Dissipation production in a closed two-level quantum system as a test of the irreversibility of the dynamics

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Irreversible behavior in open stochastic dynamical systems is quantified by stochastic entropy production, a property that measures the difference in likelihoods of forward and subsequent backward system evolution. But for a closed system, governed by deterministic dynamics, such an approach is not appropriate. Instead, we can consider the difference in likelihoods of forward and "obverse" behavior: the latter being a backward trajectory initiated at the same time as the forward trajectory. Such a comparison allows us to define "dissipation production," an analog of stochastic entropy production. It quantifies the breakage of a property of the evolution termed "obversibility" just as stochastic entropy production quantifies a breakage of reversibility. Both are manifestations of irreversibility. In this study we discuss dissipation production in a quantum system. We consider a simple, deterministic, two-level quantum system characterized by a statistical ensemble of state vectors, and we provide numerical results to illustrate the ideas. We consider cases that both do and do not satisfy an Evans-Searles Fluctuation Theorem for the dissipation production, and hence identify conditions under which the system displays time-asymmetric average behavior: an arrow of time.

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I. INTRODUCTION

Irreversible behavior, such as the melting of an ice cube, is ubiquitous in everyday life. Such behavior is traditionally characterized by a monotonic rise in entropy in accordance with the second law of thermodynamics [1]. This allows the past to be distinguished from the present, characterizing the future as the direction of time in which entropy increases [2].

However, given that the laws governing microscopic motion are time-reversal symmetric, we require a satisfactory understanding of the emergence of macroscopic irreversibility, as did Boltzmann at the advent of the study of thermodynamics. One proposed explanation is known as the Past Hypothesis, which posits that entropy increases globally because the universe started from a state of low entropy, making it likely that all conceivable evolutions lead to its increase. Irreversibility would then ultimately depend on the initial conditions taken by a system. The persistent impact of initial conditions may have philosophical, as well as physical, consequences, which can be explored [3].

Recent developments in nonequilibrium statistical mechanics offer the possibility of quantifying irreversibility given an initial state and a specification of the dynamics, namely, to evaluate the degree to which a process manifests an arrow of time. However, rather different approaches need to be taken for open and closed systems.

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Mean stochastic entropy production [4] has been developed as a measure of irreversibility for *open* systems. It is intimately connected to the development of subjective uncertainty and loss of information [5] brought about by underspecified environmental interactions. It explores a failure of mechanical reversibility, namely, a distinction between the likelihoods of forward and subsequent backward evolution trajectories under suitable preparation. A connection can be established with thermodynamic entropy change. Progress has been made within this framework in understanding entropy production in open classical dynamical systems, as well as in studying the average [6] and single realization quantum entropy production in quantum systems in the weak coupling limit [7,8]. Recently, stochastic entropy production in open quantum systems has received further attention within a framework of quantum state diffusion [9,10].

However, for systems that are closed and dynamically deterministic, the rate of change of mean stochastic entropy production is zero, making this quantity unsuitable as a measure of irreversibility. Nevertheless, distinctively irreversible behavior can emerge even in closed systems, so an alternative approach to its quantification needs to be employed. Total correlation [11–13] has been considered, though a proof of its second law-like behavior is lacking. The quantity that has received most attention as a measure of irreversibility in closed dynamical systems is the *dissipation function* [14–16], which can be shown to increase in time in a manner that resembles entropy. The purpose of this study is to extend the use of this approach to a closed quantum system.

To this end, we consider a measure of irreversibility that derives from a difference in likelihoods of a forward and a so-called *obverse* trajectory (to be defined) under deterministic, mechanically reversible dynamics. To distinguish this from the stochastic entropy production that tests the reversibility, we call this a test of the *obversibility* of the dynamics, a concept that has previously been investigated in classical situations [16,17]. In the next section we provide a definition of obversibility and quantify its failure using *dissipation production* (or, less succinctly, the time-integrated modified dissipation function [17], a generalization of the time-integrated dissipation function [14]). We evaluate dissipation production and explore some of its properties for a simple two-level quantum system. We demonstrate that dissipation production may be computed for individual realizations of the system dynamics, that its average over all possible realizations is never negative, and that in certain situations its probability density function (PDF) can satisfy a symmetry known as the Evans-Searles Fluctuation Theorem (ESFT). This property of the dissipation function played an important role in motivating its use as a measure of irreversibility. The ESFT is the "original" fluctuation relation, a set of statements about probability distributions that have found wide use in nonequilibrium statistical physics [18]. We identify the conditions under which the ESFT is satisfied. When it is violated, situations emerge where the expected dissipation production of the system as it evolves into the future differs from its expected evolution into the past, thus providing an arrow of time.

II. METHODS

A. Measures of irreversibility

Classically, the forward trajectory taken by a system is simply the path it follows from an initial configuration defined by a point in the coordinate phase space, Γ_A, to a final configuration, Γ_B, after a time t. In a quantum setting, the configurations might correspond to initial and final state vectors ψ_A and ψ_B, specified by a collection of complex amplitudes $\tilde{\Gamma}_A$ and $\tilde{\Gamma}_B$, respectively, with reference to a chosen basis set.

In order to proceed, we require an inversion operator M^T which has the effect of transforming the final configuration reached at the end of the forward trajectory into an appropriate starting point from which the backward trajectory can commence under the *time-reversed* dynamics, those designed to return the system after a further time t to an inverted version of the starting configuration for the forward trajectory. In a classical situation, this transformation is *velocity inversion*, $v \to M^T v = -v$ [17]. However, the equivalent inversion in the quantum case (for a spin zero particle) is complex conjugation of the wave function, $\psi \to \psi^*$, as this sets up conditions for a time-reversed solution to the Schrödinger equation with the appropriately time-reversed Hamiltonian [19]. We associate a set of amplitudes $\tilde{\Gamma}^*$ with each ψ^* and define M^T such that $M^T\tilde{\Gamma} = \tilde{\Gamma}^*$.

Thus, starting from Γ_B in the classical or $\tilde{\Gamma}_B$ in the quantum case, the application of an inversion operator M^T followed by (time-)reversed dynamics over a further time period t returns a system to the inverted form of the original state Γ_A or $\tilde{\Gamma}_A$, if the dynamics are mechanically reversible. The red and blue trajectories in Fig. 1 illustrate this.

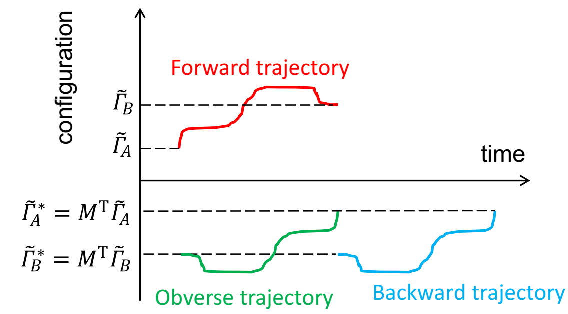

FIG. 1. Trajectories in configuration space. Stochastic entropy production is derived from the probabilities of the forward and backward trajectories (red and blue, respectively). Dissipation production depends in a similar way on probabilities for the forward and obverse trajectories (red and green, respectively). The operator M^T corresponds to a time-reversal transformation.

For open systems with indeterminate dynamics, such that the evolution is represented in terms of probabilities, a return to the starting configuration is not assured, and the degree of failure of reversibility can be quantified using the stochastic entropy production Δs_t for the forward trajectory, defined as

$$\Delta s_t = \ln \frac{p(\tilde{\Gamma}_A, 0)d\tilde{\Gamma}_A\, T(\tilde{\Gamma}_A \to \tilde{\Gamma}_B)}{p(\tilde{\Gamma}_B, t)d\tilde{\Gamma}_B\, P_I(\tilde{\Gamma}_B \to \tilde{\Gamma}_B^*)\, T(\tilde{\Gamma}_B^* \to \tilde{\Gamma}_A^*)} \tag{1}$$

in notation suitable for a quantum setting. Replacing $\tilde{\Gamma}_{A,B}$ with $\Gamma_{A,B}$ gives the appropriate expression for the classical stochastic entropy production. In Eq. (1), $p(\tilde{\Gamma}, \tau)$ is the PDF of the quantum amplitudes, $\tilde{\Gamma}$, at time τ, such that $p(\tilde{\Gamma}, \tau)d\tilde{\Gamma}$ is the probability that the configuration of the system lies in the region of phase space $d\tilde{\Gamma}$ about $\tilde{\Gamma}$. $p(\tilde{\Gamma}, \tau)$ in this context is essentially the classical probability density of selecting a certain quantum state vector from an ensemble of possibilities. Each quantum state vector is itself associated with probabilities for obtaining one outcome or another upon projective measurement of observables, though we restrict ourselves here to considering deterministic quantum evolution *without* measurement.

$T(\tilde{\Gamma} \to \tilde{\Gamma}')$ is the probability for a transition from $\tilde{\Gamma}$ to $\tilde{\Gamma}'$ according to the dynamics in a time interval of length t. The probability for the inversion $P_I(\tilde{\Gamma}_B \to \tilde{\Gamma}_B^*)$ in the denominator of Eq. (1) might be omitted since it is unity, though its presence makes more apparent the precise nature of the two processes that are being compared. The inversion operation is taken to act instantaneously. The idea of Eq. (1) is to compare the probability of a forward path from $\tilde{\Gamma}_A$ to $\tilde{\Gamma}_B$, in a time interval of length t, with the probability of starting from a configuration $\tilde{\Gamma}_B$ at time t, conditioned on evolution from $t = 0$, inverting it, and then having it evolve to configuration $\tilde{\Gamma}_A^*$ under the dynamics for a further time t. For stochastic dynamics, the ratio of initial to final increments $d\tilde{\Gamma}_A/d\tilde{\Gamma}_B$ is unity and can be omitted.

However, for closed systems with deterministic dynamics, Δs_t vanishes since the transition probabilities T are replaced by deterministic mappings of the state, taken with unit probability. The evolution of $\tilde{\Gamma}_A$ to $\tilde{\Gamma}_B$ might be represented by the operation S_t, the backward trajectory by S_t^*, and, including the inversions, the reversibility of the dynamics corresponds to

TABLE I. Comparison of measures of irreversibility. For simplicity, and a more compact expression, we assume that the deterministic dynamics conserve increments in configuration space. $p(\widetilde{\Gamma}, t)$ is the PDF describing an ensemble of sets of probability amplitudes $\widetilde{\Gamma}$ that define the state vector and T is a transition probability under stochastic dynamics.

Procedure	Compare likelihood of forward *then* backward paths	Compare likelihood of forward *or* obverse paths
Concept tested	Reversibility	Obversibility
Quantifying property	Stochastic entropy production $\Delta s_t = \ln\frac{p(\widetilde{\Gamma}_A,0)T(\widetilde{\Gamma}_A\to\widetilde{\Gamma}_B)}{p(\widetilde{\Gamma}_B,t)T(\widetilde{\Gamma}_B^*\to\widetilde{\Gamma}_A^*)}$	Dissipation production $\omega_t = \ln\frac{p(\widetilde{\Gamma}_A,0)}{p(\widetilde{\Gamma}_B,0)}$
Measure of irreversibility for	Open systems	Closed systems

$M^T S_t^* M^T S_t \widetilde{\Gamma}_A = \widetilde{\Gamma}_A$. By conservation of probability we have $p(\widetilde{\Gamma}_B, t)d\widetilde{\Gamma}_B = p(\widetilde{\Gamma}_A, 0)d\widetilde{\Gamma}_A$ and hence $\Delta s_t = 0$. There is no stochastic entropy production since there is no change in the subjective uncertainty of the adopted state brought about by the passage of time.

For closed, deterministic systems we therefore need a different quantity with which to measure irreversibility. A suitable quantity called the *dissipation production* has been employed in classical situations [17], developing earlier work by Evans *et al.* [14]. Rather than comparing the likelihoods of the forward and (subsequent) backward trajectories to quantify irreversibility through stochastic entropy production, dissipation production compares the likelihoods of the forward and *obverse* trajectories. In the quantum situation, the obverse trajectory takes the inverted final configuration, $\widetilde{\Gamma}_B^*$, via the reversed dynamics, S_t^*, to the inverted initial configuration $\widetilde{\Gamma}_A^*$, but the reverse evolution is started at time *zero*, rather than at time t, which distinguishes it from the backward trajectory, which is the reversal of a *previous* forward trajectory. The ideas are illustrated by the red and green trajectories in Fig. 1. We assume that the probability density at $t = 0$ is nonvanishing for all possible final configurations. By comparing the likelihood that a system adopts configuration $\widetilde{\Gamma}_A$ at $t = 0$ with the likelihood that it adopts $\widetilde{\Gamma}_B$, we can quantify the failure of *obversibility*, a counterpart to the reversibility that is tested by the stochastic entropy production. Such failure is necessarily and sufficiently a consequence of the properties of the initial probability density over the configuration space, rather than of the dynamics.

The dissipation production is therefore defined as $\omega_t = \ln[p(\widetilde{\Gamma}_A, 0)d\widetilde{\Gamma}_A/p(\widetilde{\Gamma}_B, 0)d\widetilde{\Gamma}_B]$, where $\widetilde{\Gamma}_A$ and $\widetilde{\Gamma}_B$ are related by the mapping $\widetilde{\Gamma}_B = S_t\widetilde{\Gamma}_A$. To make a more exact parallel with the definition of stochastic entropy production in Eq. (1), dissipation production could be written less concisely as

$$\omega_t = \ln\frac{p(\widetilde{\Gamma}_A, 0)d\widetilde{\Gamma}_A\, \widetilde{T}(\widetilde{\Gamma}_A \to \widetilde{\Gamma}_B)}{p(\widetilde{\Gamma}_B, 0)d\widetilde{\Gamma}_B\, P_I(\widetilde{\Gamma}_B \to \widetilde{\Gamma}_B^*)\, \widetilde{T}(\widetilde{\Gamma}_B^* \to \widetilde{\Gamma}_A^*)}, \tag{2}$$

where the transition probabilities $\widetilde{T}$ are unity since we are considering deterministic dynamics under which $\widetilde{\Gamma}_A$ inevitably evolves into $\widetilde{\Gamma}_B$, and $\widetilde{\Gamma}_B^*$ into $\widetilde{\Gamma}_A^*$ (the latter under reversed dynamics). Hence the $\widetilde{T}$ can be omitted, together with the inversion probability $P_I(\widetilde{\Gamma}_B \to \widetilde{\Gamma}_B^*)$ in the denominator.

Unlike stochastic entropy production, which compares the likelihood of a system evolving forward and then *subsequently* evolving backward, dissipation production is a comparison of the probabilities of *one event or another*. The evolution under S_t taking $\widetilde{\Gamma}_A$ to $\widetilde{\Gamma}_B$ and the evolution under S_t^* taking $\widetilde{\Gamma}_B^*$ to $\widetilde{\Gamma}_A^*$ are considered in the same time interval. A comparison of the tests for reversibility and obversibility is made in Table I.

Dissipation production is zero when configurations $\widetilde{\Gamma}_A$ and $\widetilde{\Gamma}_B$ are equally likely to be selected at $t = 0$. In such a case we say the specific evolution is *obversible*. If they are not equally likely, but the evolution interval is short such that $\widetilde{\Gamma}_B$ lies close to $\widetilde{\Gamma}_A$, the dissipation production will be small. However, $\widetilde{\Gamma}_B^*$ will typically be distant from $\widetilde{\Gamma}_A$ even after a short time interval. This is why it is important to define dissipation production in terms of a ratio of $p(\widetilde{\Gamma}_A, 0)$ to $p(\widetilde{\Gamma}_B, 0)$ rather than to $p(\widetilde{\Gamma}_B^*, 0)$, in order that it should vanish for a time interval of zero duration.

B. Bloch sphere representation

We consider a two-level quantum system characterized by a general state vector written in ket notation as

$$|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle, \tag{3}$$

where $\cos(\theta/2)$ and $e^{i\phi}\sin(\theta/2)$ are the amplitudes specifying the associated configuration $\widetilde{\Gamma}$. We can use θ and ϕ or Cartesian coordinates defined as

$$x = \sin\theta\cos\phi, \quad y = \sin\theta\sin\phi, \quad z = \cos\theta \tag{4}$$

to represent system configurations as points on the surface of a Bloch sphere [20]. Trajectories are then paths from an initial point on the Bloch sphere to another point representing the evolved configuration.

Unitary evolutions of a two-level quantum system, represented by the mapping S_t, generate continuous paths on the Bloch sphere, by analogy with a classical trajectory through coordinate phase space. Without loss of generality, we consider the mapping of $|\psi\rangle$ from an initial to a final state to be a rotation with unitary

$$S_t(\hat{\mathbf{n}}, \alpha(t)) = \mathbb{I}\cos(\alpha/2) - i\hat{\mathbf{n}}\cdot\hat{\boldsymbol{\sigma}}\sin(\alpha/2), \tag{5}$$

where $\hat{\mathbf{n}}$ is the (normalized) axis of rotation, α is the angle of rotation, and $\hat{\boldsymbol{\sigma}}$ is the vector of Pauli matrices. The angle of rotation depends on the duration of the evolution. Forward and obverse trajectories created by such a mapping are illustrated in Fig. 2. For a time-independent Hamiltonian, the trajectories are precisely rotations on the Bloch sphere, with the angle rotated proportional to elapsed time, but the mapping under Eq. (5) can also represent the final outcome of motion under a Hamiltonian that is time-dependent. As we are considering only deterministic evolution, no measurement process is involved, as this would introduce uncertainty of eigenstate projection into the dynamics.

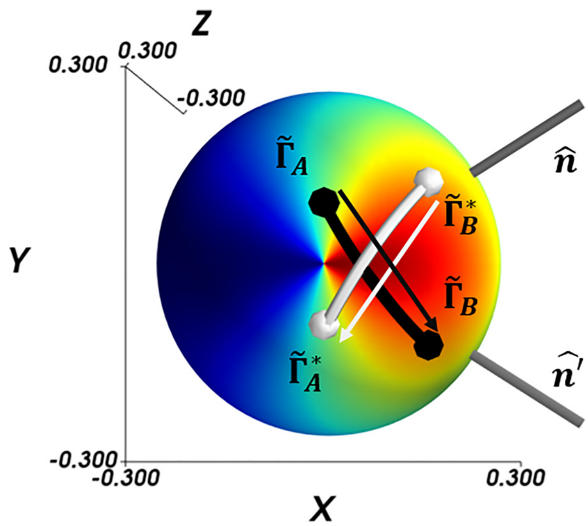

FIG. 2. Forward ($\tilde{\Gamma}_A$ to $\tilde{\Gamma}_B$) and obverse ($\tilde{\Gamma}^*_B$ to $\tilde{\Gamma}^*_A$) trajectories shown on the Bloch sphere, shown in black and white, respectively. The coloration of the sphere denotes the probability density of the initial configuration (red is high, blue low). The forward and obverse trajectories are produced by rotations about the $\hat{\mathbf{n}}$ and $\hat{\mathbf{n}}'$ axes, respectively.

In the Bloch sphere representation, the inversion operation, complex conjugation, is the transformation $\phi \to -\phi$. Furthermore, the dynamics conserve areas on the surface of the Bloch sphere, in the sense that a patch of size $d\tilde{\Gamma}_A$ is mapped under rotation to an equal size patch $d\tilde{\Gamma}_B$. We shall therefore be able to omit these increments in the definition of the dissipation production.

The choice of basis used to specify the ensemble of quantum state vectors is arbitrary, determining only which states are located at the poles of the Bloch sphere. As unitary transformations are rotations on the Bloch sphere, a change of basis merely alters the reference axes but not any feature such as the PDF displayed upon it. As the dissipation production is defined in terms of this PDF, the particular choice of basis will therefore not affect the values of ω_t.

C. Mathematical properties of dissipation production

1. Nonnegativity of mean dissipation production

It can be shown that the mean or expectation value of dissipation production is never negative. This property indicates that, just like stochastic entropy production, dissipation production satisfies a second law-like relation: it is *expected* to increase as time passes [21].

To prove the nonnegativity of the mean dissipation production, we start with the expression for the mean, which is

$$\langle \omega_t \rangle = \int p(\tilde{\Gamma}, 0) \ln \frac{p(\tilde{\Gamma}, 0)}{p(\tilde{\Gamma}_t, 0)}\, d\tilde{\Gamma}, \tag{6}$$

where $\tilde{\Gamma}$ and $\tilde{\Gamma}_t = S_t\tilde{\Gamma}$ are configurations and $p(\tilde{\Gamma}, \tau)$ is the PDF over configurations at time τ. Angled brackets represent an average. Note that this expression takes the form of a Kullback-Leibler (KL) divergence D_{KL} [22] between two PDFs, which is never negative. Formally, we could define $q(\tilde{\Gamma}, 0) = p(\tilde{\Gamma}_t, 0)$ such that $\langle \omega_t \rangle = D_{KL}(p||q)$. Note that this differs from a KL divergence between the initial and final PDFs $p(\tilde{\Gamma}, 0)$ and $p(\tilde{\Gamma}, t)$, which can correspond to the mean stochastic entropy production in certain circumstances.

Alternatively, it can be shown that the mean dissipation production is a nonnegative quantity by considering the average of its negative exponential:

$$\langle e^{-\omega_t} \rangle = \int p(\tilde{\Gamma}, 0) \frac{p(\tilde{\Gamma}_t, 0)}{p(\tilde{\Gamma}, 0)}\, d\tilde{\Gamma} = \int p(\tilde{\Gamma}_t, 0)\, d\tilde{\Gamma}. \tag{7}$$

Since $p(\tilde{\Gamma}_t, 0)$ is a normalized PDF, and the transformation $\tilde{\Gamma} \to \tilde{\Gamma}_t$ has a Jacobian of unity, we can write $\langle e^{-\omega_t} \rangle = 1$. Since $e^{-z} \geqslant 1 - z,\ z \in \mathbb{R}$, it follows that $\langle e^{-\omega_t} \rangle \geqslant 1 - \langle \omega_t \rangle$ allowing us to conclude that $\langle \omega_t \rangle \geqslant 0$. It should be noted that this emerges for both positive and negative t, namely, evolution into the future and into the past relative to the starting condition.

2. The Evans-Searles fluctuation theorem

A *fluctuation relation* [14,16,23] quantifies the extent to which a property such as stochastic entropy production evolves in a direction counter to that dictated by the second law of thermodynamics, recognizing that the latter holds only on average. The implication of such a relation is that fluctuations that "break" the second law are exponentially unlikely and are never apparent on a macroscopic scale.

Stochastic entropy production is known to obey a number of fluctuation relations [24]. Similarly, the dissipation production ω_t can satisfy a result known as the Evans-Searles Fluctuation Theorem (ESFT) in certain situations. Indeed, the ESFT provided the model and template for the later development of fluctuation relations.

The (rather abstract) requirements for deriving the ESFT [16,17] are that the probabilities of a pair of starting configurations, related by a mapping M^R, should be equal (i.e., a symmetry of the PDF exists), and there are trajectories yielding equal and opposite dissipation productions whose starting points are also related by M^R. These conditions can be expressed as

$$p(M^R\tilde{\Gamma}, 0) = p(\tilde{\Gamma}, 0) \tag{8}$$

and

$$\omega_t(\tilde{\Gamma}) = -\omega_t(M^R\tilde{\Gamma}_t). \tag{9}$$

M^R is a transformation that can be more general than the inversion map M^T used in Sec. II. Recall that $\tilde{\Gamma}_t = S_t\tilde{\Gamma}$ is the configuration to which $\tilde{\Gamma}$ evolves after time t. Given these two conditions, the derivation of the ESFT proceeds as follows. The PDF of dissipation production is

$$P(\omega) = \int d\tilde{\Gamma}\, p(\tilde{\Gamma}, 0)\delta[\omega_t(\tilde{\Gamma}) - \omega], \tag{10}$$

and we use the definition of ω_t from Sec. II to write

$$\begin{aligned} P(\omega) &= \int d\tilde{\Gamma}\, p(\tilde{\Gamma}, 0) e^{\omega_t(\tilde{\Gamma})} \frac{p(\tilde{\Gamma}_t, 0)}{p(\tilde{\Gamma}, 0)} \delta[\omega_t(\tilde{\Gamma}) - \omega] \\ &= e^{\omega} \int d\tilde{\Gamma}\, p(\tilde{\Gamma}_t, 0)\delta[\omega_t(\tilde{\Gamma}) - \omega]. \end{aligned} \tag{11}$$

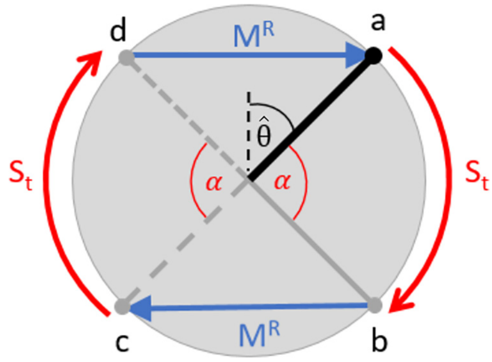

FIG. 3. Cross section of the Bloch sphere, looking down the rotation axis of the dynamics, geometrically illustrating that $M^R S_t M^R S_t = \mathbb{I}$. To see this, consider a point a on the surface of the Bloch sphere, with its position specified by angle $\hat{\theta}$. Application of evolution operator S_t will rotate this point to b: $\hat{\theta} \to \hat{\theta} + \alpha$. Then M^R will map b to c: $\hat{\theta} + \alpha \to 2\pi - (\hat{\theta} + \alpha)$. Applying S_t again sends c to d: $2\pi - (\hat{\theta} + \alpha) \to 2\pi - (\hat{\theta} + \alpha) + \alpha = 2\pi - \hat{\theta}$. A final application of M^R returns d to a.

Now we use the condition given in Eq. (9) to obtain

$$P(\omega) = e^{\omega} \int d\widetilde{\Gamma}_t p(\widetilde{\Gamma}_t, 0)\delta[-\omega_t(M^R\widetilde{\Gamma}_t) - \omega]. \tag{12}$$

Finally, Eq. (8) and a transformation of the integration measure give

$$\begin{aligned} P(\omega) &= e^{\omega} \int d(M^R\widetilde{\Gamma}_t)p(M^R\widetilde{\Gamma}_t, 0)\delta[\omega_t(M^R\widetilde{\Gamma}_t) + \omega] \\ &= e^{\omega}P(-\omega). \end{aligned} \tag{13}$$

This is the ESFT. Proofs in the literature employ a transformation that time inverts the evolved state, namely, an M^R given by M^T, but the result can clearly hold in more general circumstances. With $M^R = M^T$ we can employ the identity $M^T S_t^* M^T S_t = \mathbb{I}$ to show that condition (9) follows from (8), as long as the protocol of the dynamics is symmetric over the interval, i.e., $S_t^* = S_t$. The ESFT has previously been considered to arise in the complicated circumstances where the latter holds *and* the initial PDF is symmetric in the time-reversal operation.

We anticipate that the ESFT emerges in more general circumstances if the relation $M^R S_t M^R S_t = \mathbb{I}$ holds. This places a requirement on M^R: in our system the operation it represents must be a reflection in the plane containing the axis of rotation of the transformation S_t that implements the dynamics of the evolution. The requirement $p(M^R\widetilde{\Gamma}, 0) = p(\widetilde{\Gamma}, 0)$ further enforces a more stringent restriction that M^R is also a reflection in the plane of symmetry of the PDF. To see this, we can associate the operations as rotations about the axis and reflections in the plane as illustrated in Fig. 3.

In short, in situations where the rotation axis representing the evolution S_t lies in a plane of symmetry of the PDF of the initial state of the system, we shall observe an ESFT.

It is worth commenting on why the ESFT is of interest. When it holds, Eq. (13) shows clearly that the probability of a negative dissipation production is exponentially lower than the probability of a positive dissipation production of the same magnitude. Even though positive mean dissipation production holds quite generally, second law-like behavior of dissipation production becomes very apparent when the ESFT is satisfied. Second, the ESFT can be used to derive a symmetry in dissipation production into the past and future, to which we now turn.

3. Symmetry of mean dissipation production into future and past

Provided that the conditions for obtaining an ESFT are met, specifically that $M^R S_t M^R S_t = \mathbb{I}$ and $p(M^R\widetilde{\Gamma}, 0) = p(\widetilde{\Gamma}, 0)$, we can show that the mean dissipation production is the same for evolution into the past and the future. Starting from the mean dissipation production for evolution into the past:

$$\langle \omega_{-t} \rangle = \int p(\widetilde{\Gamma}, 0) \ln \frac{p(\widetilde{\Gamma}, 0)}{p(S_{-t}\widetilde{\Gamma}, 0)} d\widetilde{\Gamma}, \tag{14}$$

we recast as

$$\langle \omega_{-t} \rangle = \int p(M^R\widetilde{\Gamma}, 0) \ln \frac{p(M^R\widetilde{\Gamma}, 0)}{p(S_{-t}M^R\widetilde{\Gamma}, 0)} dM^R\widetilde{\Gamma}, \tag{15}$$

and apply $S_{-t}M^R = M^R S_t$ and Eq. (8) to get

$$\begin{aligned} \langle \omega_{-t} \rangle &= \int p(M^R\widetilde{\Gamma}, 0) \ln \frac{p(M^R\widetilde{\Gamma}, 0)}{p(M^R S_t\widetilde{\Gamma}, 0)} dM^R\widetilde{\Gamma} \\ &= \int p(\widetilde{\Gamma}, 0) \ln \frac{p(\widetilde{\Gamma}, 0)}{p(S_t\widetilde{\Gamma}, 0)} d\widetilde{\Gamma}, \end{aligned} \tag{16}$$

and hence $\langle \omega_{-t} \rangle$ is equal to the mean dissipation production for forward evolution, $\langle \omega_t \rangle$. However, in situations in which the ESFT is violated, we do not expect this result to hold, the implication being that the initial ensemble will exhibit different mean dissipation productions into the past and the future: a time asymmetry in expected failure of obversibility.

III. RESULTS

In order to demonstrate the range of behavior of dissipation production, we restrict ourselves to considering simple evolutions of the system represented by rotation matrices

$$S_{jk}(\hat{\boldsymbol{n}}, t) = \begin{cases} \cos^2 \frac{t}{2} + \sin^2 \frac{t}{2}\left(2\hat{n}_j^2 - 1\right), & \text{if } j = k \\ 2\hat{n}_j\hat{n}_k \sin^2 \frac{t}{2} - \varepsilon_{jkl}\hat{n}_l \sin t & \text{if } j \neq k \end{cases}, \tag{17}$$

where ε_{jkl} is the Levi-Civita symbol, the rotation angle α is equal to the elapsed time, t, and $(\hat{n}_x, \hat{n}_y, \hat{n}_z)$ is the rotation axis.

We consider four initial probability density functions over the Bloch sphere, specified using a combination of spherical polar and Cartesian coordinates:

Case 1: $p(\theta, \phi, t = 0) = (4\pi)^{-1}(1 + z)$ which is rotationally symmetric about the z axis.

Case 2a: $p(\theta, \phi, 0) = (4\pi)^{-1}(1 + \cos\theta)(1 + \cos\phi)$, which is symmetric with respect to the transformation $\phi \to -\phi$ and hence has mirror symmetry in the xz plane.

Case 2b: $p(\theta, \phi, 0) = (4\pi)^{-1}(1 + \cos\theta)[1 + \cos(\phi + \pi/4)]$, which is *not* symmetric with respect to the transformation $\phi \to -\phi$ but does have a plane of symmetry which passes through the z axis.

Case 3: $p(\theta, \phi, 0) = (8\pi)^{-1}(1 + \cos\theta)(2 + \cos\phi + \sin 2\phi)$, which is *not* symmetric with respect to the transformation $\phi \to -\phi$ and has no planes of symmetry.

Case 1 and Cases 2a and 2b are illustrated in Fig. 4, while the fully asymmetric Case 3 is shown later in this paper in Fig. 8.

In Fig. 5 we show PDFs of the dissipation production, ω_t, for Case 1, using rotations about the x axis through various angles to represent the transformation S_t over various times. The shape of the PDFs in Case 1 broadens as the elapsed time increases. These can be used to compute the logarithm of the ratio of probabilities of equal and opposite values of ω_t, and if a plot of this quantity against ω_t gives a straight line with unit gradient, then an ESFT holds. Since the PDF in Case 1 has rotational symmetry about the z axis, any axis of rotation defining S_t will lie in a plane of symmetry of the PDF, meeting the requirements for an ESFT described earlier. The inset in Fig. 5 demonstrates an ESFT for an example rotation of 2.1 radians about the x axis (i.e., $t = 2.1$).

To confirm further the conditions required to obtain an ESFT, we consider the more complicated Case 2a, which involves more structure in the initial PDF. For three evolutions consisting of rotation by $2\pi/3$ about each of the Cartesian axes, we generate Fig. 6. An ESFT holds for rotations about the x and z axes, which lie in the plane of symmetry of the PDF on the Bloch sphere, but it fails for rotation about the y axis which does not.

We also consider Case 2b, which is a rotated version of the PDF in Case 2a. It can be demonstrated numerically that an ESFT is satisfied for evolution corresponding to rotation about the z axis and remains violated for rotation about the y axis, but in contrast with Case 2a, an ESFT does *not* now hold for rotation about the x axis as this axis does not lie in the plane of symmetry of the Case 2b initial PDF.

When we observe an ESFT, we also expect symmetric behavior for the mean dissipation production for evolution into the future and the past, as discussed in Sec. II C 3. Figure 7, depicting $\langle\omega_t\rangle$ in Cases 2a and 2b for rotations about the z axis, illustrates this. Notice that mean dissipation production is nonnegative for the entire range of the rotation angle. Small angles of rotation give a small mean dissipation production, since in these instances there is little difference between the two configurations being compared.

The nonnegativity is universal and independent of choice of axis or Bloch sphere PDF, but the time-symmetric behavior accompanies only situations which satisfy an ESFT. We verify this by investigating Bloch sphere PDF Case 3, which has no planes of symmetry, and hence cannot give an ESFT, regardless of evolution rotation axis. Figure 8 demonstrates the associated time asymmetry in mean dissipation production for an example rotation about the z axis.

These considerations allow us to identify initial ensembles of quantum states which will exhibit time-asymmetric average behavior under a reversible unitary evolution. The dynamics are time-reversal symmetric, but the initial condition is not.

Table II specifies which combinations of PDF and rotation lead to the emergence of an ESFT. The results confirm that an ESFT depends on the relationship between the chosen rotation

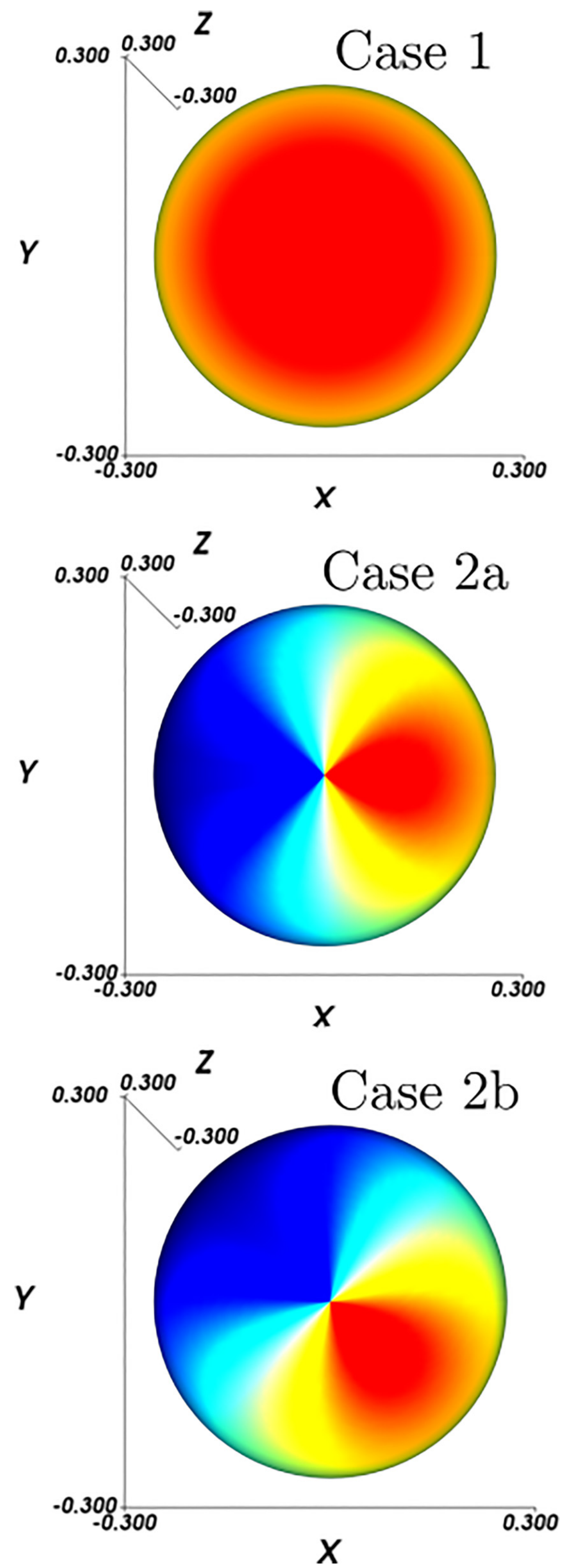

FIG. 4. Color denotes the magnitude of the PDF describing the initial ensemble at points on the Bloch sphere as viewed from the positive z direction: red is high, blue is low. Case 1: PDF with rotational symmetry about the z axis. Case 2a: PDF symmetric in the xz plane. Case 2b: PDF symmetric in plane passing through the z axis.

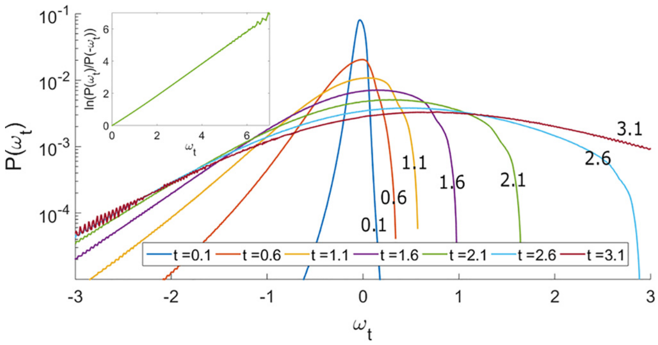

FIG. 5. Dissipation production for Case 1 depicted as PDFs for various elapsed times (i.e., rotations about the x axis). The inset confirms that an Evans-Searles Fluctuation Theorem (ESFT) holds for $t = 2.1$.

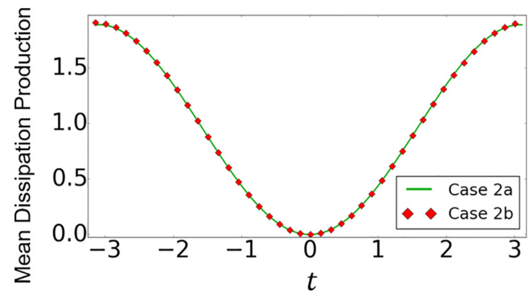

FIG. 7. Comparison of $\langle\omega_t\rangle$ for rotations of angle t about the z axis in Cases 2a and 2b. As both PDFs have a plane of symmetry passing through the z axis, there is symmetry in mean dissipation production for evolution into the future and the past. Furthermore, $\langle\omega_t\rangle$ is the same for both cases.

axis and the symmetry of the PDF on the Bloch sphere: when the rotation axis lies in a plane of symmetry of the PDF, the ESFT is upheld. The message is that the ESFT is by no means a universal feature.

IV. CONCLUSIONS

In quantum systems undergoing deterministic evolution, the statistical ensemble that represents subjective uncertainty with regard to the initial state vector can be used to specify the likelihood of observing a particular trajectory and its "obverse" counterpart, the latter being a reversal of the events of the forward trajectory, but starting at the same time. We test for irreversibility of behavior through the failure of *obversibility* (a property distinct from, but closely related to, *reversibility*), which we quantify with *dissipation production*. This first study of dissipation production in a quantum system extends the use of the concepts beyond the classical realm previously considered [17]. In particular, we are able to determine whether a system with a particular PDF describing the initial ensemble will exhibit time asymmetry in expected behavior under a particular process.

We have studied a simple two-level system, and our principal aim has been to identify conditions under which the dissipation production satisfies an Evans-Searles Fluctuation Theorem (ESFT), from which it follows that it evolves on average into the past in the same way as into the future. The evolution of states on the Bloch sphere after a given time interval under deterministic dynamics can be represented by a rotation about a specified axis, and the criterion for the validity of the ESFT is that this axis should lie in a plane of symmetry of the PDF describing the initial ensemble. It is also straightforward to demonstrate that the average dissipation production can never be negative, which makes it potentially a measure of irreversibility.

Obversibility is distinct from reversibility. The latter is upheld here owing to the deterministic unitary dynamics of an isolated system. Reversibility is essentially the property that the effects of carrying out a process can be undone by inverting velocities, carrying out a reverse process, and then inverting velocities again (in classical circumstances). Obversibility is the property that a process and its reverse starting from the same ensemble (its "obverse") may take place with equal likelihood [17].

Dissipation production is a consequence of a failure of obversibility and plays a role that is similar to,

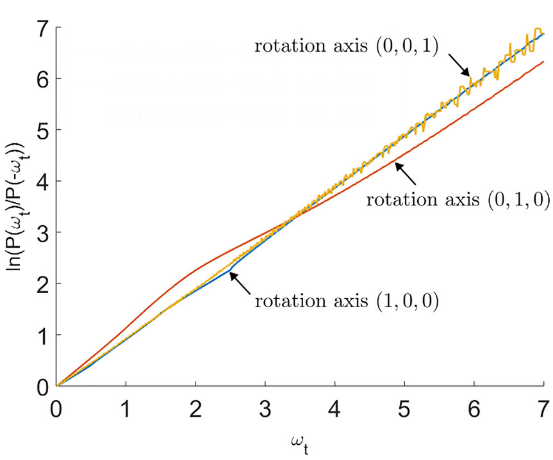

FIG. 6. The ESFT states that a PDF of dissipation production should satisfy $\ln[P(\omega_t)/P(-\omega_t)] = \omega_t$. Case 2a violates the ESFT for evolution consisting of a rotation about the y axis, which does not lie in the plane of symmetry of the PDF, while it is satisfied for rotations about the other Cartesian axes, through which the plane of symmetry does pass.

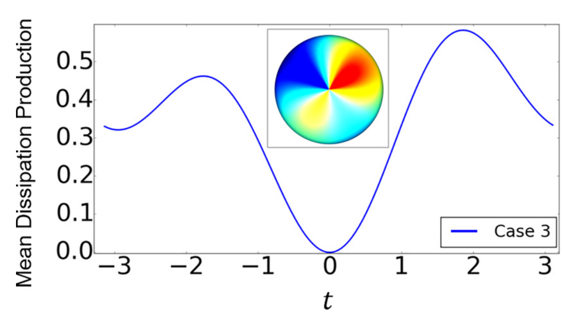

FIG. 8. $\langle\omega_t\rangle$ for rotations of angle t about the z axis in Case 3, for which a view of the PDF is shown as an inset. This PDF does *not* have a plane of symmetry passing through the rotation axis and an asymmetry in $\langle\omega_t\rangle$ for evolution into the future and the past emerges as a consequence.

TABLE II. Satisfaction of an ESFT for various cases of Bloch sphere PDFs when configurations are rotated by the dynamics about the Cartesian axes.

Axis	Case 1	Case 2a	Case 2b	Case 3
x	Yes	Yes	No	No
y	Yes	No	No	No
z	Yes	Yes	Yes	No

but distinct from, the stochastic entropy production that arises from a failure of reversibility. In a nonequilibrium stationary state, dissipation production and entropy production are synonymous, but this is not the case in more general situations. We have therefore broadened our understanding of quantities that might characterise the arrow of development in time. Furthermore, we have been able to demonstrate that time-asymmetric expected behavior for a closed quantum system can arise from certain asymmetries in the PDF describing the ensemble of initial states, a situation analogous to the Past Hypothesis. Dissipation production depends only on the probabilities of adopting particular states. It relies on classical uncertainties that reflect a lack of knowledge of the initial state, rather than quantum uncertainties due to a lack of predictability with regard to the outcomes of measurement. In any case, we have excluded the latter from our considerations.

We anticipate that the methods described here are readily applicable to larger systems, such as two qubits, since the tools required to calculate dissipation production (namely, PDFs of the system configuration and appropriate reversal and evolution operators) can be readily defined. For a general system it is likely that the ESFT will be upheld only under very special circumstances. These will always include situations where the PDF describing the initial ensemble obeys time-reversal symmetry and the protocol of dynamics is time-symmetric about its midpoint, as envisaged by Evans [14], but these are, nevertheless, rather exacting requirements.

We have seen that the failure of obversibility can be used as an indicator of irreversibility in a closed system where mechanical reversibility is respected. Such a failure can also be used as an indicator of irreversibility in systems that are *open* to the environment. The dynamics of such systems are mechanically irreversible and characterized by stochastic entropy production, but we could also compute dissipation production by inserting appropriate transition probabilities into Eq. (2). The relationship between reversibility and obversibility needs to be developed, giving further consideration to the role of initial conditions in generating time asymmetry of the irreversibility measures. Exploring dissipation production and obversibility in open quantum situations is hence an avenue for further research.

ACKNOWLEDGMENT

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[1] H. J. Kreuzer, *Nonequilibrium Thermodynamics and Its Statistical Foundations* (Clarendon Press, Oxford, 1981).
[2] J. L. Lebowitz, Boltzmann's entropy and time's arrow, Phys. Today **46**, 32 (1993).
[3] D. Z. Albert, *Time and Chance* (Harvard University Press, Cambridge, MA, 2009).
[4] U. Seifert, Entropy Production along a Stochastic Trajectory and an Integral Fluctuation Theorem, Phys. Rev. Lett. **95**, 040602 (2005).
[5] J.-P. Eckmann and D. Ruelle, Ergodic theory of chaos and strange attractors, Rev. Mod. Phys. **57**, 617 (1985).
[6] S. Deffner and E. Lutz, Nonequilibrium Entropy Production for Open Quantum Systems, Phys. Rev. Lett. **107**, 140404 (2011).
[7] J. M. Horowitz and J. M. Parrondo, Entropy production along nonequilibrium quantum jump trajectories, New J. Phys. **15**, 085028 (2013).
[8] C. Elouard, N. K. Bernardes, A. R. Carvalho, M. F. Santos, and A. Auffèves, Probing quantum fluctuation theorems in engineered reservoirs, New J. Phys. **19**, 103011 (2017).
[9] D. Matos, L. Kantorovich, and I. J. Ford, Stochastic entropy production for continuous measurements of an open quantum system, J. Phys. Commun. **6**, 125003 (2022).
[10] C. L. Clarke and I. J. Ford, Stochastic entropy production associated with quantum measurement in a framework of Markovian quantum state diffusion, arXiv:2301.08197 (2023).
[11] S. Watanabe, Information theoretical analysis of multivariate correlation, IBM J. Res. Dev. **4**, 66 (1960).
[12] D. L. Zhou, Irreducible Multiparty Correlations in Quantum States without Maximal Rank, Phys. Rev. Lett. **101**, 180505 (2008).
[13] T. Kang and S.-W. Li, The local relaxation and correlation production in the quantum Ising model, arXiv:2211.03050 (2022).
[14] D. J. Evans, E. G. D. Cohen, and G. P. Morriss, Probability of Second Law Violations in Shearing Steady States, Phys. Rev. Lett. **71**, 2401 (1993).
[15] D. J. Evans and D. J. Searles, Causality, response theory, and the second law of thermodynamics, Phys. Rev. E **53**, 5808 (1996).
[16] D. J. Evans and D. J. Searles, The fluctuation theorem, Adv. Phys. **51**, 1529 (2002).
[17] I. J. Ford, Measures of thermodynamic irreversibility in deterministic and stochastic dynamics, New J. Phys. **17**, 075017 (2015).
[18] R. E. Spinney and I. J. Ford, Fluctuation relations: A pedagogical overview, in *Nonequilibrium Statistical Physics of Small Systems: Fluctuation Relations and Beyond*, edited by R. J. Klages, W. Just, and C. Jarzynski (Wiley-VCH, Weinheim, 2013), pp 3–56.
[19] F. Haake, *Quantum Signatures of Chaos* (Springer Science & Business Media, 2013).
[20] M. A. Nielsen and I. Chuang, *Quantum Computation and Quantum Information* (AAPT, 2002).

[21] J. C. Reid, D. J. Evans, and D. J. Searles, Communication: Beyond Boltzmann's H-theorem: Demonstration of the relaxation theorem for a non-monotonic approach to equilibrium, J. Chem. Phys. **136**, 021101 (2012).

[22] S. Kullback and R. A. Leibler, On information and sufficiency, Ann. Math. Stat. **22**, 79 (1951).

[23] R. Harris and G. Schütz, Fluctuation theorems for stochastic dynamics, J. Stat. Mech.: Theory Exp. (2007) P07020.

[24] G. E. Crooks, Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences, Phys. Rev. E **60**, 2721 (1999).