{\text{id}}(W) e^{-\eta W} dW. \quad (234)$$

The m th cumulant of $P_F^{\text{id}}(W)$ is then found from $(-1)^m (\partial^m / \partial \eta^m) \Phi_\eta |_{\eta=0}$. Following lines akin to those presented in Sec. IV.A [see Eq. (85)], one can use Hölder's

inequality to obtain a family of lower bounds for the average work (first cumulant), which read

$$\beta\langle W \rangle \geq -\frac{\beta}{\eta}\Phi_\eta, \quad \eta \geq 0, \quad (235)$$

and

$$\beta\langle W \rangle \leq \frac{\beta}{|\eta|}\Phi_\eta, \quad \eta \leq 0. \quad (236)$$

We now connect this family of bounds to the notions of work extraction and work of formation. To this end, we assume that $\rho_S = \rho_S^{\text{th}} = e^{-\beta H_S}/Z_S$. The scenario will thus be akin to that of the work of formation since we want to form the final state $\rho'_S = V_S \rho_S V_S^\dagger$ from an initially thermal state. There is one difference, though, which is that here we are also changing the Hamiltonian from H_S to H'_S during the process.

Using Eq. (232) we may write Φ_η as (Esposito, Harbola, and Mukamel, 2009)

$$\Phi_\eta = \ln \text{tr}_S [e^{-(\eta/2)H'_S} V_S e^{(\eta/2)H_S} \rho_S e^{(\eta/2)H_S} V_S^\dagger e^{-(\eta/2)H'_S}]. \quad (237)$$

Defining also $\rho_S^{\prime\text{th}} = e^{-\beta H'_S}/Z'_S$ as the thermal state at the final Hamiltonian H'_S , one may show that Φ_η can be written as

$$\Phi_\eta = -\frac{\eta}{\beta} S_{1-\eta/\beta}(\rho'_S \| \rho_S^{\prime\text{th}}) - \eta \Delta F, \quad (238)$$

where $\Delta F = -T \ln Z'_S/Z_S$ is the difference in equilibrium free energies. The cumulant generating function is thus directly associated with the Rényi divergences [Eq. (201)], which are the central objects in the resource theory of thermodynamics (recall the discussion in Sec. III.F).

VII. APPLICATIONS

A. The SWAP engine

One of the prime applications of entropy production is in the description of quantum heat engines. Four-stroke engines are reviewed in Sec. VII.B. Here we begin by describing a particularly simple model called the SWAP engine (Allahverdyan, Hovhannisyan, and Mahler, 2010; Campisi, 2014; Uzdin and Kosloff, 2014; Campisi, Pekola, and Fazio, 2015). The basic idea is summarized in Fig. 6. The working fluid comprises two nonresonant qubits, with energy gaps ϵ_a and ϵ_b . The machine operates in two strokes, as depicted in Fig. 6(a). In the first stroke each qubit interacts with its own environment, kept at temperatures T_a and T_b , respectively. During this stroke the qubits do not interact. Moreover, it is assumed that this step is a thermal operation so that the change in energy of each qubit is entirely associated with the heat that flows to each bath (Sec. III.D). In the second stroke, the baths are uncoupled and the qubits are put to interact by means of a partial SWAP. No heat is involved. However, since the qubits are not resonant, the partial SWAP will have an associated work cost.

In the simplest case, one can assume that the thermalization in the first stroke is complete and that the SWAP in the second stroke is full. Since thermalization is complete, after the first stroke the state of the system will be $\rho_A^{\text{th}} \otimes \rho_B^{\text{th}}$. The partial SWAP then changes this to $\rho_B^{\text{th}} \otimes \rho_A^{\text{th}}$. The work associated with this process is the total change in energy of both qubits $W = \Delta H_a + \Delta H_b$, which can be written as

$$W = -(\epsilon_a - \epsilon_b)(f_a - f_b), \quad (239)$$

where $f_i = (e^{\beta_i \epsilon_i} + 1)^{-1}$ is the probability of finding each qubit in the excited state (the Fermi-Dirac function). The swapped state $\rho_B^{\text{th}} \otimes \rho_A^{\text{th}}$ is then made to interact with the baths at temperatures T_a and T_b , causing the system to go back to

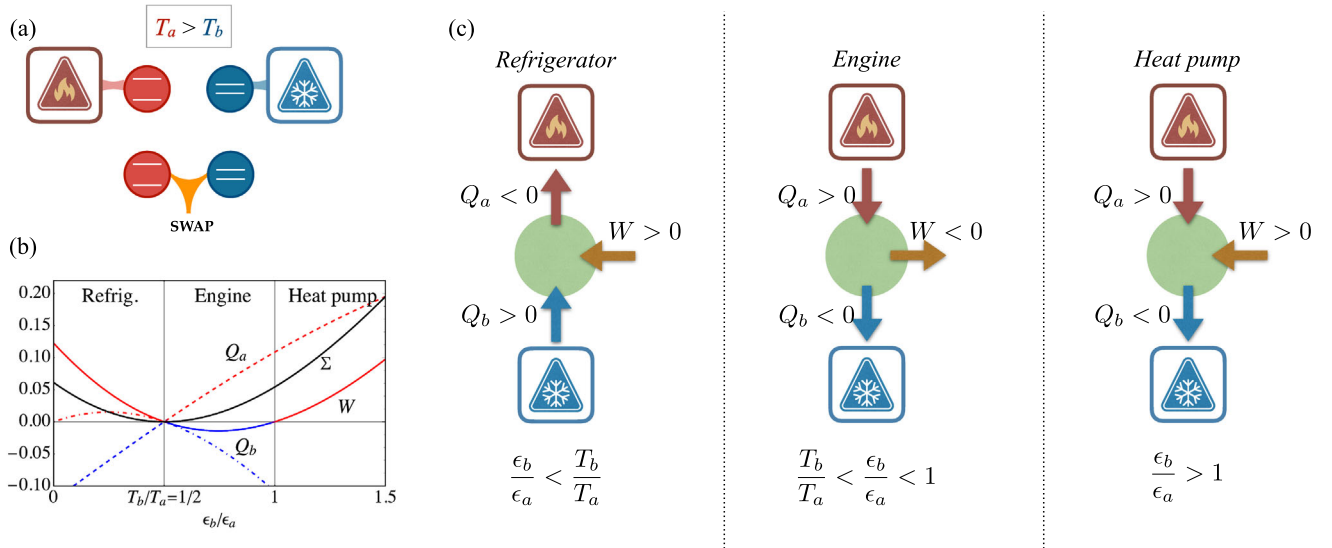


FIG. 6. (a) The two strokes of a SWAP engine. (b) Average thermodynamic quantities and entropy production as a function of ϵ_b/ϵ_a for $T_b/T_a = 1/2$. All energetic quantities are plotted in units of $\epsilon_a = 1$. (c) Operation regimes of the SWAP engine.

the original state $\rho_A^{\text{th}} \otimes \rho_B^{\text{th}}$. The heat exchanged with each bath in this case will then be

$$Q_a = \epsilon_a(f_a - f_b), \quad (240)$$

$$Q_b = \epsilon_b(f_b - f_a). \quad (241)$$

Since the process is cyclic, one can verify that $W + Q_a + Q_b = 0$.

The values of W , Q_a , and Q_b are plotted in Fig. 6(b). We define heat and work as positive when energy enters the system. Depending on the relation between ϵ_b/ϵ_a and T_b/T_a , the engine can offer three regimes of operation: refrigerator, engine, and accelerator. The meaning of the different regimes is diagrammatically explained in Fig. 6(c).

Since the thermalization strokes are thermal operations, the entropy produced in each cycle will be simply given by Eq. (4), with $\Delta S_S = 0$, as

$$\Sigma = -\beta_a Q_a - \beta_b Q_b = -(\beta_a \epsilon_a - \beta_b \epsilon_b)(f_a - f_b). \quad (242)$$

Equation (242) is always non-negative since it has the form $-(x-y)[f(x)-f(y)]$, where $f(x) = (e^x + 1)^{-1}$ is monotonically decreasing in x . As a consequence $f(x) - f(y)$ will always have the opposite sign of $x - y$ for any x and y . Hence, $\Sigma \geq 0$. Equation (242) is plotted in black in Fig. 6(b).

Taking $T_a > T_b$, for concreteness we can characterize the efficiency of the engine in each operating regime by (Callen, 1985)

$$\text{COP} = \frac{|Q_b|}{W} = \frac{\epsilon_b}{\epsilon_a - \epsilon_b}, \quad \frac{\epsilon_b}{\epsilon_a} < \frac{T_b}{T_a}, \quad (243)$$

$$\eta = \frac{|W|}{Q_a} = 1 - \frac{\epsilon_b}{\epsilon_a}, \quad \frac{T_b}{T_a} < \frac{\epsilon_b}{\epsilon_a} < 1, \quad (244)$$

$$\text{COP}_h = \frac{Q_a}{W} = \frac{\epsilon_a}{\epsilon_b - \epsilon_a}, \quad \frac{\epsilon_b}{\epsilon_a} > 1, \quad (245)$$

where COP stands for coefficient of performance. The machine thus always operates at Otto efficiency. As Molitor and Landi (2020) recently showed, there is an entire class of two-stroke engines for which this turns out to be the case.

The Carnot point corresponds to $\epsilon_b/\epsilon_a = T_b/T_a$. This point is special because, even though we get $\Sigma = 0$, we also get $Q_a = Q_b = W = 0$. Thus, at the Carnot point nothing happens; see Fig. 6(b). Another special point is at $\epsilon_b = \epsilon_a$, where $W = 0$ but $Q_a = -Q_b \neq 0$. At this point all heat that flows from the hot bath is converted into heat for the cold bath, so that no net output work occurs.

For $\epsilon_b/\epsilon_a > 1$ heat continues to flow from hot to cold and, in addition, one also has to provide a finite work input ($W > 0$). This regime is called an accelerator. In the refrigerator regime, work is consumed to make heat flow from cold to hot. In an accelerator, work is consumed to make heat flow from hot to cold, but ‘‘faster.’’ From a thermodynamical point of view accelerators are interesting because their performance is directly related to the existence of an excess entropy

production, which turns out to have a clear interpretation. The following argument is general and not restricted to the SWAP engine. We begin by substituting $Q_b = -W - Q_a$ into Eq. (4) for the entropy production, which yields $\Sigma = (\beta_b - \beta_a)Q_a + \beta_b W$. In an accelerator $Q_a > 0$ and $W > 0$. Hence, there is a minimum entropy production associated with it, which is when $W = 0$, which reads $\Sigma_{\min} = (\beta_b - \beta_a)Q_a$. This is thus the entropy production associated with the natural flow of heat from hot to cold. The coefficient of performance of the accelerator is defined as the amount of heat that can be extracted from the hot bath divided by the associated work cost ($\text{COP}_h = Q_a/W$) as in Eq. (245). With some rearrangement, we can write this as

$$\text{COP}_h = \frac{\beta_b Q_a}{\Sigma - \Sigma_{\min}}. \quad (246)$$

Thus, we see that the efficiency of an accelerator actually depends on the excess entropy production $\Sigma - \Sigma_{\min}$, which represents the extra irreversibility introduced by the additional work used to pump the heat.

B. Stroke-based engines

We now turn to a description of more general, four-stroke engines. We focus on how to apply the framework of Sec. III, and, in particular, the basic *SE* map in Eq. (28), to this specific problem. We consider a four-stroke engine, where unitary (work only) maps in the system are riffled between dissipative interactions with a hot and a cold bath (which may involve both heat and work). The corresponding circuit diagram is depicted in Fig. 7.

We consider the engine’s operation in a collisional model sense (Sec. V.A). The system is initially prepared in an arbitrary state ρ_S . In each stroke, it interacts with two baths *H* and *C* prepared in states ρ_H and ρ_C . For ease of mind, we imagine that these represent a hot and cold bath, respectively. The following results, however, are actually true for any bath state, not just a thermal one. Each cycle of the engine is divided into four strokes, as follows. The first and third strokes involve unitary interactions V_1 and V_3 acting only on the system. The second stroke refers to the interaction with the hot bath by means of a unitary U_{SH} . Similarly, the fourth stroke is between *S* and *C*, with a unitary U_{SC} . The global state of *SHC* after each stroke will then be given by

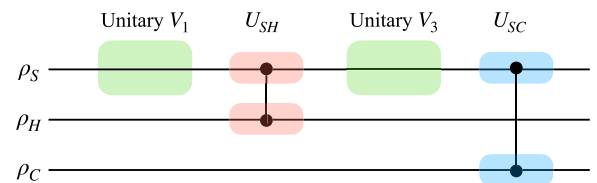


FIG. 7. Circuit diagram of a four-stroke heat engine composed of two unitaries V_1 and V_3 interlaced with two dissipative interactions with a hot and a cold bath, respectively.

$$\begin{aligned}
 \rho_{SHC}^{(1)} &= [V_1 \rho_S V_1^\dagger] \rho_H \rho_C = \rho_S^{(1)} \rho_H \rho_C, \\
 \rho_{SHC}^{(2)} &= U_{SH} [\rho_S^{(1)} \rho_H] U_{SH}^\dagger \rho_C = \rho_{SH}^{(2)} \rho_C, \\
 \rho_{SHC}^{(3)} &= [V_3 \rho_{SH}^{(2)} V_3^\dagger] \rho_C = \rho_{SH}^{(3)} \rho_C, \\
 \rho_{SHC}^{(4)} &= U_{SC} \rho_{SH}^{(3)} \rho_C U_{SC}^\dagger,
 \end{aligned} \tag{247}$$

where care was taken in highlighting at each step which Hilbert spaces the unitaries act in and what the structure of the resulting state is. Combining all strokes, the state at the end of the cycle will thus be

$$\rho_{SHC}^{(4)} = U_{SC} V_3 U_{SH} V_1 (\rho_S \rho_H \rho_C) V_1^\dagger U_{SH}^\dagger V_3^\dagger U_{SC}^\dagger. \tag{248}$$

Notice that all unitaries have a common support on S and therefore in general do not commute. Tracing over H and C leads to the following stroboscopic map for the system:

$$\rho_S' := \Phi(\rho_S) = \text{tr}_{HC} \{ U_{SC} V_3 U_{SH} V_1 (\rho_S \rho_H \rho_C) V_1^\dagger U_{SH}^\dagger V_3^\dagger U_{SC}^\dagger \}. \tag{249}$$

This state is then to be used as input state for the next cycle, which is constructed with fresh new baths ρ_H and ρ_C .

Proceeding in this way, one can construct finite-time engines operating under arbitrary conditions. The state of the system after each complete cycle is obtained from the previous one by applying the map Φ . After many cycles are performed, the system will usually reach a limit cycle ρ_S^* satisfying $\rho_S^* = \Phi(\rho_S^*)$. Once the limit cycle is reached, the engine's operation becomes periodic and any function of state, which may include the system energy or entropy, no longer changes. The limit cycle shares many similarities with NESSs. In fact, the limit cycle can be viewed as a stroboscopic NESS, in the sense that if viewed only at integer steps the system no longer changes. Internally, however (i.e., inside each cycle), its state is constantly changing.

The entropy production in each stroke is given by the general expression (30). The first and third strokes are unitary and no entropy is produced. Thus, $\Sigma = \Sigma_H + \Sigma_C$, which can be further split into

$$\Sigma = \mathcal{I}_{\rho_{SH}^{(2)}}(S:H) + S(\rho_H^{(2)} \parallel \rho_H) + \mathcal{I}_{\rho_{SC}^{(4)}}(S:C) + S(\rho_C^{(4)} \parallel \rho_C). \tag{250}$$

Equation (250) is useful if one is interested in analyzing the individual contributions of the mutual information and entropies relative to the total entropy production. Instead, if one is interested only in Σ itself, it is simpler to use Eq. (34) to express it in terms of the entropy flux Φ , which in this case becomes

$$\Sigma = \Delta S_S + \Phi_H + \Phi_C, \tag{251}$$

where $\Delta S_S = S(\rho_S^{(4)}) - S(\rho_S)$ is the net change in entropy of the system in a full cycle and

$$\Phi_i = \text{tr}_i \{ (\rho_i - \rho_i') \ln \rho_i \}, \quad i = H, C, \tag{252}$$

is the entropy flux to baths H and C , with ρ_i' denoting the state of the bath after it interacts with the system.

Equation (251) shows that the familiar structure for the entropy production, in terms of changes in entropy of the system and fluxes to the bath, also holds quite generally for any stroke-based engine with the structure of Fig. 7. What is important to realize is that this also includes arbitrary initial states for the environments that are not necessarily thermal. In fact, note that no mention has to be made of heat and work or the associated conundrums. Equation (250) or (251) thus provides a fully information-theoretic definition of irreversibility for a cyclic engine. If the bath happens to be thermal, then Eq. (251) reduces to the familiar result $\Sigma = \Delta S_S + \beta_H Q_H + \beta_C Q_C$.

In the limit cycle the first term in Eq. (251) vanishes and we are left only with $\Sigma = \Phi_H + \Phi_C$. It is crucial, however, to notice that this does not imply $\Sigma_H = \Phi_H$ and $\Sigma_C = \Phi_C$. This would in fact be inconsistent, as one of the two fluxes is in general negative. The net entropy production rate Σ coincides in the limit cycle with the net flux $\Phi_H + \Phi_C$. But individually they do not. The individual contributions Σ_H and Σ_C are interesting, as they quantify the contribution of each dissipation channel to the system's irreversibility. But the only way to assess them is through Eq. (250).

C. Squeezed baths

In this section we discuss the thermodynamics of squeezed reservoirs. These types of baths can be used, for instance, as a resource to operate heat engines above Carnot efficiency, as discussed theoretically by [Abah and Lutz \(2014\)](#) and [Roßnagel et al. \(2014\)](#) and as implemented experimentally by [Klaers et al. \(2017\)](#). Here we focus on how to formulate the entropy production for this problem, which was first put forth by [Manzano et al. \(2016\)](#).

We begin by reviewing the basics of squeezing. Consider a single bosonic mode b with Hamiltonian $H = \Omega(b^\dagger b + 1/2)$. We say b is prepared in a squeezed thermal state when its density matrix has the form

$$\rho = S(z) \rho_{\text{th}} S^\dagger(z), \tag{253}$$

where $\rho_{\text{th}} = e^{-\beta H} / Z$ is the thermal state and

$$S(z) = e^{(1/2)(z^* b^2 - z b^{\dagger 2})}, \quad z = r e^{i\theta}, \tag{254}$$

is the squeezing operator, with complex parameter z . The action of $S(z)$ on annihilation operators is given by

$$S(z) b S^\dagger(z) = b \cosh(r) + e^{i\theta} b^\dagger \sinh(r). \tag{255}$$

From this, one may readily compute the expectation values of the second moments in the state of Eq. (253) as

$$\langle b^\dagger b \rangle + 1/2 = (\bar{n} + 1/2) \cosh(2r), \tag{256}$$

$$\langle bb \rangle = (\bar{n} + 1/2) e^{i\theta} \sinh(2r), \tag{257}$$

where $\bar{n} = e^{\beta\Omega} - 1$ is the Bose-Einstein distribution related to the thermal part of Eq. (253). In terms of quadratures

$q = (b + b^\dagger)/\sqrt{2}$ and $p = i(b^\dagger - b)/\sqrt{2}$, if $\theta = 0$ we get $\langle q^2 \rangle = e^{2r}(\bar{n} + 1/2)$ and $\langle p^2 \rangle = e^{-2r}(\bar{n} + 1/2)$, so the variance of q is stretched by e^{2r} , while that of p is squeezed by e^{-2r} . When $\theta \neq 0$ something analogous happens, but in a different direction of the (q, p) plane.

From a thermodynamic perspective, the squeezed state in Eq. (253) can be viewed as a generalized Gibbs ensemble (GGE) akin to the grand-canonical state $e^{-\beta(H-\mu\hat{N})}$ (where μ is the chemical potential and \hat{N} is the particle number operator). This can be made more transparent by noting that, from Eq. (255), one has $S(z)HS^\dagger(z) = \cosh(2r)H + \sinh(2r)A$, where $A = \Omega(e^{i\theta}b^{\dagger 2} + e^{-i\theta}b^2)/2$ is what we henceforth refer to as asymmetry (Manzano *et al.*, 2016) (in the sense that $\langle A \rangle$ measures how asymmetric, or compressed, the compressed Gaussian in phase space is). Equation (253) can then be written in the GGE form

$$\rho = \frac{1}{Z} e^{-\beta[\cosh(2r)H + \sinh(2r)A]}. \quad (258)$$

There is, though, one fundamental difference with respect to the usual grand-canonical state, namely, that, unlike H and \hat{N} , the operators H and A do not commute. GGEs of this form are called non-Abelian (Manzano, Parrondo, and Landi, 2020).

We now use the results developed in Sec. III to formulate the entropy production of a system interacting with a squeezed thermal bath. We do so using the standard von Neumann entropy. This therefore represents an alternative to the phase-space approach discussed in Sec. V.H. The system is assumed to be arbitrary (it does not have to be bosonic) and the bath is taken to be a collection of bosonic modes b_k , with Hamiltonian $H_E = \sum_k \Omega_k (b_k^\dagger b_k + 1/2)$ and prepared in a squeezed thermal state of the form (253), viz.,

$$\rho_E = \prod_k \rho_k = \prod_k S_k(z_k) \rho_k^{\text{th}} S_k^\dagger(z_k), \quad (259)$$

where $\rho_k^{\text{th}} = (1 - e^{-\beta\Omega_k}) e^{-\beta\Omega_k b_k^\dagger b_k}$ is the thermal state and $S_k(z_k)$ is the squeezing operator (254) for mode b_k , with parameter $z_k = r_k e^{i\theta_k}$. For now we allow each r_k to be different.

The system and bath are then put to interact via an arbitrary unitary U , according to the map (28). The entropy produced in the process is given by Eq. (36). This can be simplified by inserting Eq. (258) for $\ln \rho_E$, leading to

$$\begin{aligned} \Sigma = \Delta S_S + \beta \sum_k \left\{ \Omega_k \cosh(2r_k) \Delta \langle b_k^\dagger b_k \rangle \right. \\ \left. + \frac{\Omega_k}{2} \sinh(2r_k) (\Delta \langle b_k^\dagger b_k^\dagger \rangle e^{i\theta_k} + \Delta \langle b_k b_k \rangle e^{-i\theta_k}) \right\}, \quad (260) \end{aligned}$$

where $\Delta \langle \mathcal{O}_E \rangle = \text{tr} \{ \mathcal{O}_E (\rho'_E - \rho_E) \}$ is the change in the expectation value of a bath observable during the process. It is essential to note that, in line with what was discussed in Sec. III, all terms except the first actually refer to changes in quantities of the bath, not the system. For this reason, the entropy production cannot in general be computed solely from

knowledge of the changes that take place in S (as we discuss later).

Since the bath is not thermal, Eq. (260) cannot be written in the Clausius form $\Sigma = \Delta S_S + \beta \Delta Q_E$. We assume for concreteness that all modes are squeezed by the same amount: $r_k = r$ and $\theta_k = \theta$. The second term in Eq. (260) then becomes proportional to the heat flux ($\Delta Q_E = \sum_k \Omega_k \Delta \langle b_k^\dagger b_k \rangle$). Moreover, the last term becomes proportional to the change in asymmetry as follows:

$$\Delta A_E = \sum_k \frac{\Omega_k}{2} (e^{i\theta} \Delta \langle b_k^\dagger b_k^\dagger \rangle + e^{-i\theta} \Delta \langle b_k b_k \rangle). \quad (261)$$

Equation (260) thus becomes

$$\Sigma = \Delta S_S + \beta [\cosh(2r) \Delta Q_E + \sinh(2r) \Delta A_E]. \quad (262)$$

Equation (262) resembles the entropy produced during an interaction with a grand-canonical bath. The last two terms represent the changes in the corresponding thermodynamic charges ΔQ_E and ΔA_E , each multiplied by the corresponding thermodynamic affinities $\beta \cosh(2r)$ and $\beta \sinh(2r)$. This matches the previously discussed intuition of the squeezed state as a GGE. For instance, one could have a situation where no heat flows to the bath ($\Delta Q_E = 0$), but entropy is still produced due to a flow of asymmetry.

For generic system Hamiltonians and system-environment interactions, it is not possible to write Eq. (262) solely in terms of system quantities. The situation is entirely analogous to that of strict energy conservation [Eq. (50)]. For a concrete example, suppose that the system is a single bosonic mode described by annihilation operator a and $H_S = \omega a^\dagger a$, while the bath is also comprised of a single mode, with operator b and $H_E = \omega b^\dagger b$ (i.e., resonant with S). As Manzano, Parrondo, and Landi (2020) showed, the only Gaussian unitary that preserves both energy and asymmetry for two modes is of the form

$$U_{SE} = \exp\{gt(a^\dagger b - b^\dagger a)\}. \quad (263)$$

The choice of phase here is crucial. A generic interaction of the form $ga^\dagger b + g^* b^\dagger a$ preserves the number of quanta (and hence the energy since S and E are assumed to be resonant). But in general it does not preserve the asymmetry. Only for the specific choice of phase in Eq. (263) will we have both $[U_{SE}, a^\dagger a + b^\dagger b] = 0$ and $[U_{SE}, aa + bb] \neq 0$. In this case $\Delta Q_E = -\Delta Q_S$ and $\Delta A_E = -\Delta A_S$, so Eq. (262) can be expressed solely in terms of system-related quantities. Alternatively, we can write Σ as in Eq. (47), with ρ_S^* now being the GGE (258), which will be a global fixed point (Sec. III.A) of the map.

Last, we discuss the continuous-time version of this process, where the system evolves instead according to the Lindblad master equation

$$\begin{aligned} \frac{d\rho_S}{dt} = \gamma(N+1)[a\rho_S a^\dagger - \frac{1}{2}\{a^\dagger a, \rho_S\}] + \gamma N[a^\dagger \rho_S a - \frac{1}{2}\{aa^\dagger, \rho_S\}] \\ - \gamma M[a^\dagger \rho_S a^\dagger - \frac{1}{2}\{a^{\dagger 2}, \rho_S\}] - \gamma M^*[a\rho_S a - \frac{1}{2}\{a^2, \rho_S\}]. \quad (264) \end{aligned}$$

Here $\gamma \geq 0$ is the damping rate and $N + 1/2 = (\bar{n} + 1/2) \cosh(2r)$ and $M = (\bar{n} + 1/2) e^{i\theta} \sinh(2r)$ are the parameters imposed by the squeezed thermal bath; see Eqs. (256) and (257). Equation (264) can be derived using the usual Born-Markov-secular approximations (Breuer and Petruccione, 2007) or using a collisional model, exactly as described in Sec. V.C. From knowledge only of the master equation (264), it is not possible to define the entropy production. But if one assumes that the master equation was derived via interactions that are both energy and asymmetry preserving (at least approximately), then we can use a continuous-time version of Eq. (47), i.e.,

$$\dot{\Sigma} = -\frac{d}{dt} S(\rho_S(t) \| \rho_S^*). \quad (265)$$

It was shown by Manzano (2018) that, if the strong fixed-point hypothesis does not hold, Eq. (265) will nonetheless still describe a part of the entropy production, namely, the so-called nonadiabatic component associated with the entropy production needed to reach the stationary state.

D. Quantum heat

We now turn to another application of thermodynamics beyond standard thermal systems. Elouard, Herrera-Martí, Clusel, and Auffèves (2017) considered a generalization of the first and second laws of thermodynamics for a situation where the interaction with a heat bath is replaced by a set of quantum measurements. In its simplest formulation, the process can be described as follows. The system starts in a pure state $|\psi_0\rangle$. At evenly spaced times $n\Delta t$, $n = 0, 1, \dots$, one applies a projective measurement described by an orthonormal basis $\{|k_n\rangle\}$. These sets may be different at different times, which is left implicit in the additional index n in $|k_n\rangle$.

On the other hand, in between jumps from $n\Delta t^+$ to $(n+1)\Delta t^-$ the system evolves unitarily from $|k_n\rangle$ to $|\psi_{n+1}^-\rangle = U_{n+1,n}|k_n\rangle$, where $U_{n+1,n}$ is the unitary generating this evolution. At time $(n+1)\Delta t$ it then undergoes another quantum jump to one of the states $|k_{n+1}\rangle$. The probability associated with this jump is

$$p(k_{n+1}|k_n) = |\langle k_{n+1} | \psi_{n+1}^- \rangle|^2 = |\langle k_{n+1} | U_{n+1,n} | k_n \rangle|^2, \quad (266)$$

which thus depends only on the previous state $|k_n\rangle$. A quantum trajectory for this process up to time $n\Delta t$ is then specified by the set of quantum numbers $\gamma_n = (k_0, \dots, k_n)$. Using Eq. (266), the corresponding path probability reads

$$\mathcal{P}_F[\gamma_n] = p(k_n|k_{n-1})p(k_{n-1}|k_{n-2}) \cdots p(k_1|k_0)p(k_0), \quad (267)$$

where $p(k_0) = |\langle k_0 | \psi_0 \rangle|^2$. If the initial state is an element of $\{|k_0\rangle\}$, then $p(k_0)$ becomes deterministic.

From Eq. (267) one can readily compute the probability of the final state, which reads

$$p(k_n) = \sum_{k_1, \dots, k_{n-1}} \mathcal{P}_F[\gamma_n]. \quad (268)$$

Equation (268) can then be used to define the reverse process, where the system starts in $|k_n\rangle$ with probability $p(k_n)$, then

evolves backward by applying the time-reversed unitaries $U_{n,n+1}^\dagger$. Since $|\langle k_n | U_{n,n+1}^\dagger | k_{n+1} \rangle|^2 = |\langle k_{n+1} | U_{n+1,n} | k_n \rangle|^2 = p(k_{n+1}|k_n)$, the time-reversed path probability becomes

$$\mathcal{P}_B[\gamma] = p(k_1|k_0) \cdots p(k_{n-1}|k_{n-2})p(k_n|k_{n-1})p(k_n). \quad (269)$$

The entropy production is defined as in Eq. (58), which simplifies in this case to

$$\sigma[\gamma_n] = \ln \frac{\mathcal{P}_F[\gamma_n]}{\mathcal{P}_B[\gamma_n]} = \ln \frac{p(k_0)}{p(k_n)} \quad (270)$$

since all conditional terms in \mathcal{P}_F and \mathcal{P}_B cancel out.

The two terms in Eq. (270) are interpreted as follows. The contribution $\ln p(k_n)$ is the entropy production associated with the randomness that is built up by the stochastic jumps caused by the projective measurements. The term $\ln p(k_0)$, on the other hand, is related to the fact that even the first measurement is nondeterministic; this randomness is of purely quantum origin, as it is associated with the fact that $|\psi_0\rangle$ has some finite coherence in the basis $\{|k_0\rangle\}$. The exact result, however, could also be obtained if we were to assume that the initial state of the system were an incoherent mixture. Thus, the term $\ln p(k_0)$ refers to the general randomness stemming from the first measurement, irrespective of whether this randomness is classical or quantum.

The stochastic entropy production (270) satisfies a fluctuation theorem by construction. Moreover, averaging it over the forward distribution (267) one finds

$$\langle \sigma[\gamma_n] \rangle = S(p(k_n)) - S(p(k_0)) \geq 0, \quad (271)$$

where $S(p) = -\sum_n p_n \ln p_n$ is the classical Shannon entropy. The positivity of Eq. (271) is actually a subtle feature of projective measurements related to the fact that $p(k_n)$ and $p(k_0)$ are linked through a doubly stochastic matrix (Nielsen and Chuang, 2000). Specifically, from Eqs. (267) and (268), we can write $p(k_n) = \sum_{k_0} \mathcal{M}(k_n, k_0)p(k_0)$, where

$$\mathcal{M}(k_n, k_0) = \sum_{k_1, \dots, k_{n-1}} p(k_n|k_{n-1})p(k_{n-1}|k_{n-2}) \cdots p(k_1|k_0) \quad (272)$$

is doubly stochastic [$\sum_{k_n} \mathcal{M}(k_n, k_0) = \sum_{k_0} \mathcal{M}(k_n, k_0) = 1$]. Owing to the data processing inequality, it then follows that the entropy of $p(k_n)$ is always larger than or equal to that of $p(k_0)$, which thus implies the positivity of the average entropy production in Eq. (271).

Although Eq. (270) provides a consistent definition of entropy production, it is not possible to expect any relation between σ and thermodynamic quantities such as heat and work, which appears in the original Clausius inequality (4) (Mohammady, Auffèves, and Anders, 2020). While notions of heat and work can still be defined (Elouard, Herrera-Martí, Clusel, and Auffèves, 2017) since the states in question are never thermal in shape, entropy production and heat have no straightforward relation to each other. We also mention that such notions of heat and work do not take into account the energy cost itself of performing a projective measurement,

something that has recently been put under scrutiny (Guryanova, Friis, and Huber, 2020).

E. Infinitesimal quenches

We continue here our review of the nonequilibrium lag, which was first discussed in Sec. III.F. But now we focus on the specific scenario of infinitesimal quenches. All ideas and notations are the same as in Sec. III.F. One of the difficulties in characterizing the nonequilibrium lag is its dependence on the form of the work protocol $H(\lambda(t))$. Or, equivalently, the form of the unitary V in Fig. 2. This can be simplified by considering quantum quenches (Fusco *et al.*, 2014). That is, one assumes that the protocol taking $H_i \rightarrow H_f$ is much faster than the typical timescales of the system, so the evolution can be taken as instantaneous. This therefore amounts to setting $V \simeq 1$ so that the final state coincides with the initial one ($\rho' = \rho_i^{\text{th}}$). The basic idea is therefore that the changes in the Hamiltonian are so fast that the system has no time to respond, so even though $H_i \rightarrow H_f$ the system stays frozen at ρ_i^{th} . After the quench, many things can happen. If the system is isolated, it will evolve according to the new Hamiltonian H_f (Calabrese and Cardy, 2005). And if it is coupled to a bath, it will eventually thermalize, changing from $\rho_i^{\text{th}} \rightarrow \rho_f^{\text{th}}$.

All equations in Sec. III.F are simplified in this case. In particular, Eq. (67) becomes

$$\Sigma = S(\rho_i^{\text{th}} \parallel \rho_f^{\text{th}}), \quad (273)$$

while the CGF (75) transforms to

$$K(\lambda) = (\lambda - 1)S_\lambda(\rho_i^{\text{th}} \parallel \rho_i^{\text{th}}) = -\lambda S_{1-\lambda}(\rho_i^{\text{th}} \parallel \rho_i^{\text{th}}). \quad (274)$$

The two expressions for $K(\lambda)$ coincide due to the properties of the Rényi divergences.

In the quantum quench scenario, the nonequilibrium lag depends only on the initial and final work parameters λ_i and λ_f ; it becomes independent of the specific protocol $\lambda(t)$ taking one to the other. An additional simplification can be obtained for infinitesimal quenches. That is, when $\lambda_i = \lambda$ and $\lambda_f = \lambda + \delta\lambda$, with $\delta\lambda$ taken to be small. In this case Eqs. (273) and (274) can be expanded in a power series in $\delta\lambda$, greatly simplifying the problem.

We start with Eq. (273). It is convenient to write it in terms of the average work and equilibrium free energy [Eq. (68)]. In the quench scenario this becomes

$$\Sigma = \beta \text{tr}\{(H_f - H_i)\rho_i^{\text{th}}\} - \beta \Delta F. \quad (275)$$

We can now series expand each term in powers of $\delta\lambda$. We write $H_i = H(\lambda) \equiv H$ and $H_f = H(\lambda + \delta\lambda)$, leading to $H_f - H_i = (\partial H / \partial \lambda)\delta\lambda + (1/2)(\partial^2 H / \partial \lambda^2)\delta\lambda^2 + \dots$. We expand ΔF in a similar way. From equilibrium statistical mechanics, however, it follows that for thermal states

$$\left\langle \frac{\partial H}{\partial \lambda} \right\rangle = \frac{\partial F}{\partial \lambda}. \quad (276)$$

Hence, the terms of the order of $\delta\lambda$ in Eq. (275) cancel out, meaning that the first nonzero contribution will be of the order of $\delta\lambda^2$ (as it must since $\Sigma \geq 0$):

$$\Sigma = \frac{\beta \delta \lambda^2}{2} \left\{ \left\langle \frac{\partial^2 H}{\partial \lambda^2} \right\rangle - \frac{\partial^2 F}{\partial \lambda^2} \right\}. \quad (277)$$

Note how $\langle W \rangle \sim \delta\lambda$, while $\Sigma \sim \delta\lambda^2$. That is, the first order contribution to the average work is exactly canceled out by the contribution from ΔF .

One can always choose the work protocol such that it appears linearly in the Hamiltonian, that is, such that $H(\lambda) = H_0 + \lambda H_1$. In this case the first term in Eq. (277) vanishes and one is left with the simpler expression

$$\Sigma = -\frac{\beta \delta \lambda^2}{2} \frac{\partial^2 F}{\partial \lambda^2}, \quad (278)$$

which shows that the nonequilibrium lag is simply the thermal susceptibility to λ , a concept widely studied in equilibrium statistical mechanics.

The relation to the susceptibility makes it particularly inviting to study infinitesimal quenches in systems presenting a quantum phase transition as a function of λ . This problem was first studied by Dornier *et al.* (2012), who analyzed the transverse-field Ising model. A quantum phase transition strictly occurs only at $T \rightarrow 0$, while the nonequilibrium lag scenario involves a thermal state at finite temperature. Notwithstanding, reflections of the $T = 0$ critical point can still be felt at low temperatures. This is precisely what was observed by Dornier *et al.* (2012), who found that the entropy production diverges logarithmically at the critical point in the limit $T \rightarrow 0$ (while showing a sharp peak for finite T).

In the ensuing years, there have been several papers dedicated to an understanding of the critical properties of the nonequilibrium lag. An extension to the general XY model was given by Bayocboc and Paraan (2015), and the more exotic XZY - YZX model was studied by Zhong and Tong (2015). Recently a general group-theoretic framework suitable for arbitrary quadratic Hamiltonians was introduced by Fei and Quan (2019), who generalized the previous results. An analysis of the related Lipkin-Meshkov-Glick model (which can be viewed as the long-range analog of the transverse-field Ising model) was given by Campbell (2016). All of these papers referred to continuous transitions. The extension to discontinuous transitions was discussed by Mascarenhas *et al.* (2014). Finally, the extension to consider the full statistics [instead of just the first moment (273)] was recently put forth by Fei *et al.* (2020).

To shed further light on the physics behind Eq. (278), it is necessary to determine whether H_i and H_f commute or, equivalently, whether H and $\partial H / \partial \lambda$ commute (Fusco *et al.*, 2014). The reason why this matters is that differentiating $F = -T \ln \text{tr}(e^{-\beta H(\lambda)})$ with respect to λ is not trivial if H and $\partial H / \partial \lambda$ do not commute. In fact, this can be readily seen from the following Baker-Campbell-Hausdorff expansion, which is applicable to an arbitrary operator $M(\lambda)$:

$$\partial_\lambda e^{M(\lambda)} = \left\{ M' + \frac{1}{2}[M, M'] + \frac{1}{3!}[M, [M, M']] + \dots \right\} e^{M(\lambda)}, \quad (279)$$

where $M' = \partial_\lambda M$. Thus, if H and $\partial_\lambda H$ commute, one can readily write $\partial_\lambda e^{-\beta H} = -\beta(\partial_\lambda H)e^{-\beta H}$. But if they do not one must use Eq. (279) instead, where new terms appear that are associated with the commutator $[M, M']$. Because of the cyclic property of the trace, this effect turns out to be irrelevant when computing the first derivative $\partial F/\partial\lambda$, which is why Eq. (276) is actually always true. But for the second derivative in Eq. (278), this is crucial.

Another way to deal with this is to introduce the following Feynman integral representation:

$$\frac{\partial}{\partial\lambda} e^{-\beta H} = \beta \int_0^1 dy e^{-\beta y H} (\partial H/\partial\lambda) e^{-\beta(1-y)H}. \quad (280)$$

Using Eq. (280) to compute $-\partial^2 F/\partial\lambda^2$, one eventually finds the following result for Eq. (278) (Scandi *et al.*, 2020):

$$\Sigma = \frac{\beta^2}{2} \int_0^1 dy \text{cov}_i^y(\delta H, \delta H), \quad (281)$$

where $\delta H = H_f - H_i = \delta\lambda(\partial H/\partial\lambda)$ and

$$\text{cov}_i^y(A, B) = \text{tr}[A(\rho_i^{\text{th}})^y B(\rho_i^{\text{th}})^{1-y}] - \text{tr}(A\rho_i^{\text{th}})\text{tr}(B\rho_i^{\text{th}}) \quad (282)$$

is the so-called y covariance. Equation (282) represents a generalization of the notion of covariance to the case of noncommuting operators. When $[H, \delta H] = 0$, the y covariance simplifies to the usual covariance. In this case the integral in y can be performed explicitly, leading to

$$\Sigma = \frac{\beta^2}{2} \text{var}(\delta H). \quad (283)$$

Conversely, when $[H, \delta H] \neq 0$, this is no longer true.

This commutativity issue can also be analyzed from the perspective of the probability distribution $P(\sigma)$ defined in Eq. (70). The transition probabilities in the case of quenches simplify to $p(m_f|n_i) = |\langle m_f|n_i \rangle|^2$. If $[H, \delta H] = 0$, they therefore trivialize. But if $[H, \delta H] \neq 0$, one may still find nontrivial transitions.

The relevance of these results lies in their connection with quantum coherence (Miller *et al.*, 2019). The case of $[H, \delta H] = 0$ represents a quench that changes the energy levels of the system but keeps the same eigenbasis. Conversely, $[H, \delta H] \neq 0$ indicates that, in addition to the change in energy, the eigenbasis is also rotated so that ρ_i^{th} will be coherent in the basis of H_f . As a consequence, there will be an additional entropy production associated with the loss of coherence in the thermalization process (Santos *et al.*, 2019).

This can be made more patent by introducing the Wigner-Yanase-Dyson skew information (Hansen, 2008) $I_y(\rho, A) = -(1/2)\text{tr}\{[\rho^y, A][\rho^{1-y}, A]\}$, which quantifies the coherence between A and ρ , in the sense that it gauges the degree with which ρ and A fail to commute. $I_y(\rho, A)$ is always

non-negative and 0 if and only if $[\rho, A] = 0$. In terms of this, one can rewrite Eq. (281) as

$$\Sigma = \frac{\beta^2}{2} \text{var}(\delta H) - \mathcal{Q}, \quad (284)$$

where $\mathcal{Q} = (\beta^2/2) \int_0^1 dy I_y(\rho_i^{\text{th}}, H_f)$ is a new contribution measuring the incompatibility of the final Hamiltonian with the initial state of the system. Compared with Eq. (283), the result in Eq. (284) shows how a lack of commutativity modifies the average entropy production.

The same analysis can also be made for the full CGF (274), as done by Scandi *et al.* (2020). The result is compactly expressed as

$$K(\lambda) = -\frac{\beta^2}{2} \int_0^\lambda dx \int_x^{1-x} dy \text{cov}_i^y(\delta H, \delta H). \quad (285)$$

When $[H, \delta H] = 0$, Eq. (285) reduces to

$$K_{\text{comm}}(\lambda) = -\frac{\beta^2 \lambda(1-\lambda)}{2} \text{var}(\delta H). \quad (286)$$

From Eq. (286), one appreciates that K satisfies the Jarzynski equation $K(\lambda = 1) = \ln\langle e^{-\sigma} \rangle = 0$. In addition, it satisfies the stronger Gallavotti-Cohen symmetry $K(\lambda) = K(1-\lambda)$, which implies that $P(\sigma)$ obeys an exchange fluctuation theorem $P(\sigma)/P(-\sigma) = e^\sigma$, or, put differently, that the probability distribution of the time-reversed process is the same as that of the forward one. This is a consequence of the infinitesimal or slow nature of this process and does not happen for non-infinitesimal quenches.

Since Eq. (286) is quadratic in λ , $P(\sigma)$ must be a Gaussian distribution whose mean is Eq. (283), while the variance reads

$$\text{var}(\sigma) = \beta^2 \text{var}(\delta H). \quad (287)$$

Comparing Eq. (287) to Eq. (283), we arrive at the fluctuation-dissipation theorem (Callen and Welton Theodore, 1951) relating the mean and variance of the entropy production $\langle\sigma\rangle = (1/2)\text{var}(\sigma)$.

When $[H, \delta H] \neq 0$, however, the fluctuation-dissipation relation (FDR) no longer holds. Equation (287) for the variance turns out to remain unchanged, but the mean is modified to Eq. (284), hence the two quantities are now related by

$$\langle\sigma\rangle = \frac{1}{2}\text{var}(\sigma) - \mathcal{Q}. \quad (288)$$

The FDR is therefore broken due to the presence of the coherent term (Miller *et al.*, 2019). We mention in passing that the FDR for general quantum processes was also recently discussed by Mehboudi, Sanpera, and Parrondo (2018), who showed the nontrivial role of the so-called symmetric logarithmic derivative, a concept widely used in quantum metrology.

Returning now to the noncommuting case [Eq. (285)], it is also possible to rewrite the CGF as

$$K(\lambda) = K_{\text{comm}}(\lambda) + \frac{\beta^2}{2} \int_0^\lambda dx \int_x^{1-x} dy I_y(\rho_i^{\text{th}}, H_f).$$

This shows how the presence of coherence makes $P(\sigma)$ non-Gaussian, as the last term makes K nonpolynomial in λ . Another consequence of this result concerns cumulants of the order of 3 or higher. Since K_{comm} is quadratic, it will contribute only to the first two cumulants. All higher order cumulants will therefore come from the second term. In fact, using Leibniz' integral rule together with Eq. (72), one arrives at

$$\kappa_n = -(-1)^n \beta^2 \frac{\partial^{n-2}}{\partial \lambda^{n-2}} I_\lambda(\rho_i^{\text{th}}, H_f), \quad n \geq 3. \quad (289)$$

Using this result, Scandi *et al.* (2020) showed that all higher order cumulants are actually positive ($\kappa_n > 0$ for $n \geq 3$).

The previous discussion refers to a single quench from H_i to H_f . However, this can now be used as a building block to study coherence in more general slow processes. We imagine a process where $H(t)$ is changed slowly, with the system permanently in contact with a heat bath at fixed temperature. Following Nulton *et al.* (1985) and Crooks (1998), we can divide this process into a series of discrete, infinitesimal steps. At each step H changes slightly from H_i to H_{i+1} (the quench). After this quench, the system is allowed to relax back to thermal equilibrium, but now at the new Hamiltonian H_{i+1} . Using this construction, one may build a slow process where the system is in thermal equilibrium throughout but, notwithstanding, the entropy production can still be quantified. In fact, the net entropy production will simply be the sum of the entropy produced in each quench: $\sigma = \sigma_1 + \dots + \sigma_N$. And since the system fully thermalizes at each step, σ_i 's are statistically independent. The full CGF is hence $K_\sigma(\lambda) = \sum_{i=1}^N K_{\sigma_i}(\lambda)$, and the intuition from a single quench directly carries over to a slow (noninfinitesimal) process.

F. Dissipative phase transitions: Basic models

We recall the notion of NESSs discussed in Sec. I; they occur when a system is coupled simultaneously to multiple reservoirs. The hallmark of such states is a finite entropy production rate $\dot{\Sigma}$. In certain situations, NESSs can also present phase transitions. In the classical literature these usually go by the name of “nonequilibrium transitions” and in the quantum literature by the name of “dissipative phase transitions” (for concreteness, we henceforth use the latter). Since NESSs are characterized by a finite $\dot{\Sigma}$, it is therefore only natural to ask how $\dot{\Sigma}$ behaves across a dissipative transition. This is the issue that we explore in this section. For classical systems the situation is somewhat well understood. Conversely, in the quantum case there are dramatically few studies on the topic. Here we will try to discuss both scenarios together. Before discussing the thermodynamics, though, we begin by reviewing some of the prototypical models of dissipative phase transitions, as these may not be as widely known by the community working in stochastic and quantum thermodynamics.

Classically, dissipative phase transitions are usually studied in lattice models described by stochastic thermodynamics. This is well illustrated by the model studied by Tomé and de Oliveira (2012), corresponding to a 2D classical Ising model coupled to two baths at different chemical potentials. One bath couples only to the even sites of the lattice and the other to the odd sites (thus forming a checkerboard pattern). The lattice has a total of N sites, each described by a classical spin variable $\sigma_i = \pm 1$. The configurations of the system are described by the vector $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_N)$, where $\sigma_i = \pm 1$ and the spins interact with the typical nearest-neighbor Ising energy $E = -J \sum_{\langle i, j \rangle} \sigma_i \sigma_j$, where $\langle i, j \rangle$ means a sum over nearest neighbors. The probability distribution $p(\boldsymbol{\sigma})$ is assumed to evolve according to the Pauli equation

$$\frac{dp(\boldsymbol{\sigma})}{dt} = \sum_{i=1}^N \{w_i(\boldsymbol{\sigma}^i) p(\boldsymbol{\sigma}^i) - w_i(\boldsymbol{\sigma}) p(\boldsymbol{\sigma})\}, \quad (290)$$

where $\boldsymbol{\sigma}^i = (\sigma_1, \dots, -\sigma_i, \dots, \sigma_N)$ and $w_i(\boldsymbol{\sigma})$ is the single spin-flip transition rate $\sigma_i \rightarrow -\sigma_i$ at site i , each characterized by a temperature T_i and a chemical potential μ_i . Tomé and de Oliveira (2012) assumed all $T_i = T$ and used an alternating chemical potential pattern of $\mu_i = \mu$ for odd sites and $\mu_i = -\mu$ for even sites.

In the quantum domain, lattice models can be constructed with unusual types of dissipation. This acquires particular relevance in the context of ultracold atoms in optical lattices. For instance, Diehl *et al.* (2008) considered a 2D bosonic lattice, with each site characterized by an annihilation operator a_i and evolving according to the Lindblad master equation

$$\frac{dp}{dt} = -i[H, \rho] + \sum_{\ell} \kappa_{\ell} [L_{\ell} \rho L_{\ell}^{\dagger} - \frac{1}{2} \{L_{\ell}^{\dagger} L_{\ell}, \rho\}], \quad (291)$$

where $H = -J \sum_{\langle i, j \rangle} a_i^{\dagger} a_j + (U/2) \sum_i a_i^{\dagger} a_i^{\dagger} a_i a_i$ is the Bose-Hubbard Hamiltonian. Diehl *et al.* (2008) discussed the nontrivial effects that come about from using jump operators acting on nearest-neighbor sites of the form $L_{\ell} = L_{ij} = (a_i^{\dagger} + a_j^{\dagger})(a_i - a_j)$. These operators do not change the number of particles. Instead, they cause only a phase-sensitive decoherence: the term $a_i - a_j$ annihilates antisymmetric superpositions of the pair (i, j) , whereas $(a_i^{\dagger} + a_j^{\dagger})$ recycles it toward a symmetric state. This dissipator therefore induces phase locking, which is characteristic of Bose-Einstein condensates. It thus represents a novel type of dissipation with a clear quantum signature.

Notwithstanding this bout of interest in lattice systems, it turns out that quantum models of dissipative phase transitions have actually been around for many decades, particularly in the quantum optical community. The reason is that they often occur in nonlinear optical systems coupled to optical cavities, such as the Dicke model (Dicke, 1954) or the optical parametric oscillator (Drummond, McNeil, and Walls, 1981). These models are dissipative due to the characteristic photon losses of optical cavities. The transition in this case is driven by an external pump laser, which increases the number of photons in the cavity and thus the rate at which the nonlinear processes take place. Criticality is marked by a threshold

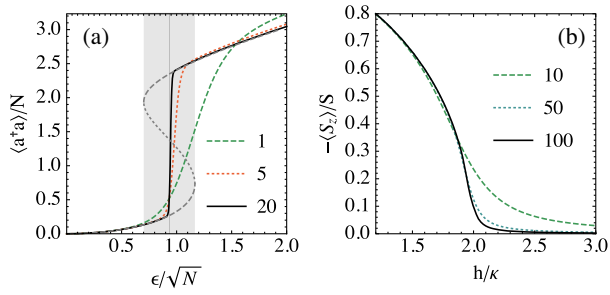


FIG. 8. Examples of dissipative transition. (a) Average photon number for the Kerr bistability model (292), with $\kappa = 1/2$, $\Delta = -2$, and $U = 1/N$, where N is a parameter used to tune the thermodynamic limit. The various curves correspond to $N = 1, 5$, and 20 (long-dashed green curve, short-dashed red curve, and solid black curve, respectively) and were computed by numerically finding the steady state of Eq. (292). We also show as a dashed light gray curve the semiclassical result expected for optical bistability, showing that there is a region where there are two possible solutions. (b) Steady-state magnetization of the macrospin model (293) computed for $S = 10, 50$, and 100 (dashed, dotted, and solid curves, respectively).

pump intensity at which the quantum state of the cavity changes abruptly. This class of models is called driven dissipative. The simplest such model is that of Kerr bistability (Drummond and Walls, 1980; Casteels, Fazio, and Ciuti, 2017), which is defined as follows by a single bosonic model a evolving according to the Lindblad equation in a rotating frame at the frequency of the pump:

$$\frac{d\rho}{dt} = -i[H, \rho] + \kappa[\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}], \quad (292)$$

where $H = \Delta a^\dagger a + (U/2)a^\dagger a^\dagger a a + i\epsilon(a^\dagger - a)$. Here Δ is the cavity detuning, U is the nonlinear interaction, and ϵ is the external pump. For certain parameters, this model may exhibit a discontinuous transition as a function of the pump ϵ , which is reminiscent of the phenomenon of optical bistability. This is illustrated in Fig. 8(a). For the transition to take place, one must define an appropriate thermodynamic limit, which corresponds to $U \rightarrow 0$ and $\epsilon \rightarrow \infty$ while keeping $U\epsilon^2$ finite or, equivalently, one could introduce a fictitious integer N such that $U \rightarrow U/N$ and $\epsilon \rightarrow \epsilon\sqrt{N}$. The curves in Fig. 8(a) were computed numerically for different values of N . From a statistical mechanical point of view, driven-dissipative models are mean-field models since the strong confinement of the optical cavity makes the interactions between the atoms in the nonlinear medium long ranged (“everyone interacts with everyone”).

Dissipative phase transitions share many similarities with quantum phase transitions, as well as important differences; see Table II. As with any transition, they stem from a competition between different drives. Thus, just as quantum phase transitions are driven by the competition between two noncommuting terms in the Hamiltonian, the drives in dissipative phase transitions can be any two (or more) terms generating the open-system dynamics. Now, however, there are more possibilities. Not only can there be a competition between two dissipative mechanisms, such as two reservoirs at

TABLE II. Dissipative phase transitions compared to quantum phase transitions. Adapted from Kessler *et al.*, 2012.

	Quantum	Dissipative
Operator	Hamiltonian $H(g)$	Liouvillian $\mathcal{L}(g)$
Spectra	Energy eigenvalues $H(g) \psi_i\rangle = E_i(g) \psi_i\rangle$	Eigenvalues $\mathcal{L}(g)\rho = \lambda_i(g)\rho$
State	Ground state $H(g) \psi_0\rangle = E_0(g) \psi_0\rangle$	NESS $\mathcal{L}(g)\rho_{ss} = 0$
Gap	Energy gap $\Delta(g) = E_1(g) - E_0(g)$	Liouvillian gap $\Re[\lambda_1]$

different temperatures, but also a competition between a dissipative and a unitary (and hence coherent) term, as is the case in Eqs. (291) and (292).⁸ A simple but elegant example is a macrospin of size S described by spin operators S_x, S_y , and S_z and evolving according to the Lindblad master equation

$$\frac{d\rho}{dt} = -i h[S_x, \rho] + \frac{2\kappa}{S} \left[S_- \rho S_+ - \frac{1}{2} \{S_+ S_-, \rho\} \right]. \quad (293)$$

This describes a competition between a dissipative term favoring the south pole (lowest eigenstate of S_z) and a unitary contribution corresponding to a transverse field. This model is reminiscent of the Dicke model for collective atom interactions and has been studied since the 1970s; see Schneider and Milburn (2002) and references therein.⁹ In the thermodynamic limit (which in this case indicates that $S \rightarrow \infty$) the model presents a phase transition at a critical field $h_c = 2\kappa$. This is illustrated in Fig. 8(b), where we plot the order parameter $\langle S_z \rangle_{ss}$ as a function of h . For $h < h_c$ the dissipative part wins and the system tends to align toward the south pole, making $\langle S_z \rangle_{ss}$ nonzero and negative (when $h = 0$ the steady state is precisely the south pole). Conversely, for $h > h_c$ the two terms mix together to produce a disordered state with $\langle S_z \rangle_{ss} = 0$.

G. Dissipative phase transitions: Entropy production

Having introduced some of the basic models and features of dissipative phase transitions, we now turn to the question of how the entropy production behaves as one crosses the critical point. We begin with classical systems. In this case much more is known since the entropy production can be more readily computed. For systems described by a Pauli master equation such as Eq. (148), the entropy production can be computed from the general formula in Eq. (163), which contemplates the presence of multiple heat baths; see Sec. V.F for more details.

The entropy production rate in classical transitions is found to be always finite but becomes nonanalytic at the critical point. For continuous transitions, it always presents a kink, meaning its derivative with respect to the driving parameter is

⁸This is not a quantum effect and may well occur in classical stochastic systems, such as those governed by a Fokker-Planck equation.

⁹The steady state ρ_{ss} can actually be found analytically, as Puri and Lawande (1979) showed.

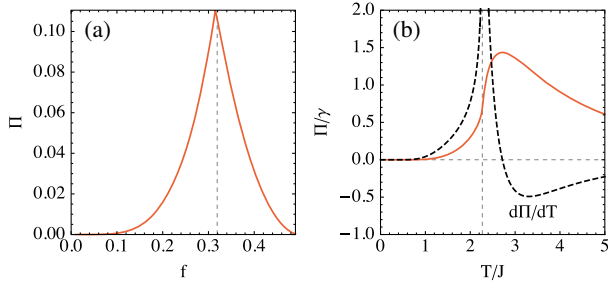


FIG. 9. Example of behavior of $\dot{\Sigma}$ across a continuous dissipative transition. (a) Mean-field majority vote model given by Noa *et al.* (2019), where f is the so-called misalignment parameter. (b) Two-bath Ising model of Tomé and de Oliveira (2012), where the transition is driven by the temperature T . In both cases $\dot{\Sigma}$ is continuous across the transition but has a kink at the critical point, implying that the derivative of $\dot{\Sigma}$ is discontinuous. It is also possible, as shown in (b), that the derivative presents a logarithmic discontinuity.

discontinuous. This is illustrated in Fig. 9(a). The derivative can also diverge logarithmically, as shown in Fig. 9(b) (the critical exponent of this divergence is associated with the equilibrium specific heat of the system). Notwithstanding, $\dot{\Sigma}$ itself is always finite. This behavior was found in both analytical and numerical Monte Carlo simulations in a variety of models (Crochik and Tomé, 2005; Tomé and de Oliveira, 2012; Shim, Chun, and Noh, 2016; Zhang and Barato, 2016; Herpich and Esposito, 2019; Noa *et al.*, 2019).

For discontinuous transitions, on the other hand, $\dot{\Sigma}$ is finite but has a discontinuity at the phase coexistence region. This was encountered in numerous models (Zhang and Barato, 2016; Herpich, Thingna, and Esposito, 2018; Noa *et al.*, 2019) and is exemplified by Fig. 10. Figure 10(a) corresponds to the same model used in Fig. 9(a), which can actually be tuned to present both continuous and discontinuous transitions across the critical point. Figure 10(b), on the other hand, was based on Zhang and Barato (2016) and corresponds to a classical Ising model subject to an oscillating magnetic field. This is therefore somewhat different from the NESS scenario that we have been discussing, as there is only one bath. But the explicit time-dependent drive yields similar physics.

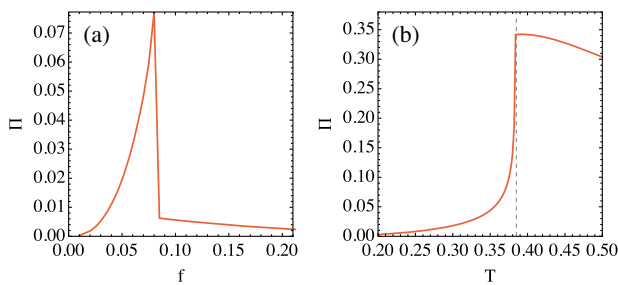


FIG. 10. Similar to Fig. 9 but exemplifying $\dot{\Sigma}$ across discontinuous transitions. (a) Majority vote model. This is the same model used in Fig. 9(a), which can be tuned from a continuous to a discontinuous transition depending on the parameter range. From Noa *et al.*, 2019. (b) Ising model subject to an oscillating field. Adapted from Zhang and Barato, 2016.

The underlying mechanisms that lead to this kind of behavior were established recently by Noa *et al.* (2019). They involve the stochastic fluctuations of the entropy production close to criticality, which, due to the central limit theorem, can be approximated by a sum of Gaussians. These results show that the previously mentioned behaviors for both continuous and discontinuous transitions are in fact universal for systems described by Pauli equations breaking a discrete Z_2 symmetry. Whether they extend to other types of discrete symmetries remains to be proved. The results of Herpich and Esposito (2019), who studied a q -state Potts model, seem to indicate that they do.

Next we turn to the quantum case. Little is known about the behavior of the entropy production in quantum dissipative phase transitions. Not only are the models difficult to simulate or experiment with, but computing $\dot{\Sigma}$ presents an additional challenge. As discussed in Sec. III, the definition of entropy production requires knowledge of the specific system-bath interactions involved. With the exception of standard thermal baths, it is not possible to estimate $\dot{\Sigma}$ solely from the reduced dynamics. This acquires additional relevance in light of the fact that most dissipators studied in the context of dissipative phase transitions are actually not thermal. This is the case in Eq. (291). It is also true for driven-dissipative systems, such as for Eqs. (292) and (293), which are effectively equivalent to zero-temperature baths.

To our knowledge, the only studies on this issue have been in driven-dissipative systems (the driven optical cavity is loaded with a nonlinear medium) (Brunelli *et al.*, 2018; Goes, Fiore, and Landi, 2020). In such systems, even though the standard formulation of $\dot{\Sigma}$ is not available (since the baths are at zero temperature) one can approach the problem using the phase-space formulation discussed in Sec. V.H.

What is found is that the entropy production rate can be decomposed into two terms as

$$\dot{\Sigma} = \dot{\Sigma}_u + \dot{\Sigma}_d. \quad (294)$$

The first term is related to the unitary dynamics and behaves exactly like the entropy production in classical systems; see Figs. 9 and 10. The reason why this is so is not yet fully understood. The second term $\dot{\Sigma}_d$, on the other hand, is related to the dissipative part and behaves like a susceptibility. As a consequence, it can diverge at the critical point. These results therefore indicate that the entropy production in the quantum domain may have contributions that behave fundamentally differently than their classical counterparts.

We review two specific models of entropy production in dissipative phase transitions that were studied by Goes, Fiore, and Landi (2020). We first look at the discontinuous transition of the Kerr model in Eq. (292). Figure 11 shows both contributions in Eq. (294) as a function of the pump ϵ for several values of N (the parameter controlling the thermodynamic limit; see Fig. 8). The curves have been plotted so as to yield a data collapse whose properties can help one to infer the nature of each contribution. The horizontal axes are rescaled to $N(\epsilon/\epsilon_c - 1)$, whereas the vertical axis is rescaled not for $\dot{\Sigma}_u$ but instead by $1/N$ for $\dot{\Sigma}_d$. This means that $\dot{\Sigma}_u$ is intensive,

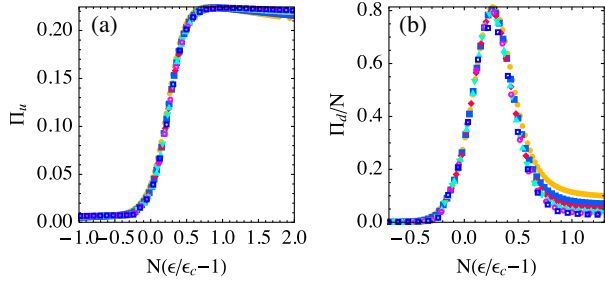


FIG. 11. The two contributions in Eq. (294) to the entropy production for the Kerr bistability model (292). The points correspond to different values of N and have been plotted so as to yield a data collapse; see the text for more details.

while $\dot{\Sigma}_d$ is extensive. As a consequence, for large N the dominant contribution will be from $\dot{\Sigma}_d$.

The behavior of $\dot{\Sigma}_u$ matches exactly what is found in classical systems [see Fig. 10(b)] and can be understood using the phenomenological two-Gaussian model of Noa *et al.* (2019). Conversely, the behavior of $\dot{\Sigma}_d$ follows the variance of the order parameter $\langle \delta a^\dagger \delta a \rangle$, where $\delta a = a - \langle a \rangle$. This contribution therefore behaves like a susceptibility. As it is a direct consequence of quantum fluctuations, it corresponds to an additional contribution to $\dot{\Sigma}$ of pure quantum origin.

The other model, which was studied by Goes, Fiore, and Landi (2020), was the driven-dissipative Dicke model, described by a master equation identical to Eq. (292) but with the Hamiltonian

$$H = \omega_s S_z + \omega a^\dagger a + \frac{2\lambda}{N} (a + a^\dagger) S_x, \quad (295)$$

where S_i are macrospin operators of size $S = N/2$. The Dicke model describes an optical cavity with mode a and loss κ coupled to a nonlinear medium, modeled as a macrospin S .

In this model the driving stems from the Dicke interaction $(a + a^\dagger) S_x$, which is related to the field generating the optical lattice and whose effect is to populate the cavity with a finite number of photons; see Baumann *et al.* (2010) for more details. The entropy production of this model was also studied experimentally by Brunelli *et al.* (2018), which is reviewed in Sec. VIII.D. The theoretical predictions for this model are shown in Fig. 12. As one can see, once again $\dot{\Sigma}_u$ behaves exactly as in the classical case [see Fig. 9(a)], whereas $\dot{\Sigma}_d$ behaves like a susceptibility and therefore diverges at the critical point.

H. Effects of non-Markovian dynamics on entropy production

In this section we aim to explore potential connections between entropy production and the possible non-Markovian character of the system-environment dynamics. The flavor of such potential connections is provided by Eq. (30). First, the assumptions that underlie it involve a certain degree of control over the environment E , which, as remarked in Sec. III.A, might well have the same dimensions as S . This is entailed by the finite-size corrections to these expressions discussed in Sec. IV.A. Second, Eq. (30) implies the possibility that, due to

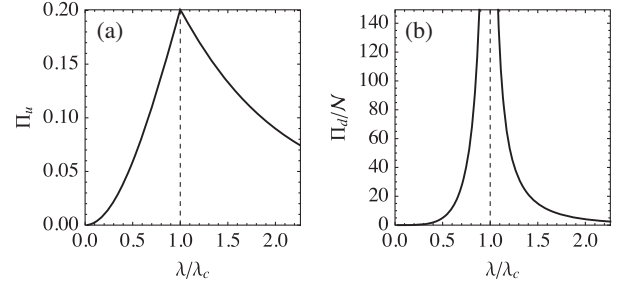


FIG. 12. The two contributions in Eq. (294) to the entropy production for the driven-dissipative Dicke model in Eq. (295). The critical point occurs at $\lambda_c = \sqrt{\omega_0(\kappa^2 + \omega^2)}/\omega$.

the globally unitary system-environment interaction, both S and E are affected. These features are strongly suggestive of influences of a potential backflow of information, from the environment back to the system, that has been pinpointed as one of the fundamental mechanisms for the emergence of non-Markovianity in the reduced dynamics of S (Breuer *et al.*, 2016; de Vega and Alonso, 2017).

Specifically, Breuer, Laine, and Piilo (2009) defined a process as non-Markovian if there is a pair of initial states $\rho_S^{1,2}(0)$ of the system and a time t of its dynamics such that

$$\frac{d}{dt} D(\rho_S^1(t), \rho_S^2(t)) > 0. \quad (296)$$

Here $D(\rho_1, \rho_2) = \|\rho_1 - \rho_2\|/2$ is the trace distance between two states $\rho_{1,2}$ (with $\|\cdot\|$ the trace-1 norm of a matrix). The framework set by Breuer, Laine, and Piilo (2009) was based on the contractivity of the trace distance under positive trace-preserving maps: a breakdown of contractivity makes the distance between the two states grow [and thus Eq. (296) hold], signaling non-Markovianity in the ensuing evolution.

The identification of the reasons for the nonmonotonic behavior of the trace distance under non-Markovian dynamics is evidently key for the characterization of open-system dynamics. In this regard, one can demonstrate the following theorem (Mazzola *et al.*, 2012).

Theorem 5.—For any quantum process described by a completely positive map with an associated system-environment interaction ruled by the propagator $U = e^{-iHt}$, we have

$$\frac{d}{dt} D(\rho_S^1(t), \rho_S^2(t)) \leq \frac{\mathcal{E}(t) + \mathcal{C}(t)}{2}, \quad (297)$$

with $\mathcal{E}(t) = \min_{k=1,2} \|\text{Tr}_E\{H, \rho_S^k(t) \otimes [\rho_E^1(t) - \rho_E^2(t)]\}\|$ and $\mathcal{C}(t) = \|\text{Tr}_E\{H, [\chi_{SE}^1(t) - \chi_{SE}^2(t)]\}\|$. Here $\rho_{S(E)}^k(t) = \text{Tr}_{E(S)}[U \rho_{SE}^k U^\dagger]$ are the reduced states of the system (environment) at time t and $\chi_{SE}^k(t) = \rho_{SE}^k(t) - \rho_S^k(t) \otimes \rho_E^k(t)$ are matrices that encode the correlations between S and E .

Equation (297) identifies the two mechanisms that underpin the occurrence of the backflow responsible for non-Markovian dynamics, namely, the possibility that, in light of the dynamical nature of the environment (as previously remarked), the state of E changes in time (as encompassed by \mathcal{E}), and the potential setting of system-environment correlations (here quantified by the boundary term \mathcal{C}). Compare this result with

the entropy production rate, which is obtained by differentiating Eq. (30) with respect to time as follows:

$$\dot{\Sigma} = \frac{d}{dt} \mathcal{I}_{\rho'_{SE}}(S':E') + \frac{d}{dt} S(\rho'_E || \rho_E). \quad (298)$$

While $\Sigma \geq 0$, the same is not necessarily true for the rate $\dot{\Sigma}$. Theorem 6 resonates directly with this result for $\dot{\Sigma}$. The quantity \mathcal{E} is in close correspondence to $dS(\rho'_E || \rho_E)/dt$ and \mathcal{C} with $d\mathcal{I}_{\rho'_{SE}}(S':E')/dt$. This therefore shows that, even though the trace distance measure (296) and the entropy production (30) are defined in terms of different information-theoretic quantities, the mechanisms that underlie both are similar in spirit; put differently, negativities in the entropy production rate can be viewed as a witness of non-Markovianity (Strasberg and Esposito, 2019). Contrast this with the contractivity property of Markov processes, which enjoys a good physical interpretation in the context of quantum (and indeed stochastic) thermodynamics, as it entails the positivity of the entropy production rate.

Next consider a time-dependent system-bath interaction Hamiltonian given by $H_{\text{tot}}(\lambda_t) = H(\lambda_t) + V + H_E$, with $H(\lambda_t)$ a driving term for the system, H_E the Hamiltonian of the bath, V their mutual coupling term, and λ_t a work parameter. Owing to the coupling between system and bath, which may well be strong, the equilibrium state of the system is not necessarily of the Gibbs form with respect to $H(\lambda)$. Moreover, the initial state of the system-bath compound might not be factorized, thus entailing the potential emergence of non-Markovianity.

Yet we need to characterize such an equilibrium state in order to be able to define the entropy production and its rate. To do so, it is convenient to introduce the following so-called Hamiltonian of mean force (Kirkwood, 1935):

$$H^{\text{mf}}(\lambda_t) = -\frac{1}{\beta} \ln \frac{\text{Tr}_B[e^{-\beta H_{\text{tot}}(\lambda_t)}]}{Z_B}, \quad (299)$$

with Z_B the partition function of the equilibrium state of the bath. Equation (299) describes the energy of the reduced state of the system if the global system-bath state is in equilibrium. Following Strasberg and Esposito (2019), we can introduce the nonequilibrium free energy $F(t) = \langle H^{\text{mf}}(\lambda_t) + (1/\beta) \ln \rho_S(t) \rangle$, with $\rho_S(t)$ an arbitrary state of the system at time t . This leads to the following formal definition of work:

$$W(t) = \int_0^t dt' \text{Tr}_S \left[\frac{dH(\lambda_{t'})}{dt'} \rho_S(t') \right], \quad (300)$$

which is structurally identical to the definition in the classical case. Using the previous definitions, we have

$$W(t) = \text{Tr}_{SE}[\rho_{SE}(t)H_{\text{tot}}(\lambda_t)] - \text{Tr}_{SE}[\rho_{SE}(0)H_{\text{tot}}(\lambda_0)], \quad (301)$$

where $\rho_{SB}(t)$ is the instantaneous state of the total system-bath compound.

If we now take the following coarse-grained, mean-force version of the equilibrium state of the system:

$$\pi_S(\lambda_t) = \frac{e^{-\beta H^{\text{mf}}(\lambda_t)}}{Z^{\text{mf}}(\lambda_t)}, \quad (302)$$

the entropy production rate may be defined as $\dot{\Sigma}(t) = -\partial_t S(\rho_S(t) || \pi_S(\lambda_t))$, which is equivalent to

$$\Sigma(t) = \beta[W(t) - \Delta F(t)] = \delta S(t) - \delta S(0), \quad (303)$$

with $\delta S(t) = S(\rho_{SE}(t) || \pi_{SE}(\lambda_t)) - S(\rho_S(t) || \pi_S(\lambda_t))$. The variation in quantum relative entropy at a generic time t , with and without the inclusion of the bath [here $\pi_{SE}(\lambda_t)$ is the total system-bath Gibbs state and $\pi_S = \text{Tr}_B(\pi_{SE})$] (Strasberg and Esposito, 2019). The monotonicity of the quantum relative entropy entails that $\delta S(t) \geq 0 \forall t$. Therefore, $\Sigma(t) \geq 0$ provided that $\delta S(0) = 0$, which happens in two noticeable cases: (a) if the system-bath compound is initially prepared in the global Gibbs state $\pi_{SE}(\lambda_0)$ and (b) for the class of zero-discord system-bath states (mathematically implying the condition $[H(\lambda_0), V] = 0$).

The entropy production rate thus cannot be expressed as the relative entropy associated with the irreversible relaxation of the state of the system toward equilibrium. As a result, a relation between the sign of the entropy production rate and the occurrence of non-Markovian effects is not immediately apparent, even for undriven systems. Notice that this is in contrast to the case of undriven classical open-system dynamics, for which it is possible to establish that the negativity of the entropy production rate directly implies the non-Markovian nature of the dynamics under scrutiny. The fact that Eq. (303) requires the consideration of the bath with which the system interacts is a testament to the view, according to which a self-consistent formulation of the second law of thermodynamics for general (i.e., in principle non-Markovian) open quantum systems should not be based on the sole reduced-state dynamics of the system, as illustrated by Marcantoni *et al.* (2017). The relation between the conditions for the observation of non-Markovianity and the achievement of negative entropy production is currently an open question (Bhattacharya *et al.*, 2017; Popovic, Vacchini, and Campbell, 2018)

A different approach to the inclusion of the global system-bath compound in the description of the thermodynamics of the system can be taken when considering the case of weak yet non-negligible S - E couplings (Rivas and Huelga, 2012; Rivas, 2019). In these conditions, the dynamics of the system might exhibit non-Markovian features in light of the breakdown of divisibility conditions. We assume the initial system-bath state to be the tensor product of the equilibrium states $\rho_E^{\text{th}} = e^{-\beta H_E}/Z_E$ and $\rho_S^{\text{th}} = e^{-\beta H_S}/Z_S$, i.e., $\rho_{SE}(0) = \rho_S^{\text{th}} \otimes \rho_E^{\text{th}}$, and a time-independent system Hamiltonian. Under the assumption of negligible system-bath coupling, the total Gibbs state of the compound is well approximated by such an initial state, that is, $\rho_{SE}^{\text{th}} \simeq \rho_{SE}(0)$. As the global Gibbs state is a stationary state of the dynamics, the Gibbs state of the system ρ_S^{th} would be a steady state of the reduced dynamics in the refined weak-coupling limit. However, this is not true at a finite time t . We call Λ_t^R the map propagating the initial state of the system in the refined weak-coupling limit. Following an

argument similar to that pursued when introducing the mean-force Hamiltonian, one can set

$$\Lambda_t^R(\rho_S^{\text{th}}) = e^{-\beta H_S^R(t)} / e^{-\beta H_S^R(t)}, \quad (304)$$

with $Z_S^R(t) = Z_S$, in light of the trace-preserving nature of the dynamical map. Moreover, H_S^R is the refined Hamiltonian of the system given by

$$H_S^R(t) = -\frac{1}{\beta} \ln \Lambda_t^R(e^{-\beta H_S}). \quad (305)$$

In analogy with the standard formulation in the weak-coupling limit, we define the refined average instantaneous energy $E^R(t) = \text{Tr}_S[\rho_S(t)H_S^R(t)]$, which reduces to the standard weak-coupling value at $t=0$ and approaches $E(t) = \text{Tr}_S[\rho_S(t)H_S]$ as $t \rightarrow \infty$, when Λ_t^R approaches a Davies semigroup and $H_S^R(t) \rightarrow H_S$. As we are considering a time-independent process, the change in energy of the system equals the amount of refined heat $Q^R(t)$ flowing to and from the system, so

$$\begin{aligned} Q^R(t) &= \int_0^t dt' \dot{E}^R(t') \\ &= \int_0^t dt' \text{Tr}_S[\dot{\rho}_S(t')H_S^R(t') + \rho_S(t')\dot{H}_S^R(t')]. \end{aligned} \quad (306)$$

As the map at hand is completely positive, the quantum relative entropy will satisfy contractivity upon application of Λ_t^R so that

$$S(\Lambda_t^R[\rho_S(0)] \| \Lambda_t^R(\rho_S^{\text{th}})) \leq S(\rho_S(0) \| \rho_S^{\text{th}}), \quad (307)$$

which gives

$$\Sigma^R(t) = \Delta S(t) - \beta Q^R(t) \geq 0, \quad (308)$$

with $\Delta S(t) = S(t) - S(0)$. The integral form of Eq. (307) is not accidental: as the map under scrutiny is in general nondivisible, the differential form of the second law is in general not valid, thus preventing a definite sign of the entropy production rate of the process (Rivas, 2019). Albeit resulting from a much more intricate derivation, the same conclusion can be drawn for a general time-dependent process entailing the performance of work.

More recent work has elaborated on this approach, providing a way to address the general case of a system coupled to a thermal bath through arbitrarily strong coupling rates (Seifert, 2016; Jarzynski, 2017; Miller and Anders, 2017; Strasberg and Esposito, 2017). In particular, Rivas (2020) proposed a framework encompassing general initial states (including correlated ones of system and bath) through which it is possible to show that, in a completely positive divisible map induced by a time-independent Hamiltonian, the entropy production rate is always positive. This plants the seed for the clear-cut link between thermodynamics and Markovianity in the quantum regime suggested in Theorem 5.

VIII. EXPERIMENTAL ASSESSMENT OF QUANTUM ENTROPY PRODUCTION

In recent years there have been many experiments on nonequilibrium thermodynamics in the microscopic domain. In this section we opt to review some representative results, with a focus on those contributions that specifically characterize the entropy production.

A. Assessment at the level of quantum trajectories

To investigate the physical origin of irreversibility, Batalhão *et al.* (2015) addressed the dynamics of a nuclear spin-1/2 system (^{13}C -labeled chloroform molecule in a liquid sample) that is initially prepared in a thermal state and driven out of equilibrium by a fast quench generated by a time-modulated radio-frequency (rf) field producing a time-dependent Hamiltonian H_t^F . A backward process was also realized by driving the system with the time-reversed Hamiltonian ($H_t^B = H_{\tau-t}^F$) with the system prepared in an equilibrium state of H_0^B . The work probability distributions of the forward and backward processes $P_{F,B}(W)$ are related via the Tasaki-Crooks fluctuation relation (Crooks, 1999; Tasaki, 1999)

$$P_F(W)/P_B(-W) = e^{\beta(W-\Delta F)}. \quad (309)$$

Equation (309) characterizes the positive and negative fluctuations of the quantum work W along single realizations. It holds for arbitrary driving protocols, especially beyond the linear response regime, and is a generalization of the second law, to which it reduces on average as $\langle \Sigma \rangle = \beta(\langle W \rangle - \Delta F) \geq 0$.

The Hamiltonian driving the forward process was taken to be $H_t^F = 2\pi\hbar\nu(t)[\sigma_x \cos \phi(t) + \sigma_y \sin \phi(t)]$, with $\phi(t) = \pi t/2\tau$ and $\sigma_{x,y,z}$ the Pauli spin operators and $\nu(t) = \nu_0(1-t/\tau) + \nu_\tau t/\tau$ the linear modulation of the rf-field frequency over time τ from value $\nu_0 = 1.0$ kHz to $\nu_\tau = 1.8$ kHz. Figure 13 reports some of the trajectories followed by the system in both the forward and backward processes.

The degree of irreversibility arising from such dynamics was quantified by measuring the probability distribution $P(\Sigma)$ of the irreversible entropy production using the Tasaki-Crooks relation in Eq. (309). This was assessed using nuclear magnetic resonance (NMR) spectroscopy (Oliveira *et al.*, 2007) and the method described by Dorner *et al.* (2013), Mazzola, De Chiara, and Paternostro (2013), and Batalhão *et al.* (2014). From this the forward and backward work distributions $P_{F,B}(W)$ can be determined and from them β , W , and ΔF ; hence, the entropy produced during each process can be extracted. The measured nonequilibrium entropy distribution is shown in Fig. 14. Both positive and negative values occur owing to the stochastic nature of the problem. However, the mean entropy production is positive (red arrow), which is in full agreement with the second law ($\langle \Sigma \rangle \geq 0$).

B. Assessment of the effects of quantum measurements

The experimental tracking of individual trajectories probed by continuous measurements allowed Harrington *et al.* (2019)

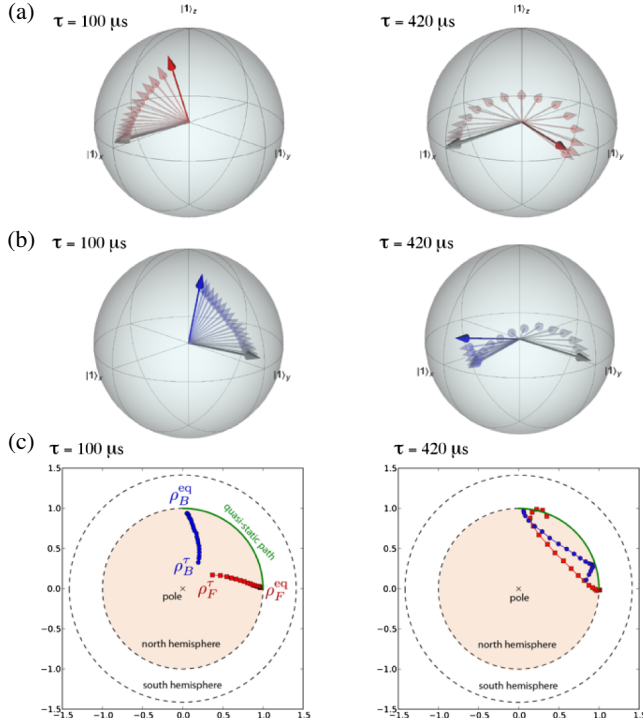


FIG. 13. (a) [(b)] Evolution of the Bloch vector of the forward (backward) spin-1/2 state ρ_F^F ($\rho_{\tau-t}^B$) during a quench of the transverse magnetic field in the experiment reported on by Batalhão *et al.* (2015) that was obtained via quantum state tomography. A sampling of 21 intermediate steps was used. The initial magnetization (gray arrow) is parallel to the external driven rf field, aligned along the positive x (y) axis for the forward (backward) process. The final state is represented as a red (blue) arrow pointing nearly to the north pole of the sphere. (c) Polar projection (indicating only the magnetization direction) of the Bloch sphere with the trajectories of the spin. Green lines represent the path followed in a quasistatic ($\tau \rightarrow \infty$) process. From Batalhão *et al.*, 2015.

to assess the irreversibility of a system affected by continuous weak measurements. A scheme of principle of the employed setting is shown in Fig. 15. The experimental platform

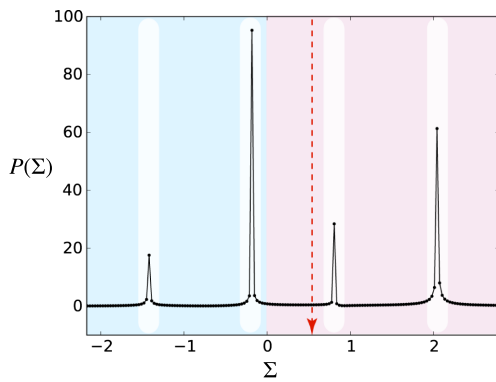


FIG. 14. Distribution of irreversible entropy production. Black dots represent the measured negative and positive values of the entropy production Σ of the spin-1/2 system after a quench of the transverse magnetic field of duration $\tau = 100 \mu\text{s}$. The mean entropy production (dashed red arrow) is positive, which is in agreement with the second law. From Batalhão *et al.*, 2015.

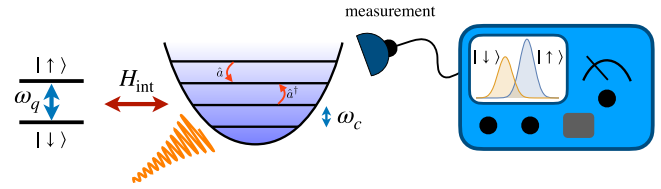


FIG. 15. Scheme of principle of the experiment reported on by Harrington *et al.* (2019). A two-level system whose states $\{|\uparrow\rangle, |\downarrow\rangle\}$ differ in frequency by ω_q is coupled through the dispersive Hamiltonian H_{int} to a harmonic oscillator of frequency $\omega_c \neq \omega_q$. The interaction term correlates the states of the two-level system to a quadrature of the oscillator. The state of the two-level system is measured by probing the oscillator resonance with a microwave pulse that acquires a phase shift that depends on whether the two-level system is prepared in $|\uparrow\rangle$ or $|\downarrow\rangle$.

involved a superconducting transmon two-level system coupled to a microwave cavity through the dispersive-coupling interaction term $H_{\text{int}} = -\chi a^\dagger a \sigma_z$. Here a and a^\dagger are the annihilation and creation operators of the cavity field, while σ_z is the z -Pauli pseudospin operator for the two-level system. The rate χ determines a pseudo-spin-dependent phase shift $2|\chi|$, acquired with a microwave tone used to probe the field's resonance, which in turn is used to acquire information on the two-level system. The signal collected from the cavity field is probed in n time steps t_k ($k = 0, 1, \dots, n-1$), which provide the set of records $\{r_k\}$ that allow for the piecewise reconstruction of individual trajectories of the two-level system. Formally, the statistics of the measurement records and the corresponding measurement dynamics can be described through the action of a generalized measurement, defined by the operators M_{r_k} that update the density matrix of the two-level system at step k , from ρ_k to $\rho_{k+1} = M_{r_k} \rho_k M_{r_k}^\dagger / \text{tr}[M_{r_k} \rho_k M_{r_k}^\dagger]$. A time-reversed measurement process is realized by reversing the dynamics for a single measurement update step. Formally, this is described by the time-reversed measurement operators \tilde{M}_{r_k} , defined such that $\tilde{M}_{r_k} M_{r_k} \rho_k M_{r_k}^\dagger \tilde{M}_{r_k}^\dagger = d(r_k) \rho_k$, where $d(r_k)$ is a depletion coefficient, dependent on the value of the measurement record r_k and entailing the effect of the irreversibility, that unbalances the forward and time-reversed trajectories. The corresponding statistical arrow of time has a length given by

$$\mathcal{A} = \sum_k \ln \frac{P(r_k | \rho_k)}{P(-r_k | \rho_{k+1})}, \quad (310)$$

with $P(r_k | \rho_k) dr_k = \text{tr}[M_{r_k} \rho_k M_{r_k}^\dagger] dr_k$ the probability density of measurement r_k achieved when the system is prepared in ρ_k . The stochastic variable \mathcal{A} is distributed according to a probability distribution $\mathcal{P}(\mathcal{A})$ that satisfies the fluctuation theorem (Harrington *et al.*, 2019) $\mathcal{P}(\mathcal{A}) = e^{\mathcal{A}} \mathcal{P}(-\mathcal{A})$. A related result, aimed at quantifying the information-theoretic contribution to entropy production resulting from the continuous measurement process (Belenchia *et al.*, 2019) and implemented over a mesoscopic optomechanical system, was reported on by Rossi *et al.* (2020).

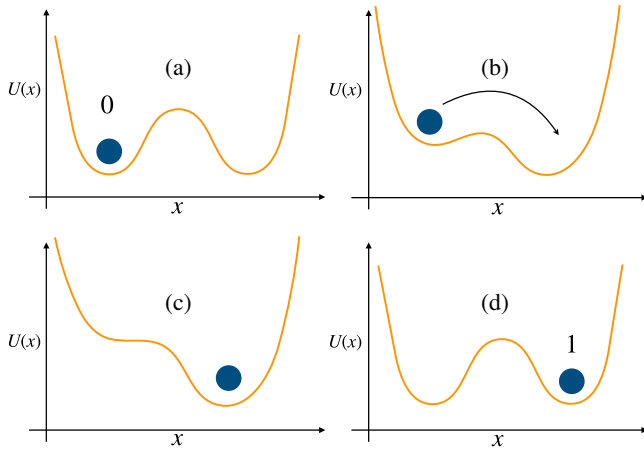


FIG. 16. Scheme of the 1-bit erasure process reported on by [Bérut *et al.* \(2012\)](#). An overamped colloidal particle (a silica bead $2\ \mu\text{m}$ in diameter) is trapped at the focus of a laser beam by an optical tweezer. The laser is focused at two distinct but closely spaced places, alternately and at a high switching rate. This provides the effective double-well potential into which the bead moves. Initially, due to thermal fluctuations the bead is equally likely to be in either one of the two wells. The erasure process always takes the particle to the rightmost well, which corresponds to the logical state 1 of a classical bit. The initial entropy of the system is thus $S_i = \ln 2$. The erasure process where the particle is moved from the left to the right well is displayed. (a) The barrier is initially high, (b),(c) then lowered and tilted to push the particle to the right well, thus switching the bit to the logical 1 state, which erases the memory. Raising the barrier again completes the erasure process. The particle is now in the right well with certainty, so the initial side that it was on has been irreversibly erased. As the process occurs in a finite time, it is stochastic in nature and the heat dissipated along a given trajectory $x(t)$ [with $x(t)$ the instantaneous position of the particle in the potential] is given by $Q = -\int_0^{\tau_{\text{cycle}}} dt \dot{x}(t) \partial U(x, t) / \partial x$, where $U(x, t)$ is the analytical form of the trapping potential and τ_{cycle} is the time taken to close an erasure cycle. The average dissipated heat is obtained by averaging Q over 600 cycles, with each started by randomly choosing the initial configuration.

C. Assessment of the nonequilibrium Landauer principle

Recent experiments have addressed erasurelike processes involving individual classical and quantum systems ([Bérut *et al.*, 2012](#); [Orlov *et al.*, 2012](#); [Jun, Gavrilov, and Bechhoefer, 2014](#); [Yan *et al.*, 2018](#); [Peterson *et al.*, 2019](#)). These experiments have contributed substantially to the resurgence of interest on the implications of Landauer's principle and its extension to general quantum contexts; see Sec. IV.A, particularly Eq. (76).

At the classical level, the space of physical configurations physically accessible to a colloidal particle has been restricted to only two, thus implementing a *de facto* 1-bit system, via the use of a modulated double-well potential ([Bérut *et al.*, 2012](#)) or a feedback-based trapping mechanism ([Jun, Gavrilov, and Bechhoefer, 2014](#)). This was used to show that the mean dissipated heat resulting from a stochastic erasure process saturates at the standard Landauer bound. Details of these experiments are provided in the captions of Figs. 16 and 17.

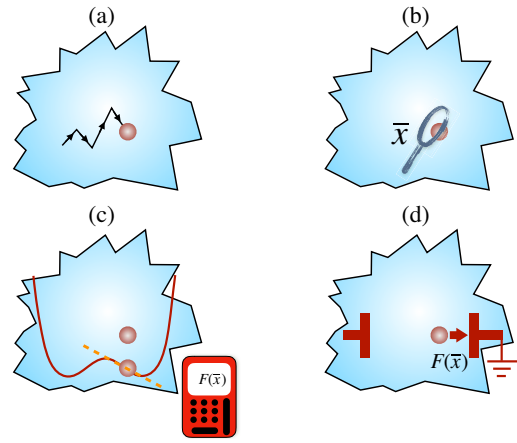


FIG. 17. Scheme of the experimental assessment of Landauer principle reported on by [Jun, Gavrilov, and Bechhoefer \(2014\)](#). (a) A 200 nm fluorescent particle moves in an aqueous solution (blue-shaded area) while (b) being monitored by a camera. A computer (c) reconstructs the position \bar{x} from the images and (d) generates a feedback electric force $F(\bar{x})$, applied via two electrodes. The force is chosen so as to create a virtual potential $V(\bar{x})$ rather than an actual one, as in Fig. 16, imposed by a computer algorithm and calculated at the estimated position \bar{x} rather than x itself. This is not a limiting feature of this implementation since, for feedback updates that are fast enough, the dynamics in such virtual potentials is known to converge asymptotically to the corresponding actual one ([Jun and Bechhoefer, 2012](#)). In the experiment reported on by [Jun, Gavrilov, and Bechhoefer \(2014\)](#), the virtual potential and the erasure process are both along the lines of Fig. 16; see [Dillenschneider and Lutz \(2009\)](#).

The nonequilibrium quantum scenario was addressed by [Peterson *et al.* \(2016\)](#) and [Yan *et al.* \(2018\)](#). [Peterson *et al.* \(2019\)](#) studied a NMR system comprising trifluoroiodoethylene molecules in acetone, whose ^{19}F nuclear spins are used to encode three two-level systems. Two of them represent the system and environment of a nonequilibrium erasure process, while the third is used as an ancilla that was instrumental in the reconstruction of the statistics of the dissipated heat (Fig. 18).

The system is prepared in the maximally mixed state $\rho_S = 1_S/2$ through a suitable set of rf pulses, thus carrying 1 bit of information and embodying a proper memory that we want to reset. The environment is instead initialized in a thermal state $\rho_E = \exp[-\beta H_E]/Z_E$ (with $Z_E = \text{Tr}[e^{-\beta H_E}]$) at an inverse temperature β that can be experimentally controlled. Here H_E is the environment Hamiltonian. Finally, the ancilla is prepared in the logical state $|0\rangle_A$. Following the approach put forward by [Goold, Poschinger, and Modi \(2014\)](#), which was adapted to the statistics of heat $P(Q)$, a method first devised for the reconstruction of the work probability distribution ([Dorner *et al.*, 2013](#); [Mazzola, De Chiara, and Paternostro, 2013](#)), it is possible to show that $P(Q) = \int \Theta(t) e^{-iQt} dt$, with

$$\Theta(t) = \text{Tr}[\rho_E v_i^\dagger \otimes \rho_S U^\dagger v_i] = \langle \sigma_x(t) \rangle_A - i \langle \sigma_y(t) \rangle_A. \quad (311)$$

This offers an operational method to infer $P(Q)$ via measurements performed on the ancilla. The latter are operated by amplifying, digitalizing, and filtering the free induction decay

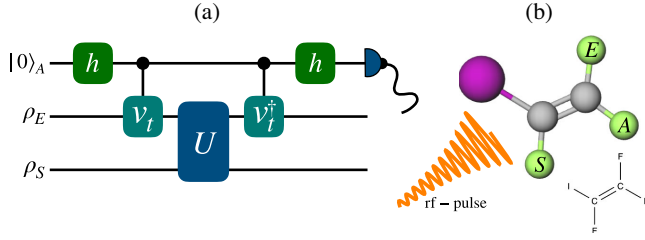


FIG. 18. (a) Quantum circuit for the reconstruction of the heat probability distribution in Eq. (311); see also Eq. (82). Here $h = (\sigma_z + \sigma_x)/\sqrt{2}$ is the Hadamard gate on the ancilla A , while $v_t = \exp[iH_E t]$ is the free evolution of the environment E . Finally, U embodies the $S + E$ unitary governing the heat-dissipation process. (b) 3D chemical structure of the trifluoroiodoethylene molecule (C_2F_3I) accommodating the nuclear spins encoding the ancilla, system, and environment. Suitably arranged rf pulses are employed to prepare and manipulate the state of such a tripartite system.

signal collected from the NMR sample through a pickup coil (Peterson *et al.*, 2019). Needless to say, the features of $P(Q)$ depend on the joint dynamics encompassed by U , while the validity of Landauer principle does not. Peterson *et al.* (2019) have chosen both a controlled-NOT and a SWAP gate as significant instances of U , with the latter providing a realization of the paradigmatic erasure process where the state of the system is changed into the initial state of E at every application of the protocol. By tomographically reconstructing the change of entropy in the state of the system following the erasure, Peterson *et al.* (2019) thus demonstrated the validity of the Landauer bound in a genuinely quantum mechanical nonequilibrium scenario.

Despite addressing quantum dynamics, such an experiment was unable to quantitatively address the information-theoretic contributions to the dissipated heat arising from the non-equilibrium quantum evolution and highlighted in Eq. (76). The reason for this is simply because such contributions were negligible in the NMR sample used by Peterson *et al.* (2019). Such an assessment was instead made possible by the tight control of the trapped-ion experiment reported on by Yan *et al.* (2018).

In such an implementation, the system is encoded in two hyperfine internal energy levels of a $^{40}\text{Ca}^+$ ion confined in a linear Paul trap, while the environment is provided by one of the vibrational modes of the particles in the trapping parabolic pseudopotential (say, the one along the z direction of the reference frame associated with the axes of the trap). Figure 19 shows a diagram of the physical configuration and the relevant part of the energy spectrum of the ion. As in the experiment of Peterson *et al.* (2019), the experiment starts with the system being prepared in a classical mixture of its logical state $\rho_S = \alpha|\downarrow\rangle_S\langle\downarrow|_S + (1 - \alpha)|\uparrow\rangle_S\langle\uparrow|_S$ (with $\alpha \in [0, 1]$ experimentally adjustable) achieved by combining a rotation in the space of states of S and spin dephasing (with no population loss). The vibrational z mode is instead left to relax to a thermal state with an average phonon number n_0 by switching off the cooling lasers for an adjustable time. The joint S - E evolution that provides the core part of the erasure protocol is given by the arrangement of a red-sideband coupling induced by a laser

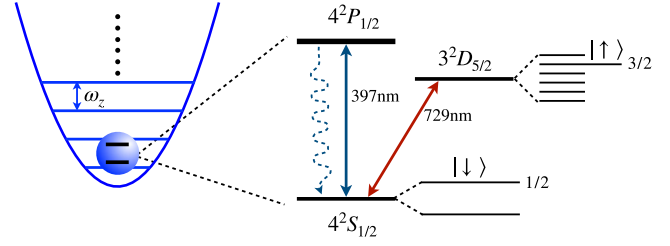


FIG. 19. Schematic diagram of the system used for the verification of the information-theoretic contributions to quantum erasure. A $^{40}\text{Ca}^+$ ion is confined in a linear Paul trap that provides an axial z pseudopotential of frequency ω_z . The ion is subjected to a magnetic field that Zeeman splits the $4^2S_{1/2}$ and $3^2D_{5/2}$ atomic states into manifolds of hyperfine levels. Among them, the $|4^2S_{1/2}, 1/2\rangle$ and $|3^2D_{5/2}, 3/2\rangle$ ones are chosen to encode the logical $|\downarrow\rangle_S$ and $|\uparrow\rangle_S$ pseudospin states of a two-level system embodying S in the erasure protocol. The vibrational z mode of the ion is used to encode the environment E , which is thus an infinite-dimensional system. From Yan *et al.*, 2018.

field driving the $729 \text{ nm } 4^2S_{1/2}, 1/2 \leftrightarrow 3^2D_{5/2}, 3/2$ transition and ruled by the Hamiltonian (Leibfried *et al.*, 2003)

$$H_{SE} = \eta \hbar \Omega (a \sigma_+ e^{i\phi} + a^\dagger \sigma_- e^{-i\phi}) / 2. \quad (312)$$

Here Ω is the Rabi frequency of the coupling, ϕ is the phase of the driving field, $\eta \simeq 0.09$ is the Lamb-Dicke parameter (Leibfried *et al.*, 2003), a (a^\dagger) is the annihilation (creation) operator of the z vibrational mode, and σ_\pm are the two-level ladder operators. Equation (312) associates the creation of a phonon with the $|\uparrow\rangle_S \rightarrow |\downarrow\rangle_S$ transition. The erasure protocol $U = e^{-iH_{SE}t}$ thus consists of the transformation $\rho_S \rightarrow |\downarrow\rangle_S$ accompanied by an increase in the energy of the environment E , which is interpreted as a process of heat dissipation from S . The setup allows for the experimental inference of the phonon number change, which gives direct access to the amount of dissipated heat and the $S(\rho'_E|\rho_E)$ term in Eq. (76). Similarly, the change of entropy in the state of the system can be directly assessed by straightforward measurements of the population of the pseudospin states. The mutual information $I_{\rho'_S}(S':E')$, on the other hand, is not directly accessible but can nonetheless be estimated, as discussed by Yan *et al.* (2018). While such an estimation affects the uncertainty associated with the evaluation of the right-hand side of Eq. (76), resulting in relatively large error bars, the experiment was successful in demonstrating the compatibility between the amount of entropy produced in the erasure process and the joint contribution coming from the information-theoretic terms.

D. Assessment of entropy production in nonequilibrium steady states

Recent efforts have been deployed to the assessment of entropy production in nonequilibrium steady states of mesoscopic quantum systems (Brunelli *et al.*, 2018). In particular, settings based on cavity optomechanics and ultracold atom systems have been used as paradigm of situations leading to nontrivial nonequilibrium steady states.

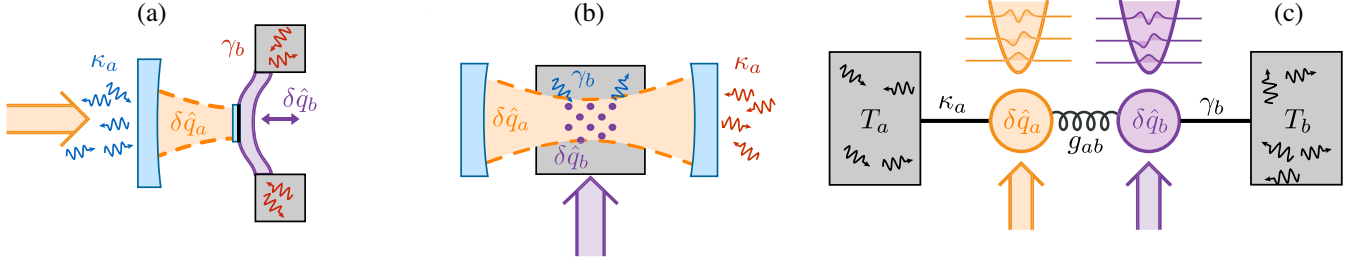


FIG. 20. (a) Optomechanical setup. A micromechanical oscillator ($\delta\hat{q}_b$) is coupled to the field mode of an optical Fabry-Perot cavity ($\delta\hat{q}_a$). For this setup only the cavity is pumped. (b) Cavity-BEC setup. The external degree of freedom of a BEC ($\delta\hat{q}_b$) is coupled to the field mode of a cavity ($\delta\hat{q}_a$). For this setup only the atoms are pumped. Red and blue jagged lines indicate heating or cooling of the subsystems via coupling to the baths. In both setups the number of excitations in the optical bath is 0, i.e., $n_{T_a} = 0$. (c) Both systems can be modeled as two quantum harmonic oscillators at frequencies ω_a and ω_b , linearly coupled with a strength g_{ab} . Each oscillator is coupled to independent local baths at temperatures T_a and T_b , respectively. The corresponding coupling rates are κ_a and γ_b . The oscillators can be pumped by an external field (purple and orange arrows). From Brunelli *et al.*, 2018.

In cavity optomechanics, the position of a mechanical oscillator accommodated in an externally driven cavity is displaced by an amount directly proportional to the number of photons in the field of the cavity itself; see Fig. 20(a). This brings the state of the mechanical system to an out-of-equilibrium steady state resulting from the competition between the coupling of the cavity field to the zero-temperature electromagnetic environment and the equilibrium phononic reservoir that affects the mechanical system (Aspelmeyer, Kippenberg, and Marquardt, 2014).

The second experimental platform that has been studied in this context comprises a Bose-Einstein condensate (BEC) loaded into a high-finesse optical cavity and illuminated by a transverse laser field; see Fig 20(b). The off-resonant photon scattering from the laser field into an initially empty cavity field mode couples the zero-momentum mode of the BEC to an excited momentum mode. The process mediates effective and tunable-in-strength (via the transverse laser beam) long-range atom-atom interactions (Mottl *et al.*, 2012). Such interaction can be brought to competition with the kinetic energy of the atoms, resulting in a structural phase transition (Landig *et al.*, 2015) akin to a Dicke phase transition (Baumann *et al.*, 2010). The cavity light field leaks through the mirrors with a heterodyne detection setup. The spectral analysis of this signal is used to infer the diverging amount of atomic density fluctuations accompanying the structural phase transition (Landig *et al.*, 2015).

In both cases, the effective interaction between the fluctuations of the field operators of the matterlike subsystems and their optical counterpart can be shown to be that of two harmonic oscillators coupled via the Hamiltonian as follows [see Fig. 20(c)]:

$$\hat{H} = \frac{\hbar\omega_a}{2}(\delta\hat{q}_a^2 + \delta\hat{p}_a^2) + \frac{\hbar\omega_b}{2}(\delta\hat{q}_b^2 + \delta\hat{p}_b^2) + \hbar g_{ab}\delta\hat{q}_a\delta\hat{q}_b. \quad (313)$$

Here $\delta\hat{q}_{a,b}$ and $\delta\hat{p}_{a,b}$ are the position and momentum fluctuation operators around the mean-field values of the two oscillators (a and b refer to the optical and mechanical and atomic oscillators, respectively), ω_p is the frequency of the driving pump fields, the oscillators have frequencies

$\omega_a = \omega_c - \omega_p$ and ω_b , ω_c is the frequency of the cavity field, and g_{ab} is the coupling strength between the modes (Brunelli *et al.*, 2018). The cavity mode is coupled to the surrounding electromagnetic vacuum with a decay rate κ_a . On the other hand, the nature of the mechanical or atomic bath is specific to the setup being considered. The optomechanical system considered by Brunelli *et al.* (2018) consisted of a Fabry-Perot cavity with one of its mirrors a doubly clamped, highly reflective mechanical cantilever. The mechanical support of the cantilever thus provided a local heat bath at room temperature responsible for the quantum Brownian motion of the mechanical system. In the cavity-BEC system, dissipation is due to the collection of excited Bogoliubov modes, which provides a bath for the condensate. In both cases, we assume that oscillator b is in contact with a bath at temperature T_b and rate γ_b . The average number of excitations in the equilibrium state of oscillator b is thus $n_{T_b} = (e^{\hbar\omega_b/k_B T_b} - 1)^{-1}$.

The linear dynamics undergone by the coupled oscillators allows for the use of the framework for the quantification of entropy production in phase space illustrated in Sec. V.H. The entropy production rate in the nonequilibrium steady state of such respective systems thus takes the form

$$\Pi \equiv \dot{\Sigma} = 2\gamma_b \left(\frac{n_b + 1/2}{n_{T_b} + 1/2} - 1 \right) + 4\kappa_a n_a = \mu_b + \mu_a, \quad (314)$$

where $n_a = \langle (\delta\hat{q}_a^2 + \delta\hat{p}_a^2 - 1) \rangle_s / 2$ and $n_b = \langle (\delta\hat{q}_b^2 + \delta\hat{p}_b^2 - 1) \rangle_s / 2$ are the average numbers of excitations in the non-equilibrium steady state of the two oscillators in excess of the zero-point motion of the respective harmonic oscillators. In the cavity optomechanics expression for μ_b , instead of the full phonon number n_b only the momentum variance $\langle \delta\hat{p}_b^2 \rangle_s$ enters, as we assume Brownian motion damping.

Equation (314) quantifies the entropic contribution of quantum fluctuations that the system has to pay to remain in its nonequilibrium steady state. The contribution is directly determined by the individual entropy flows μ_j ($j = A, B$) from the mechanical or atomic and optical oscillator to their respective environments.

Brunelli *et al.* (2018) separately reconstructed the two terms μ_a and μ_b ; see Fig. 21, which displays the experimental data

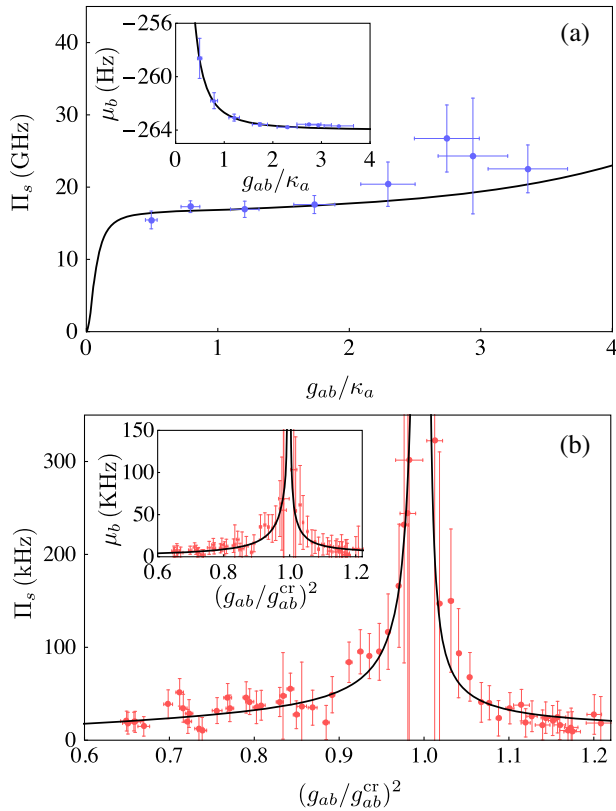


FIG. 21. Experimental assessment of the irreversible entropy production rate Π_s at the nonequilibrium steady state for (a) the cavity optomechanical system and (b) the cavity-BEC system. For the cavity-BEC setup, $g_{ab}^{cr} = \sqrt{(\kappa_a^2 + \omega_a^2)\omega_b/4\omega_a}$ is the critical parameter of the model. Insets: behavior of μ_b . The solid black lines show the theoretical predictions based on parameters extracted from experiment (Brunelli *et al.*, 2018). The blue and red dots show the experimental data for the optomechanical and cavity-BEC experiments, respectively. In (a), the vertical error bars represent statistical errors extracted from the fit, while the horizontal ones show the experimental error on the values of the parameter. In (b), the vertical and horizontal error bars represent the statistical errors from the fit and the determination of the critical point, respectively (Landig *et al.*, 2015). From Brunelli *et al.*, 2018.

together with the theoretical model. The behavior of μ_b observed for the optomechanical system is a signature of cooling: the entropy flow from the mechanical resonator to the cavity field grows with g_{ab} as the effective temperature of the resonator decreases. As for the cavity-BEC system, the divergent behavior of the entropy production rate at $g_{ab} = g_{ab}^{cr} \equiv \sqrt{(\kappa_a^2 + \omega_a^2)\omega_b/4\omega_a}$ reflects the occurrence of the Dicke phase transition: at g_{ab}^{cr} the populations of the two oscillators at the steady state diverges, resulting in the singularity of μ_a and μ_b .

IX. CONCLUSIONS

The second law has always been intimately linked with information theory. The underlying laws of physics are time-reversal invariant. Thus, how can the ensuing macroscopic

dynamics be irreversible? This is perhaps one of the deepest questions in physics, and a major source of confusion. The answer is that irreversibility is an emergent property: It emerges from the fact that information easily becomes irretrievable, when the number of degrees of freedom involved is large. A classical thermodynamic argument goes as follows: suppose that one has a gas of 10^{23} particles but can monitor the position and momenta of only $10^{23} - 1$ of them. Since the motion of the gas is highly chaotic, even this minuscule loss of information can lead to dramatic effects on the description of the remaining $10^{23} - 1$ particles, causing their dynamics to be irreversible.

This argument, however, conceals a much more dramatic effect, which becomes clear only in the full quantum treatment. To properly account for multiple degrees of freedom, it is not enough to monitor them individually; one must monitor them globally. Consider a system with N particles and density matrix $\rho_{1,\dots,N}$ (mixed or pure). Local measurements on each subsystem explore only the local corners of $\rho_{1,\dots,N}$ and are not enough to reconstruct the full state. To do that, one would also have to perform global measurements (such as Bell-like ones). Such measurements are difficult, even for two qubits. For a handful of degrees of freedom, it already easily becomes surreal. In this quantum picture, therefore, information spreads not only from 1 degree of freedom to another but also from the local to the global corners of a many-body density matrix. The basic definition (30) naturally encompasses both aspects: The mutual information accounts for the spreading of information to the various corners of ρ_{SE} , while the relative entropy accounts for the local transfer of information from the degrees of freedom of the system to those of the bath.

Compared to the approach of Eq. (30), the historical formulations of Clausius, Carnot, and Kelvin (Sec. II) were much more pragmatic, stating the second law solely in terms of heat and work, which are palpable quantities. But, although pragmatic, their scope is much less evident at first sight. For instance, demonstrating that the various principles are equivalent requires complicated constructs, involving thermal machines operating in different ways (Fermi, 1956).

A more general statement of the second law thus comes at the expense of introducing the notion of entropy. At the thermodynamic level, entropy is defined as an abstract function of state, with the property that changes in entropy for reversible processes close to equilibrium satisfy $\Delta S = Q/T$, where Q is the heat exchanged. The second law can then be formulated as “the entropy of the Universe never decreases.” For instance, if the Universe comprises a system and bath only, which interact and exchange an amount of heat Q , then $\Delta S_S + \Delta S_E \geq 0$. If in addition the bath is kept close to equilibrium, then $\Delta S_E = Q_E/T$ and the second law becomes $\Delta S_S + Q_E/T \geq 0$, which is Eq. (4). For this reason, historically the entropy production Σ was often stated as representing the change in entropy of the Universe.

The same reasoning also appears in other contexts, such as Boltzmann’s famous H theorem. For instance, Tolman (2010) analyzed a scenario of an isolated gas (the Universe) where the molecules may undergo collisions with each other, described phenomenologically using Boltzmann’s equation. The entropy in this case is given in terms of the gas’ phase-space

density. And, as a consequence of the choice of rules used for describing the collisions, it always increases.

A natural question then would be to ask whether one can carry this interpretation of Σ over to the microscopic realm. This could be called a top-down approach, where one starts with a macroscopic principle and then adapts it to the microworld. And it is the opposite of the bottom-up approach that we have followed in this review, where we started with a fully microscopic definition of Σ in terms of information-theoretic quantities, from which the classical principles emerged as particular cases.

In addition to the progress on the bottom-up approach reported on in this review, in recent years there have been significant advances in the top-down formulation of the second law. The main challenge is in the definition of thermodynamic entropy, something that the bottom-up formulation avoids since it does not interpret entropy production as the change in entropy of the Universe. The von Neumann entropy is not a good candidate for thermodynamic entropy, since it is constant under unitary evolution. In statistical mechanics one often uses the Boltzmann entropy $S = \ln \Omega$, where Ω is the number of microstates associated with a given macrostate. But this quantity is reasonable only close to equilibrium and defined only for macroscopic systems. For microscopic and mesoscopic systems, it fluctuates violently (Gupta, 1951; Pathria and Beale, 2011) and is also awkward to explicitly define. Most advances in the top-down approach have therefore focused on alternative definitions of thermodynamic entropy, such as the diagonal entropy (Polkovnikov, 2011) or, more generally, coarse-grained entropies (Šafránek, Deutsch, and Aguirre, 2019). Recently a general formalism based on an observational entropy was constructed, starting with a coarse graining of the system-bath dynamics (Strasberg and Winter, 2021).

One of the basic features of the thermodynamic entropy is that it is extensive. This is what allows one to write the entropy of the Universe as the sum of the entropies of its parts. In this regard, taking the local von Neumann entropy works well. Consider a system of N particles with the generic density matrix $\rho_{1,\dots,N}$. The sum of the von Neumann entropies of the reduced states ρ_i can be written as

$$\sum_i S(\rho_i) = S(\rho_{1,\dots,N}) + S(\rho_{1,\dots,N} \| \rho_1 \otimes \dots \otimes \rho_N), \quad (315)$$

where the last term indicates the total correlations [see Eq. (44)] measuring the distance between the global and maximally marginalized states. Now suppose initially that the N particles are in a product state but are then made to interact according to a global unitary U , leading to a final correlated state. The first term on the right-hand side of Eq. (315) does not change, since the dynamics is unitary. The second term was initially zero but evolves into something non-negative. Hence, one concludes that for any initially uncorrelated system under closed evolution $\sum_i \Delta S(\rho_i) \geq 0$. Thus, if one takes as the thermodynamic entropy the local von Neumann entropy of each subsystem, we then return to the classical statement that the entropy of the Universe cannot decrease. Most studies attempting to define a microscopic analog of the thermodynamic entropy follow somewhat similar lines.

The previous discussion emphasized some of the basic principles involved in a general formulation of the second law. Often, however, one does not have access to such “luxuries”; that is, one has access not to the full global dynamics but only to an effective description in terms of a master equation. As a consequence, Eq. (30) and the top-down approaches may not be applicable. In situations such as this, several principles have been applied in the past to define entropy production.

The most widely used by far is to postulate that the entropy flux should be $\Phi = Q_E/T$, from which one then recovers $\Sigma = \Delta S_S + \Phi$ [Eq. (4)]. This approach is both simple and effective. It also has a neat interpretation at the trajectory level (Breuer, 2003). But it has two shortcomings. First, it holds only for thermal baths and it is not obvious how to extend it to nonequilibrium reservoirs. Second, one may run into difficulties concerning what is in fact the heat Q_E , as discussed in Sec. V.

Fluctuation theorems greatly resolve these difficulties. In this case, entropy production is defined as the ratio between the path probabilities of a forward and time-reversed (backward) trajectory (Crooks, 1998). These definitions are usually regarded as fundamental. However, they require knowledge of the full path probability, which is not always available and can be hard to obtain (Spinney and Ford, 2012). Moreover, as discussed in Sec. III.E, the backward trajectory is not uniquely defined, contrary to what was initially believed.

Finally, there is also the more pragmatic approach of simply manipulating ΔS and trying to identify a term that resembles an entropy production, such as the Schnakenberg approach discussed in Sec. V.E, which is extremely popular in stochastic thermodynamics. This may seem rather *ad hoc* at first but can lead to interesting results because often the “correct” formula really stands out. Moreover, it allows one to define entropy production for arbitrary open-system dynamics, even those that are not generated by physical processes.

Many open questions still remain. However, as we have shown in this review, in the last two decades there has been substantial progress in our understanding of the basic ingredients and principles that should be involved in this endeavor. In particular, the community’s appreciation of what the second law should represent, as well as the questions that it should address, has evolved significantly. In light of the exciting advances on the experimental manipulation of coherent quantum systems, we believe that these new foundations will play a significant role in our understanding of many potential future applications, as well as in the explanation of fundamental questions.

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