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Jarzynski equality for quantum stochastic maps

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Jarzynski equality and related fluctuation theorems can be formulated for various setups. Such an equality was recently derived for nonunitary quantum evolutions described by unital quantum operations, i.e., for completely positive, trace-preserving maps, which preserve the maximally mixed state. We analyze here a more general case of arbitrary quantum operations on finite systems and derive the corresponding form of the Jarzynski equality. It contains a correction term due to nonunitality of the quantum map. Bounds for the relative size of this correction term are established and they are applied for exemplary systems subjected to quantum channels acting on a finite-dimensional Hilbert space.

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I. INTRODUCTION

Recent theoretical and experimental advances in dealing with small quantum systems has led to a growing interest in their mechanics and thermodynamics [1]. A certain amount of progress has been connected with studies of the Jarzynski equality [2] and related fluctuation theorems [3–6]. Recent attention is mainly focused on the quantum version of these results. Quantum analogs of the Jarzynski equality were first studied by Kurchan [7] and Tasaki [8]. Since then various topics connected with the fluctuation relations and the range of their validity and applicability were investigated.

There exist many ways to approach the Jarzynski equality [9–17]. Most of them are based on a dynamical description within an infinitesimal time scale. Making use of the perturbation approach, the author of Ref. [6] analyzed quantum fluctuation and work-energy theorems that focus on the time-reversal symmetry. We will advocate here a different approach applicable for systems which can be described by discrete quantum operations.

The formalism of quantum operations is one of the basic tools in studying dynamics of open quantum systems [18,19]. Fluctuation theorems for open quantum systems were recently considered in Refs. [20–24]. In particular, some results have been shown to be valid in the case of unital quantum operations, while the general case of quantum systems with time evolution described by nonunital stochastic maps remained not fully understood.

The main goal of this study is to relax the assumption of unitality and to generalize previous results for the entire class of stochastic maps, also called quantum channels. Another task of the work is to introduce a model discrete quantum dynamics acting on an N-dimensional system, which forms a useful generalization of the amplitude damping channel acting on a two-level system. This nonunital map channel and its extensions describe effects of energy loss in quantum systems due to an interaction with an environment [18,19]. Investigation of possible effects due to deviations from unitality of the map become relevant in the context of possible experimental tests of quantum fluctuation theorems.

Experimental study of fluctuation relations is easier in the classical regime [5]. Original formulations of the Jarzynski equality and the Crooks theorem were tested in experiments [25–29]. On the other hand, experimental investigation of quantum fluctuation relations is still forthcoming, although some possible experimental schemes were already discussed [30–33]. Existing proposals often deal with a single particle undergoing a unitary time evolution. Furthermore, current efforts to construct devices able to process quantum information might offer new possibilities to test quantum fluctuation relations. Notably, quantum systems are very sensitive to interaction with an environment. In this regard, fluctuations in systems with an arbitrary form of quantum evolution deserve theoretical analysis. Therefore, we do not focus our attention on a specific class of unital channels, but we study the most general form of arbitrary quantum operations.

The original formulations of the Jarzynski equality and the Tasaki-Crooks fluctuation theorem remain valid under the assumption that changes of the system state are represented by a unital quantum operation [22,23]. Attention to bistochastic maps is natural, when we deal with the Tasaki-Crooks fluctuation theorem. Indeed, its formulation involves both the forward quantum channel and its adjoint. If the latter channel preserves the trace, then the former one is necessarily unital.

Meantime, nonunital quantum channels are of interest in various respects. In this work we provide a formulation of the Jarzynski equality for arbitrary quantum operations. The contribution of our paper is twofold. First, we formulate a generalization of the Jarzynski equality for a nonunital quantum channel. Second, we investigate the problem for which the standard Jarzynski equality remains valid nonunital quantum channels.

This paper is organized as follows. In Sec. II, we introduce basic definitions and recall relevant results. The special case of unital channels and bistochastic maps is analyzed in Sec. III. In Sec. IV, we characterize nonunitality of an arbitrary quantum stochastic map while in Sec. V we generalize the corresponding Jarzynski equality for this class of maps and derive Eq. (43)—a key result of the paper. Several examples of nonunital quantum channels acting on two- and three-level systems are analyzed in Sec. VI. We investigate also a general model of nonunitary dynamics described in an arbitrary finite-dimensional Hilbert space which can be considered a generalization of the amplitude damping channel.

II. DEFINITIONS AND NOTATION

Let $\mathcal{L}(\mathcal{H})$ denote the space of linear operators on N-dimensional Hilbert space $\mathcal{H}$. By $\mathcal{L}_{\text{s.a.}}(\mathcal{H})$ and $\mathcal{L}_{+}(\mathcal{H})$, we respectively mean the real space of Hermitian operators and the set of positive ones. For arbitrary $\hat{A},\hat{B} \in \mathcal{L}(\mathcal{H})$, we define their Hilbert-Schmidt inner product by [34]

$$\langle \hat{A}\,,\hat{B}\rangle_{\text{hs}} := \text{Tr}(\hat{A}^{\dagger}\hat{B}). \tag{1}$$

This product induces the norm $\|\hat{A}\|_2 = \langle \hat{A}\,,\hat{A}\rangle_{\text{hs}}^{1/2}$. For any $\hat{A} \in \mathcal{L}(\mathcal{H})$, we put $|\hat{A}| \in \mathcal{L}_{+}(\mathcal{H})$ as a unique positive square root of $\hat{A}^{\dagger}\hat{A}$. The eigenvalues of $|\hat{A}|$ counted with multiplicities are the singular values of $\hat{A}$, written $s_j(\hat{A})$. For all real $p \geqslant 1$, the Schatten p norm is defined as [34]

$$\|\hat{A}\|_p := (\text{Tr}(|\hat{A}|^p))^{1/p} = \left(\sum_{j=1}^{N} s_j(\hat{A})^p\right)^{1/p}. \tag{2}$$

This family includes the trace norm $\|\hat{A}\|_1 = \text{Tr}|\hat{A}|$ for $p = 1$, the Hilbert-Schmidt (or Frobenius) norm $\|\hat{A}\|_2 = (\text{Tr}(\hat{A}^{\dagger}\hat{A}))^{1/2}$ for $p = 2$, and the spectral norm $\|\hat{A}\|_\infty = \max\{s_j(\hat{A}) : 1 \leqslant j \leqslant N\}$ for $p = \infty$. For all $q > p \geqslant 1$, we have

$$\|\hat{A}\|_q \leqslant \|\hat{A}\|_p. \tag{3}$$

This relation is actually a consequence of theorem 19 of the classical book of Hardy, Littlewood, and Polya [35].

For any state of the N-level system we are going to use the Bloch-vector representation, as it might be linked to experimental data [36]. By $\hat{\lambda}_j \in \mathcal{L}_{\text{s.a.}}(\mathcal{H})$, $j = 1,2,\dots,N^2-1$, we denote the generators of SU(N) which satisfy $\text{Tr}(\hat{\lambda}_j) = 0$ and

$$\text{Tr}(\hat{\lambda}_i\hat{\lambda}_j) = 2\delta_{ij}. \tag{4}$$

The factor 2 in Eq. (4) is rather traditional and may be chosen differently. Each traceless operator $\hat{X} \in \mathcal{L}_{\text{s.a.}}(\mathcal{H})$ can be then represented in terms of its Bloch vector as [19,36]

$$\hat{X} = \frac{1}{2}\sum_{j=1}^{N^2-1} \tau_j\hat{\lambda}_j, \quad \tau_j = \text{Tr}(\hat{X}\hat{\lambda}_j). \tag{5}$$

Thus, we represent a traceless Hermitian $\hat{X}$ by means of the corresponding (N^2-1)-dimensional real vector $\boldsymbol{\tau} = (\tau_1,\tau_2,\dots,\tau_{N^2-1})$. For the case $N = 2$, the generators are the standard Pauli matrices $\hat{\sigma}_j$, where $j = 1,2,3$. In the case $N = 3$, the eight Gell-Mann matrices are commonly used. In N-dimensional space $\mathcal{H}$, the completely mixed state is expressed as

$$\hat{\rho}_* = \frac{1}{N}\,\mathbb{1}, \tag{6}$$

where $\mathbb{1}$ is the identity operator on $\mathcal{H}$. For a given density matrix $\hat{\rho}$, the operator $\hat{\rho} - \hat{\rho}_*$ is traceless, whence a Bloch representation of $\hat{\rho}$ follows Refs. [19,36].

Let us consider a linear map $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$ that takes elements of $\mathcal{L}(\mathcal{H}_A)$ to elements of $\mathcal{L}(\mathcal{H}_B)$. This map is called positive if $\Phi(\hat{A}) \in \mathcal{L}_{+}(\mathcal{H}_B)$ whenever $\hat{A} \in \mathcal{L}_{+}(\mathcal{H}_A)$ [37]. To describe physical processes, linear maps have to be completely positive [18,19]. Let id_R be the identity map on $\mathcal{L}(\mathcal{H}_R)$, where the space $\mathcal{H}_R$ is assigned to a reference system. The complete positivity implies that the map $\Phi \otimes \text{id}_R$ is positive for any dimension of the auxiliary space $\mathcal{H}_R$. The authors of Ref. [38] examined an important question, whether the dynamics of open quantum systems is always linear. Further, we will consider only completely positive linear maps. A completely positive map Φ can be written by an operator-sum representation,

$$\Phi(\hat{A}) = \sum_n \hat{K}_n\hat{A}\hat{K}_n^{\dagger}. \tag{7}$$

Here, the Kraus operators $\hat{K}_n$ map the input space $\mathcal{H}_A$ to the output space $\mathcal{H}_B$. When physical process is closed and the probability is conserved, the map preserves the trace, $\text{Tr}(\Phi(\hat{A})) = \text{Tr}(\hat{A})$. This relation satisfied for all $\hat{A} \in \mathcal{L}(\mathcal{H}_A)$ is equivalent to the following constraint for the set of the Kraus operators:

$$\sum_n \hat{K}_n^{\dagger}\hat{K}_n = \mathbb{1}_A. \tag{8}$$

Here $\mathbb{1}_A$ denotes the identity operator on the input space $\mathcal{H}_A$. By the cyclic property and the linearity of the trace, formula (8) implies $\text{Tr}(\Phi(\hat{A})) = \text{Tr}(\hat{A})$ for all $\hat{A} \in \mathcal{L}(\mathcal{H}_A)$. To each linear map $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$, one assigns its adjoint map, $\Phi^{\dagger} : \mathcal{L}(\mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$. For all $\hat{A} \in \mathcal{L}(\mathcal{H}_A)$ and $\hat{B} \in \mathcal{L}(\mathcal{H}_B)$, the adjoint map is defined by [34]

$$\langle \Phi(\hat{A}),\hat{B}\rangle_{\text{hs}} = \langle \hat{A}\,,\Phi^{\dagger}(\hat{B})\rangle_{\text{hs}}. \tag{9}$$

For a completely positive map (7), its adjoint is written as $\Phi^{\dagger}(\hat{B}) = \sum_n \hat{K}_n^{\dagger}\hat{B}\hat{K}_n$. If this adjoint is trace preserving, the Kraus operators of Eq. (7) satisfy the condition

$$\sum_n \hat{K}_n\hat{K}_n^{\dagger} = \mathbb{1}_B. \tag{10}$$

In other words, we have $\Phi(\mathbb{1}_A) = \mathbb{1}_B$. In this case, the map is said to be unital [37]. If a quantum map is completely positive and the Kraus operators satisfy properties (8) and (10) the map is called bistochastic [19], as it can be considered as an analog to the standard bistochastic matrix, which acts in the space of probability vectors. A quantum map Φ can be characterized using the norm

$$\|\Phi\| := \sup\{\|\Phi(\hat{A})\|_\infty :\ \|\hat{A}\|_\infty = 1\}. \tag{11}$$

Let us quote here one of useful results concerning the norm of a map. If a map Φ is positive, then

$$\|\Phi\| = \|\Phi(\mathbb{1})\|_\infty, \tag{12}$$

see Bhatia [37], item 2.3.8. In terms of the completely mixed state (6), we have $\|\Phi\| = N\,\|\Phi(\hat{\rho}_*)\|_\infty$.

The Jamiołkowski isomorphism [39] leads to another convenient description of completely positive maps. We recall its formulation for the symmetric case if both dimensions are equal, $\mathcal{H}_A = \mathcal{H}_B = \mathcal{H}$. The principal system A is extended by an auxiliary reference system R of the same dimension N. Let $\{|n\rangle\}$ be an orthonormal basis in $\mathcal{H}$. Making use of this basis in both subspaces, we define a maximally entangled normalized pure state,

$$|\phi_+\rangle := \frac{1}{\sqrt{N}} \sum_{n=1}^{N} |n\rangle \otimes |n\rangle. \tag{13}$$

For any linear map $\Phi : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$, we assign an operator

$$\hat{\eta}(\Phi) := \Phi \otimes \mathrm{id}_R(|\phi_+\rangle\langle\phi_+|), \tag{14}$$

which acts on the extended space $\mathcal{H} \otimes \mathcal{H}$. The matrix $\hat{D}(\Phi) = N\,\hat{\eta}(\Phi)$ is usually called *dynamical matrix* or *Choi matrix* [40]. For any $\hat{X} \in \mathcal{L}(\mathcal{H})$, the action of the map Φ can be recovered from $\hat{D}(\Phi)$ by means of the relation [34]

$$\Phi(\hat{X}) = \mathrm{Tr}_R(\hat{D}(\Phi)(\mathbb{1} \otimes \hat{X}^T)), \tag{15}$$

in which $\hat{X}^T$ is the transpose operator to $\hat{X}$. The complete positivity of Φ is equivalent to the positivity of the dynamical matrix $\hat{D}(\Phi)$. The map Φ preserves the trace if and only if its dynamical matrix satisfies [34]

$$\mathrm{Tr}_A(\hat{D}(\Phi)) = \mathbb{1}. \tag{16}$$

In a shortened notation, we will write the dynamical matrix and the rescaled one as $\hat{D}_\Phi$ and $\hat{\eta}_\Phi$, respectively. Substituting the completely mixed state $\hat{\rho}_* = \mathbb{1}/N$ into Eq. (15), we obtain

$$\Phi(\hat{\rho}_*) = \mathrm{Tr}_R(\hat{\eta}_\Phi). \tag{17}$$

In the subsequent section we will examine a nonunitality operator, closely related with the partial trace (17).

III. JARZYNSKI EQUALITY FOR BISTOCHASTIC MAPS

We will consider the case in which a thermostatted system is operated by an external agent. It is assumed that this agent acts according to a specified protocol. Hence, the Hamiltonian of the system is time dependent. To formulate the Jarzynski equality, a special kind of averaging procedure is required [8,41]. Initially, we describe this procedure for arbitrary two Hermitian operators. Let us consider operators $\hat{A} \in \mathcal{L}_{\mathrm{s.a.}}(\mathcal{H}_A)$ and $\hat{B} \in \mathcal{L}_{\mathrm{s.a.}}(\mathcal{H}_B)$. In terms of the eigenvalues and the corresponding eigenstates, spectral decompositions are expressed as

$$\hat{A} = \sum_i a_i\, |a_i\rangle\langle a_i|, \tag{18}$$

$$\hat{B} = \sum_j b_j\, |b_j\rangle\langle b_j|. \tag{19}$$

The eigenvalues in both decompositions are assumed to be taken according to their multiplicity. In this regard, we treat a_i and b_j as the labels for vectors of the orthonormal bases $\{|a_i\rangle\}$ and $\{|b_j\rangle\}$. Let evolution of the system in time be represented by a quantum channel Φ. If the input state is described by an eigenstate $|a_i\rangle$, then the output of the channel is $\Phi(|a_i\rangle\langle a_i|)$. Suppose that we measure the observable $\hat{B}$ in this output state. The outcome b_j occurs with the probability

$$p(b_j|a_i) = \langle b_j|\Phi(|a_i\rangle\langle a_i|)|b_j\rangle. \tag{20}$$

This quantity can also be interpreted as the conditional probability of the outcome b_j given that the input state is $|a_i\rangle$. The trace-preserving condition implies that

$$\sum_j p(b_j|a_i) = \mathrm{Tr}(\Phi(|a_i\rangle\langle a_i|)) = 1. \tag{21}$$

The standard requirement on conditional probabilities is thus satisfied for any quantum channel. Furthermore, we suppose that the input density matrix $\hat{\rho}_A$ has the form

$$\hat{\rho}_A = \sum_i p(a_i)|a_i\rangle\langle a_i|, \tag{22}$$

where $\sum_i p(a_i) = 1$. According to Bayes's rule, one defines the joint probability distribution with elements

$$p(a_i,b_j) = p(a_i)\, p(b_j|a_i). \tag{23}$$

This is the probability that we find the system in the i-th eigenstate of $\hat{A}$ at the input and in the j-th eigenstate of $\hat{B}$ at the output. Let $f(a,b)$ be a function of two eigenvalues. Following Ref. [8], we define the corresponding average

$$\langle\!\langle f(a,b)\rangle\!\rangle := \sum_{ij} p(a_i,b_j)\, f(a_i,b_j). \tag{24}$$

Double angular brackets in the left-hand side denote the averaging over the ensemble of possible pairs of measurement outcomes. A pair of single angular brackets denotes an expectation value of an observable $\hat{A}$ in a state $\hat{\rho}$, in consistence with the standard notation common in quantum theory, $\langle\hat{A}\rangle = \mathrm{Tr}(\hat{\rho}\hat{A})$. More general forms of the described scenario were considered in Refs. [20,22].

The Jarzynski equality relates an averaged work with the difference between the equilibrium free energies. Since the notion of work pertains to a process, it cannot be represented as a quantum observable [5,42]. A more detailed discussion of the notion of work in the context of quantum fluctuation theorems was recently provided by Van Vliet [6].

In any case, the energy can be measured twice, at the initial and the final moments. The difference between outcomes of these two measurements describes the work performed on the system in a particular realization [42]. Therefore, the averaging of the form (24) is used with respect to two Hermitian operators: the initial and the final Hamiltonians $\hat{H}_0$ and $\hat{H}_1$.

Fluctuation theorems are usually obtained under the assumption that the work is determined by projective measurements at the beginning and the end of each run of the protocol. In several cases one applies, however, much broader classes of quantum measurements. Recently Venkatesh *et al.* [43] analyzed fluctuation theorems for protocols in which generalized quantum measurements are used.

In this paper we discuss the most general case of a discrete nonunitary dynamics and consider arbitrary measurements which are error-free in the following sense: With each outcome of a generalized measurement, we can uniquely identify the corresponding eigenstate of an actual Hamiltonian [43].

The system under investigation is initially prepared in the state of the thermal equilibrium with a heat reservoir. It is convenient to denote the inverse temperatures of the reservoir at the beginning and at the end of the protocol, by β_0 and β_1, respectively. In principle, these two temperatures may differ, but in the following we will eventually discuss the case in which both temperatures are equal. The initial density matrix reads

$$\hat{\omega}_0(\beta_0) = Z_0(\beta_0)^{-1}\exp(-\beta_0\hat{H}_0), \tag{25}$$

where $Z_0(\beta_0) = \mathrm{Tr}(\exp(-\beta_0\hat{H}_0))$ is the corresponding partition function. We further suppose that the transformation of states of the system is represented by a quantum channel Φ, which maps the set of density matrices of size N onto itself. In general, the final density matrix $\Phi(\hat{\omega}_0(\beta_0))$ differs from the matrix

$$\hat{\omega}_1(\beta_1) = Z_1(\beta_1)^{-1}\exp(-\beta_1\hat{H}_1), \tag{26}$$

corresponding to the equilibrium at the final moment. Here, the partition function $Z_1(\beta_1) = \mathrm{Tr}(\exp(-\beta_1\hat{H}_1))$ corresponds to the state of the thermal equilibrium with the final Hamiltonian $\hat{H}_1$.

Eigenvalues of the Hamiltonians $\hat{H}_0$ and $\hat{H}_1$ will be denoted by $\{\varepsilon_m^{(0)}\}$ and $\{\varepsilon_n^{(1)}\}$, respectively. Let channel Φ be unital. Using notation (24) for a function of two eigenvalues, we then obtain

$$\begin{aligned}\langle\langle \exp(\beta_0\varepsilon^{(0)} - \beta_1\varepsilon^{(1)})\rangle\rangle &\equiv \sum_{mn} p\big(\varepsilon_m^{(0)},\varepsilon_n^{(1)}\big)\exp\big(\beta_0\varepsilon_m^{(0)} - \beta_1\varepsilon_n^{(1)}\big)\\ &= \frac{Z_1(\beta_1)}{Z_0(\beta_0)}.\end{aligned} \tag{27}$$

This result was recently derived in Ref. [23] and earlier by Tasaki [8] under a weaker assumption of a unitary evolution. Formula (27) directly leads to the Jarzynski equality formulated for unital quantum channels.

In the approach considered the term $W_{nm} = \varepsilon_n^{(1)} - \varepsilon_m^{(0)}$ is naturally identified with the external work performed on the principal system during the process [8,24]. In the case $\beta_0 = \beta_1 = \beta$, formula (27) gives

$$\langle\langle \exp(-\beta W)\rangle\rangle = \exp(-\beta\Delta F), \tag{28}$$

where the equilibrium free energies read $F_{0,1}(\beta) = -\beta^{-1}\ln Z_{0,1}(\beta)$. Expression (28) relates, on average, the nonequilibrium external work with the difference between the equilibrium free energies, $\Delta F = F_1 - F_0$. Thus the above statement can be interpreted as a version of the original Jarzynski equality [2,9], which holds for an arbitrary unital quantum channel.

Some other approaches to obtaining the quantum Jarzynski equality were recently considered by Vedral [20] and Albash *et al.* [22]. Furthermore, formula (28) was derived in [23] directly from Eq. (27) for any bistochastic channel. In the following we shall relax the unitality condition and generalize this reasoning for nonunital quantum maps.

IV. NONUNITALITY OBSERVABLE

In this section, we introduce a notion useful to analyze the Jarzynski equality for quantum stochastic maps. In order to characterize deviation from unitality, we are going to use the following operator. For any trace-preserving map $\Phi : \mathcal{L}(\mathcal{H}_A) \to \mathcal{L}(\mathcal{H}_B)$, one assigns a traceless operator

$$\hat{G}_\Phi := \Phi(\hat{\rho}_{*A}) - \hat{\rho}_{*B}, \tag{29}$$

where $\hat{\rho}_{*A} = \mathbb{1}_A/N_A$ and $\hat{\rho}_{*B} = \mathbb{1}_B/N_B$. This operator is Hermitian, i.e., $\hat{G}_\Phi \in \mathcal{L}_{\mathrm{s.a.}}(\mathcal{H}_B)$, whenever the map Φ is Hermiticity preserving. Let us derive a useful statement about the above nonunitality operator. For given two operators $\hat{A} \in \mathcal{L}_{\mathrm{s.a.}}(\mathcal{H}_A)$, $\hat{B} \in \mathcal{L}_{\mathrm{s.a.}}(\mathcal{H}_B)$ and real parameters α, β, we introduce the density matrices

$$\hat{\varrho}_A(\alpha) := \mathrm{Tr}(\exp(-\alpha\hat{A}))^{-1}\exp(-\alpha\hat{A}), \tag{30}$$

$$\hat{\varrho}_B(\beta) := \mathrm{Tr}(\exp(-\beta\hat{B}))^{-1}\exp(-\beta\hat{B}). \tag{31}$$

Functional forms of such a kind pertain to equilibrium in the Gibbs canonical ensemble. We will consider average of the type (24) with respect to the density matrices (30) and (31) at the input and output, respectively. The following statement holds true.

Proposition 1. Let $\hat{A} \in \mathcal{L}_{\mathrm{s.a.}}(\mathcal{H}_A)$, $\hat{B} \in \mathcal{L}_{\mathrm{s.a.}}(\mathcal{H}_B)$, and let α and β be real numbers. If the input state is described by density matrix (30), then the average defined in Eq. (24) reads

$$\begin{aligned}&\langle\langle \exp(\alpha a - \beta b)\rangle\rangle\\ &\quad = \frac{N_A\mathrm{Tr}(\exp(-\beta\hat{B}))}{N_B\mathrm{Tr}(\exp(-\alpha\hat{A}))}(1 + N_B\mathrm{Tr}(\hat{\varrho}_B(\beta)\hat{G}_\Phi)).\end{aligned} \tag{32}$$

Proof. Using the linearity of the map Φ and Eq. (29), we obtain

$$\begin{aligned}\sum_i p(b_j|a_i) &= \langle b_j|\sum_i \Phi(|a_i\rangle\langle a_i|)|b_j\rangle\\ &= N_A\langle b_j|\Phi(\hat{\rho}_{*A})|b_j\rangle = \frac{N_A}{N_B} + N_A\langle b_j|\hat{G}_\Phi|b_j\rangle.\end{aligned} \tag{33}$$

Taking $p(a_i) = \mathrm{Tr}(\exp(-\alpha\hat{A}))^{-1}\exp(-\alpha a_i)$ in Eq. (23) and using Eq. (33), we represent the left-hand side of Eq. (32) in the form

$$\begin{aligned}&\sum_{ij}\frac{\exp(-\alpha a_i)}{\mathrm{Tr}(\exp(-\alpha\hat{A}))}\,p(b_j|a_i)\exp(\alpha a_i - \beta b_j)\\ &\quad = \frac{N_A}{N_B\mathrm{Tr}(\exp(-\alpha\hat{A}))}\sum_j \exp(-\beta b_j)(1 + N_B\langle b_j|\hat{G}_\Phi|b_j\rangle).\end{aligned} \tag{34}$$

The latter term is easily rewritten as the right-hand side of Eq. (32). ■

If the operator $\Phi(\mathbb{1}_A)$ is proportional to $\mathbb{1}_B$, we have $\Phi(\mathbb{1}_A) = (N_A/N_B)\mathbb{1}_B$ by the trace preservation. In this case, the right-hand side of Eq. (29) becomes zero. Then relation (32) is reduced to the previous result given for unital channels in Ref. [23]. A deviation from unitality can be quantified by norms of the operator (29). In the following, the case $N_A = N_B = N$ will be considered. That is, the input and output Hilbert spaces have the same dimension N. Note that two different quantum channels may lead to the same non-unitality observable. This Hermitian operator is traceless and belongs to the space $\mathcal{L}_{\mathrm{s.a.}}(\mathcal{H})$ of dimensionality N^2. Due to the Jamiołkowski isomorphism, the set of quantum channels is isomorphic with the set of their dynamical matrices satisfying Eq. (16). As the latter set has $N^4 - N^2$ real dimensions [19], there is no one-to-one correspondence between quantum channels and the nonunitality operators. Let us estimate the

Hilbert-Schmidt norm of the operator $\hat{G}_\Phi$ from above. The following bound holds.

Proposition 2. Let $\mathcal{H}$ be N-dimensional Hilbert space. If $\Phi : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$ is positive and trace preserving, then

$$\|\Phi(\mathbb{1}) - \mathbb{1}\|_2 \leqslant \sqrt{N(\|\Phi\| - 1)}. \tag{35}$$

Proof. As the map is positive and trace preserving, we have $\Phi(\mathbb{1}) \in \mathcal{L}_+(\mathcal{H})$ and $\mathrm{Tr}(\Phi(\mathbb{1})) = \mathrm{Tr}(\mathbb{1}) = N$. Hence, the squared Hilbert-Schmidt norm is expressed as

$$\langle \Phi(\mathbb{1}) - \mathbb{1}, \Phi(\mathbb{1}) - \mathbb{1}\rangle_{\mathrm{hs}} = \|\Phi(\mathbb{1})\|_2^2 - N. \tag{36}$$

By positivity, we obtain $\|\Phi(\mathbb{1})\|_1 = \mathrm{Tr}(\Phi(\mathbb{1})) = N$. Lemma 3 of Ref. [44] states that $\|\hat{A}\|_2^2 \leqslant \|\hat{A}\|_\infty \|\hat{A}\|_1$ for all $\hat{A} \in \mathcal{L}(\mathcal{H})$. Combining these points with Eq. (36) finally leads to

$$\|\Phi(\mathbb{1}) - \mathbb{1}\|_2^2 \leqslant N(\|\Phi(\mathbb{1})\|_\infty - 1). \tag{37}$$

The claim (35) follows from Eqs. (12) and (37). ■

Using Eq. (17) we rewrite Eq. (35) in the form

$$\|\mathrm{Tr}_R(\hat{\eta}_\Phi) - \hat{\rho}_*\|_2 \leqslant N^{-1/2}\sqrt{\|\Phi\| - 1}. \tag{38}$$

In terms of the map norm, one characterizes a deviation of the partial trace of the rescaled dynamical matrix from the completely mixed state. If the map Φ is unital one has $\Phi(\mathbb{1}) = \mathbb{1}$ and $\|\Phi(\mathbb{1})\|_\infty = 1$. Using Eq. (12), the right-hand side of Eq. (35) vanishes for unital maps. On the other hand, the condition $\|\Phi\| = 1$ immediately leads to the relation $\|\Phi(\mathbb{1}) - \mathbb{1}\|_2 = 0$. The latter is equivalent to $\Phi(\mathbb{1}) = \mathbb{1}$, since the norm cannot be equal to zero for a nonzero matrix, which completes the reasoning.

Corollary 3. Let $\Phi : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$ be positive and trace preserving. If $\|\Phi\| = 1$, then Φ is unital, i.e., $\Phi(\mathbb{1}) = \mathbb{1}$.

It is instructive to compare this result with the Russo-Dye theorem. One of its formulations says that if a positive map Φ is unital, then $\|\Phi\| = 1$ (see, e.g., point 2.3.7 of Ref. [37]). In a certain sense, Corollary 3 is a statement in the opposite direction. Namely, if a trace-preserving positive map Φ obeys $\|\Phi\| = 1$, then it is necessarily unital. Note that this conclusion pertains to all trace-preserving positive maps and not only to completely positive ones. Although legitimate quantum operations are completely positive, positive maps without complete positivity are often used as an auxiliary tool in the theory of quantum information. For instance, one of the basic methods to detect quantum entanglement is formulated in terms of entanglement witnesses and positive maps [45].

Due to (35), a deviation from unitality is characterized by the difference between the norm $\|\Phi\|$ and unity. It is possible to find an upper bound for this quantity in terms of the dimension N of the Hilbert space. From Eq. (3), we obtain $\|\Phi(\mathbb{1})\|_\infty \leqslant N = \|\Phi(\mathbb{1})\|_1$. Combining this with Eqs. (12) and (35) we get

$$\|\Phi(\mathbb{1}) - \mathbb{1}\|_2 \leqslant \sqrt{N(N-1)}. \tag{39}$$

This inequality is valid for all trace-preserving positive maps $\Phi : \mathcal{L}(\mathcal{H}) \to \mathcal{L}(\mathcal{H})$, including quantum channels with the same input and output spaces. Rescaling the above bound by the dimensionality, we have

$$\|\hat{G}_\Phi\|_2 \leqslant (\|\Phi(\hat{\rho}_*)\|_\infty - N^{-1})^{1/2} \leqslant \sqrt{1 - 1/N}. \tag{40}$$

Thus, the Hilbert-Schmidt norm of the operator $\hat{G}_\Phi = \Phi(\hat{\rho}_*) - \hat{\rho}_*$ is strictly less than 1. The left-hand side of Eq. (40) can be interpreted as the Hilbert-Schmidt distance between $\Phi(\hat{\rho}_*)$ and $\hat{\rho}_*$. This distance is maximal if inequality (40) is saturated so the output state $\Phi(\hat{\rho}_*) = |\psi\rangle\langle\psi|$ is pure. This is the case for the map generated by Kraus operators $\hat{K}_n = |\psi\rangle\langle n|$, where the $\{|n\rangle\}$ is an orthonormal basis in $\mathcal{H}$. Such a map represents a complete contraction to a pure state: For any state $\hat{\rho}$ one has $\Phi(\hat{\rho}) = |\psi\rangle\langle\psi|$. Taking $|\psi\rangle$ as a ground state one can describe in this way the process of spontaneous emission in atomic physics.

Systems near the thermal equilibrium can be treated as ergodic in the following sense: Any quantum state can be reached, directly or indirectly, from any other state. In this regard, the completely contracting channel has opposite properties, as for any initial state only a single state $|\psi\rangle$ can be reached during the process.

Using representation (5), the nonunitality operator $\hat{G}_\Phi$ can be represented in terms of its generalized Bloch vector $\boldsymbol{\tau}$ [40,46] with components $\tau_j = \mathrm{Tr}(\hat{G}_\Phi \hat{\lambda}_j)$. Therefore we arrive at a handy expression for the nonunitality operator, $\hat{G}_\Phi = (1/2)\,\boldsymbol{\tau} \cdot \hat{\boldsymbol{\lambda}}$, where $\hat{\boldsymbol{\lambda}}$ denotes the $(N^2 - 1)$-dimensional vector of generators of SU(N). We also obtain an upper bound for the modulus of the Bloch vector,

$$|\boldsymbol{\tau}| \leqslant \sqrt{2}\,(\|\Phi(\hat{\rho}_*)\|_\infty - N^{-1})^{1/2} \leqslant \sqrt{2 - 2/N}. \tag{41}$$

It follows from Eq. (40) and the expression for the squared Hilbert-Schmidt norm $\langle \hat{G}_\Phi, \hat{G}_\Phi\rangle_{\mathrm{hs}} = (1/2)\sum_{j=1}^{N^2-1} \tau_j^2$. In the case $N = 2$, the bound (41) gives $|\boldsymbol{\tau}| \leqslant 1$ for all quantum channels, as in the normalization used in this work the set of one-qubit states forms the Bloch ball of radius one. The right-hand side of Eq. (41) tends to $\sqrt{2}$ for large N.

V. JARZYNSKI EQUALITY FOR ARBITRARY STOCHASTIC MAPS

We now apply Eq. (32) in a physical setup corresponding to the context of the Jarzynski equality [1]. One assumes that a thermostatted system is acted upon by an external agent, which operates according to the prescribed protocol. The principal system is assumed to be prepared initially in the state of the thermal equilibrium with a heat reservoir. As before we denote the initial and the final inverse temperatures of the reservoir by β_0 and β_1. Therefore, the input state is described by density matrix (25). According to the actual process, the final density matrix $\Phi(\hat{\omega}_0(\beta_0))$ may differ from the state (26), which corresponds to the equilibrium at the final moment. Considering the same system, we also assume that both dimensions are equal, $N_A = N_B = N$. By substitutions, relation (32) leads to the equality

$$\langle\langle \exp(\beta_0 \varepsilon^{(0)} - \beta_1 \varepsilon^{(1)})\rangle\rangle = \frac{Z_1(\beta_1)}{Z_0(\beta_0)}(1 + N\mathrm{Tr}(\hat{\omega}_1(\beta_1)\hat{G}_\Phi)). \tag{42}$$

For unital quantum channels, the term $N\mathrm{Tr}(\hat{\omega}_1(\beta_1)\hat{G}_\Phi)$ is zero, so formula (42) forms an extension of the previous result (27) and for a unitary evolution it reduces to the result of Tasaki [8]. The right-hand side of Eq. (42) depends not only on equilibrium properties of the system but also on the realized process. The authors of Ref. [4] emphasized such a feature in connection with nonequilibrium relations for the exponentiated internal energy and heat.

Note also that concrete details of the realized quantum process are represented by means of a single operator $\hat{G}_\Phi$. To formulate fluctuation relation (42), no additional characterization of the map is required. In this regard, we need not to specify a kind of coupling between the principal system and its environment.

The quantity $W_{nm} = \varepsilon_n^{(1)} - \varepsilon_m^{(0)}$ can be identified with the external work performed on the principal system during a process [8,24]. For the case $\beta_0 = \beta_1 = \beta$, formula (42) leads to a generalized form of the Jarzynski equality for arbitrary, nonunital quantum channels,

$$\langle\langle \exp(-\beta W) \rangle\rangle = \exp(-\beta \Delta F)(1 + N\mathrm{Tr}(\hat{\omega}_1(\beta)\hat{G}_\Phi)). \quad (43)$$

This is the central result of the present work. The correction term $N\mathrm{Tr}(\hat{\omega}_1(\beta)\hat{G}_\Phi)$ characterizes a deviation induced by the nonunitality of a map. In general, this term can be positive, equal to zero, or negative. If the channel Φ is unital, then the operator $\hat{G}_\Phi$ and the correction term are equal to zero, so the standard form (28) of the Jarzynski equality is recovered. It is essential to note that the correction term may vanish also for nonunital quantum channels, provided $\mathrm{Tr}(\hat{\omega}_1\hat{G}_\Phi) = 0$.

For a convex function $y \mapsto \exp(-\beta y)$, the Jensen inequality implies $\langle\langle \exp(-\beta W)\rangle\rangle \geqslant \exp(-\beta\langle\langle W\rangle\rangle)$. Combining this with Eq. (43) gives

$$\langle\langle W\rangle\rangle \geqslant \Delta F - \beta^{-1}\ln(1 + N\mathrm{Tr}(\hat{\omega}_1(\beta)\hat{G}_\Phi)). \quad (44)$$

This inequality provides a lower bound on the average work performed on a driven quantum system. If the correction term is strictly negative, the right-hand side of Eq. (44) is strictly larger than ΔF. The latter bound is commonly known and takes place for quasistatic processes. On the other hand, positivity of the correction term will reduce this bound. It is an evidence for the fact that the averaged external work may, in principle, be less than ΔF, provided the macroscopic process investigated is sufficiently far from unitality.

It is instructive to discuss limiting cases of high and low temperatures. For sufficiently high temperatures, if $|\beta\varepsilon_n| \ll 1$ with some typical value ε_n, the correction term can be expanded as

$$N\mathrm{Tr}(\hat{\omega}_1(\beta)\hat{G}_\Phi) = NZ_1^{-1}(\beta)(-\beta\mathrm{Tr}(\hat{H}_1\hat{G}_\Phi) + O(\beta^2)). \quad (45)$$

Since the nonunitality operator $\hat{G}_\Phi$ is traceless, the expansion starts with the first-order term with respect to β. If $\mathrm{Tr}(\hat{H}_1\hat{G}_\Phi) = 0$, the right-hand side of Eq. (45) also vanishes in the first order. Within this approximation, the standard form (28) and its consequences remain valid. For very low temperatures, the correction term can be expressed in terms of the ground-state energy, $\varepsilon_0 = \min\{\varepsilon_n^{(1)}\}$. If this state is nondegenerate, we approximately write

$$N\mathrm{Tr}(\hat{\omega}_1(\beta)\hat{G}_\Phi) = N\langle\varepsilon_0|\hat{G}_\Phi|\varepsilon_0\rangle. \quad (46)$$

Neglected terms are of the order of $O(\exp(-\beta\Delta\varepsilon))$, where $\beta\Delta\varepsilon \gg 1$ and $\Delta\varepsilon > 0$ is a typical distance between nearest-neighbor levels, for instance, the energy difference between the ground state and the first excited state. Up to a high accuracy the deviation from the unitality is represented by a single matrix element $\langle\varepsilon_0|\hat{G}_\Phi|\varepsilon_0\rangle$, as probabilities of excited states becomes negligible for low temperatures. In general, this matrix element characterizes a difference of the matrix element $\langle\varepsilon_0|\Phi(\rho_*)|\varepsilon_0\rangle$ from the equiprobable value $1/N$. If the ground state is not involved in the undergoing process, the correction term vanishes. Thus, in the low-temperature limit the standard form (28) may be adequate, even if the process itself is generally far from equilibrium. We also observe that the right-hand side of Eq. (46) does not depends on the temperature.

The above results can be put into the context of the heat transfer between two quantum systems. The composite Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ is a tensor product of the Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ of individual systems. Let us rewrite Eq. (32) so the initial state of the composite system reads

$$\hat{\varrho}_{AB} := \mathrm{Tr}(\exp(-\alpha\hat{A}))^{-1}\,\mathrm{Tr}(\exp(-\beta\hat{B}))^{-1} \times \exp(-\alpha\hat{A}) \otimes \exp(-\beta\hat{B}), \quad (47)$$

where $\hat{A} \in \mathcal{L}_{\mathrm{s.a.}}(\mathcal{H}_A)$ and $\hat{B} \in \mathcal{L}_{\mathrm{s.a.}}(\mathcal{H}_B)$. Using an observable $\hat{C} := \alpha\hat{A} \otimes \mathbb{1}_B + \mathbb{1}_A \otimes \beta\hat{B}$, we may rewrite operator (47) as

$$\hat{\varrho}_{AB} = \mathrm{Tr}(\exp(-\hat{C}))^{-1}\,\exp(-\hat{C}). \quad (48)$$

Assume now that the evolution of the composite system is represented by a quantum channel $\Psi : \mathcal{L}(\mathcal{H}_{AB}) \to \mathcal{L}(\mathcal{H}_{AB})$. By corresponding substitutions in Eq. (32), we obtain

$$\langle\langle \exp(\alpha a + \beta b - c)\rangle\rangle = 1 + N_A N_B \mathrm{Tr}(\hat{\varrho}_{AB}\hat{G}_\Psi), \quad (49)$$

where $\hat{G}_\Psi = \Psi(\hat{\rho}_{*AB}) - \hat{\rho}_{*AB}$. The operator $\hat{G}_\Psi$ vanishes for unital channels and the right-hand side of Eq. (49) becomes equal to unity as discussed in Ref. [23]. We now consider the following situation. Two separated systems are initially prepared in equilibrium with the inverse temperatures β_0 and β_1, respectively. Then the combined system is initially described by the tensor product $\hat{\Omega}_{01} := \hat{\omega}_0(\beta_0) \otimes \hat{\omega}_1(\beta_1)$. Making use of Eq. (49) we obtain

$$\langle\langle \exp(\beta_0(\varepsilon^{(0)} - \varepsilon'^{(0)}) + \beta_1(\varepsilon^{(1)} - \varepsilon'^{(1)}))\rangle\rangle = 1 + N_A N_B \mathrm{Tr}(\hat{\Omega}_{01}\hat{G}_\Psi). \quad (50)$$

Following Ref. [8] we introduce the quantity

$$\Delta S := \langle\langle \beta_0(\varepsilon'^{(0)} - \varepsilon^{(0)}) + \beta_1(\varepsilon'^{(1)} - \varepsilon^{(1)})\rangle\rangle. \quad (51)$$

As the terms $\langle\langle \varepsilon'^{(0)} - \varepsilon^{(0)}\rangle\rangle$ and $\langle\langle \varepsilon'^{(1)} - \varepsilon^{(1)}\rangle\rangle$ are average variations of self-energies of the two subsystem, quantity (51) describes a contribution of these variations into a change of the total entropy. Combining Eq. (50) with the Jensen inequality finally gives a bound $\Delta S \geqslant -\ln(1 + N_A N_B \mathrm{Tr}(\hat{\Omega}_{01}\hat{G}_\Psi))$. If variations of the inverse temperatures are sufficiently small and the contributions of interaction energy are negligible, then the quantity ΔS provides an estimate of changes of the total entropy of the system [8]. If the correction term is strictly negative, then $\Delta S > 0$. Negativity of the correction term also implies $\langle\langle W\rangle\rangle > \Delta F$. Since contributions on the interaction energy are small enough, a perturbative description of the process is reasonable. On the other hand, positivity of the correction term implies $\Delta S < 0$. In such a case, contributions of the interaction can be relevant, so quantity (51) does not provide a legitimate estimate for changes of the total entropy.

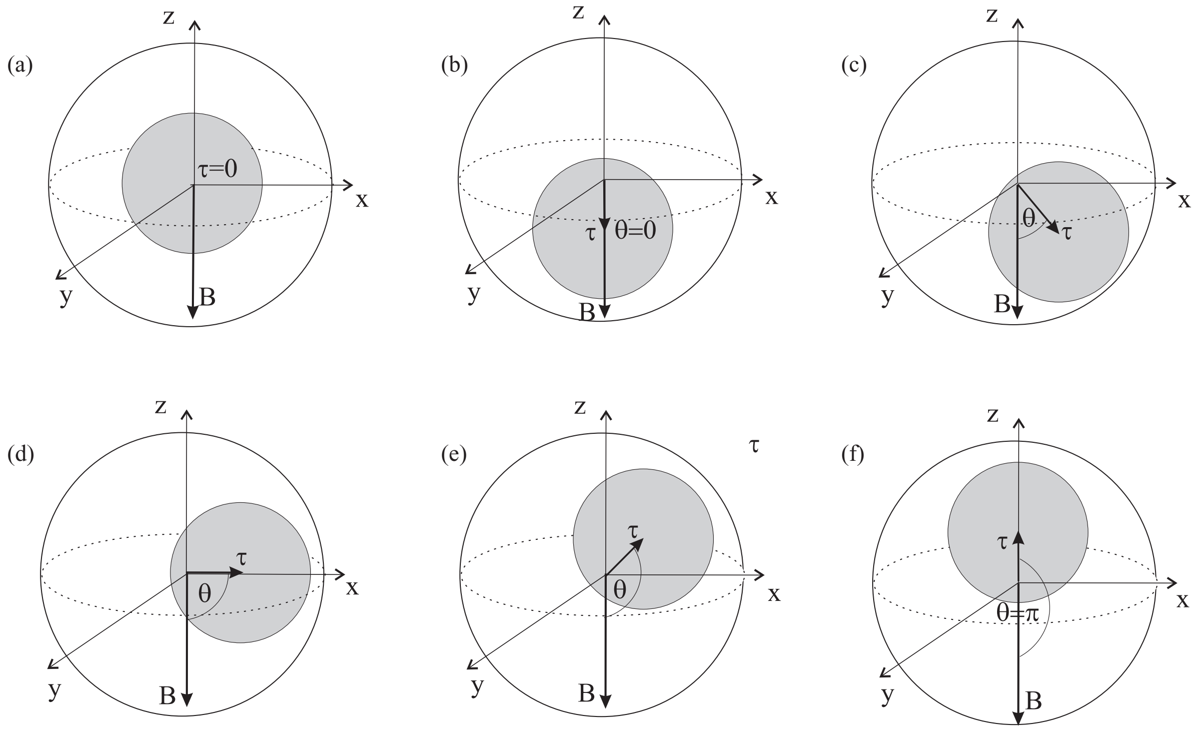

FIG. 1. One-qubit quantum channels acting on the Bloch ball. Correction term in the Jarzynski equality (43) depends on the product $\boldsymbol{\tau}\cdot\mathbf{B}$ and vanishes in the unital case (a) and in the case (d), for which both vectors are perpendicular. Correction term is maximal in the cases (b) and (f), for which these vectors are parallel.

VI. EXEMPLARY NONUNITAL QUANTUM MAPS

In this section we discuss some simple nonunital quantum channels and analyze the correction term present in the Jarzynski equality (43). Analyzed channels describe the effects of the energy loss from an interacting quantum system and can be considered as a generalization of the amplitude damping channel [18,19].

A. Two-level system

Consider the simplest case $N = 2$ representing a one qubit system. Let a magnetic moment with spin $1/2$ and a charge $-e$ be in contact with a thermal bath at the inverse temperature β. The corresponding Hamiltonian reads

$$\hat{H}_1 = -\mu_B\,\mathbf{B}\cdot\hat{\boldsymbol{\sigma}}. \tag{52}$$

Here $\mu_B = e\hbar/(2mc)$ is the Bohr magneton, $\mathbf{B}$ is the vector of an external field, and $\hat{\boldsymbol{\sigma}}$ is the vector of the three Pauli matrices. Suppose that the time evolution of the system is represented by the amplitude damping channel [18,19] described by the Kraus operators

$$\hat{K}_0 = \begin{pmatrix}\sqrt{1-p} & 0\\ 0 & 1\end{pmatrix},\quad \hat{K}_1 = \begin{pmatrix}0 & 0\\ \sqrt{p} & 0\end{pmatrix}, \tag{53}$$

with $p \in [0,1]$. For this channel the image of the maximally mixed state, $\Phi(\hat{\rho}_*)$, can be represented by the Bloch vector $\boldsymbol{\tau} = (0,0,-p)$. The length $|\boldsymbol{\tau}| = p$ of the Bloch vector characterizes the degree of the nonunitality of the map. In the original map Φ described by the operators $\hat{K}_0$ and $\hat{K}_1$ the translation vector $\boldsymbol{\tau}$ is parallel to the axis z, but this can be changed, if the nonunitary dynamics is followed by an arbitrary unitary rotation,

$$\hat{\rho} \mapsto \hat{\rho}'' = \hat{U}\,\Phi(\hat{\rho})\hat{U}^\dagger, \tag{54}$$

where $\hat{U} \in \mathrm{U}(2)$. Then the rotated translation vector $\boldsymbol{\tau}$ can take an arbitrary orientation with respect to the magnetic field, pointing along the z axis; see Fig. 1. In general, the nonunitality observable (29) reads therefore $\hat{G}_\Phi = (1/2)\,\boldsymbol{\tau}\cdot\hat{\boldsymbol{\sigma}}$. The correction term in Eq. (43) becomes then

$$2\,\mathrm{Tr}(\hat{\omega}_1(\beta)\hat{G}_\Phi) = \mathrm{Tr}(\hat{\omega}_1(\beta)\boldsymbol{\tau}\cdot\hat{\boldsymbol{\sigma}}) = p\tanh(\beta\mu_B B)\cos\theta, \tag{55}$$

where $B = |\mathbf{B}|$ and θ denotes the angle between the Bloch vector $\boldsymbol{\tau}$ and the magnetic field $\mathbf{B}$. Another interpretation of the angle θ follows from the scalar product in the Hilbert-Schmidt space of operators,

$$\langle \hat{H}_1, \hat{G}_\Phi\rangle_{\mathrm{hs}} = -p\,\mu_B B\cos\theta. \tag{56}$$

In this example, the product $|p\cos\theta|$ is a natural measure of deviation from unitality. Writing the correction term in a coordinate-independent manner, we obtain the Jarzynski equality

$$\langle\!\langle \exp(-\beta W)\rangle\!\rangle = \exp(-\beta\Delta F)(1 + \tanh(\beta\mu_B B)B^{-1}\boldsymbol{\tau}\cdot\mathbf{B}). \tag{57}$$

For high temperatures, the right-hand side of (57) reads $\exp(-\beta\Delta F)(1+\beta\mu_B\boldsymbol{\tau}\cdot\mathbf{B})$ due to $\tanh(\beta\mu_B B) \approx \beta\mu_B B$. If the translation vector is perpendicular to the external field, $\boldsymbol{\tau}\perp\mathbf{B}$, the correction term vanishes for arbitrary values of β. This case provides a concrete physical example, in which the standard form of Jarzynski equality holds for nonunital quantum channels. The absolute value of the correction term is maximal for $\boldsymbol{\tau} \parallel \mathbf{B}$. Some configurations of the vectors $\boldsymbol{\tau}$ and $\mathbf{B}$ are shown in Figs. 1(a)–1(f). A size of the correction term also depends on the temperatures and it is small in the high-temperature limit. In the low-temperature limit, $\tanh(\beta\mu_B B) \to 1$ and the right-hand side of Eq. (55) is merely reduced to $p\cos\theta$. When the parameters β, B, and θ are fixed, the correction term becomes maximal for $p = 1$. Here we deal with a spontaneous emission channel, which maps all inputs to some prescribed pure state. In the sense of Eq. (54), this prescribed state can be chosen arbitrarily.

With the above example, we can return to the discussion of the notion of work in the context of quantum fluctuation relations [5,6,42]. In the nonunital cases in Figs. 1(b) and 1(f), one has an energy shift of the "center of mass" of the set of states, resulting in maximization of the correction term. Such an effect means that one takes into account, on average, the work against the magnetic field. In Fig. 1(d), the shift is orthogonal to the field, whence no energy change occurs and the correction term vanishes.

Overall, the average energy cost due to the work against the field depends on both the length of $\boldsymbol{\tau}$ and its direction, as it is described by the last, nonunitality term in Eq. (43). Note that this term, vanishing, for instance, for any unitary evolution, is not related to average changes of the von Neumann entropy of the quantum state during nonunitary processes. As the evolution Φ is not unitary, pure states may be converted into mixed states, or mixed states into pure, due to the interaction with an environment. Thus, to produce a nonunitary map Φ, some work has to be exchanged between the principal system and the environment.

B. Three-level system

We now consider a generalized amplitude damping channel acting on a $N = 3$ quantum state and parametrized by two real numbers, $p,q \in [0,1]$. The map is described by a set of three Kraus operators. It contains a single diagonal matrix, $\hat{K}_0 = \mathrm{diag}(\sqrt{1-p},\sqrt{1-q},1)$, and two nondiagonal matrices,

$$\hat{K}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \sqrt{p} & 0 & 0 \end{pmatrix}, \quad \hat{K}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \sqrt{q} & 0 \end{pmatrix}. \tag{58}$$

For this channel we find the nonunitality observable $\hat{G}_\Phi = (1/3)\,\mathrm{diag}(-p,-q,p+q)$. As the choice $p = q = 0$ leads to the identity map, we assume in the following that $p \neq 0$ or $q \neq 0$. For a massive particle with spin 1 and charge e, we write the final Hamiltonian,

$$\hat{H}_1 = \frac{e}{mc}\,\mathbf{B}\cdot\hat{\mathbf{J}}. \tag{59}$$

Let us take the axis z such that the component $\hat{J}_z$ commutes with $\hat{G}_\Phi$, i.e., $\hat{J}_z = \hbar\,\mathrm{diag}(+1,0,-1)$. In their common eigenbasis, the two other components of the spin are expressed as

$$\hat{J}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{J}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}. \tag{60}$$

In this case, an expression for the correction term is more complicated than Eq. (55). For sufficiently high temperatures, when β is small, one has a simple approximation,

$$3\,\mathrm{Tr}(\hat{\omega}_1(\beta)\hat{G}_\Phi) = (2p+q)\beta\,\frac{e\hbar}{3mc}\,\mathbf{e}_z\cdot\mathbf{B} + O(\beta^2), \tag{61}$$

where $\mathbf{e}_z$ is the unit vector of the axis z. If $\mathbf{B} \perp \mathbf{e}_z$, the correction term vanishes in the first order with respect to β. In this respect, expression (61) is analogous to Eq. (55). On the other hand, for a generic value of the temperature, the correction term typically differs from zero. When we fix β and $\mathbf{B}$, then the correction term in the first order becomes maximal for $p = q = 1$. As in the above case $N = 2$, this choice gives a complete contraction to some pure state. In the low-temperature limit, we can rewrite Eq. (61) in the form

$$3\,\mathrm{Tr}(\hat{\omega}_1(\beta)\hat{G}_\Phi) = \left(p + \frac{q}{2}\right)\cos\theta + \frac{q}{8}\,(1 + 3\cos 2\theta), \tag{62}$$

where θ is the angle between $\mathbf{e}_z$ and $\mathbf{B}$. As mentioned above, the right-hand side of Eq. (62) neglects contributions of order $\exp(-\beta e\hbar B/(mc))$ with very large values of the exponent $\beta e\hbar B/(mc)$.

C. N-level system

Consider the following process defined for an arbitrary N-dimensional space. Let I and J be two sets of indices such that $I \cap J = \emptyset$ and $I \cup J = \{1,2,\ldots,N\}$. The map is described by a set of the Kraus operators. The first of them is chosen to be diagonal in the eigenbasis of the Hamiltonian,

$$\hat{K}_0 := \sum_{m\in I} z_m|\varepsilon_m\rangle\langle\varepsilon_m| + \sum_{n\in J}|\varepsilon_n\rangle\langle\varepsilon_n|. \tag{63}$$

For given $n \in I$ and arbitrary $m \neq n$, we define further operators,

$$\hat{K}_{mn} := a_{mn}|\varepsilon_m\rangle\langle\varepsilon_n|, \tag{64}$$

for which $\hat{K}_{mn}^\dagger\hat{K}_{mn} = |a_{mn}|^2\,|\varepsilon_n\rangle\langle\varepsilon_n|$ and $\hat{K}_{mn}\hat{K}_{mn}^\dagger = |a_{mn}|^2\,|\varepsilon_m\rangle\langle\varepsilon_m|$. For all $n \in I$ we impose a restriction,

$$|z_n|^2 + \sum_{m\neq n}|a_{mn}|^2 = 1, \tag{65}$$

whence $|z_n| \leqslant 1$ and $|a_{mn}| \leqslant 1$. Hence, condition (8) is satisfied, i.e., the considered quantum operation is trace preserving. For brevity, we put positive numbers $y_m = \sum_{n\neq m}|a_{mn}|^2$ for each $m \in \{1,2,\ldots,N\}$. An explicit form of all Kraus operators allows us to find the image of the identity operator,

$$\Phi(\mathbb{1}) = \sum_{m\in I}(|z_m|^2 + y_m)|\varepsilon_m\rangle\langle\varepsilon_m| + \sum_{n\in J}(1 + y_n)\,|\varepsilon_n\rangle\langle\varepsilon_n|. \tag{66}$$

Therefore the nonunitality observable $\hat{G}_\Phi$ is diagonal with elements $x_m = N^{-1}(|z_m|^2 + y_m - 1)$ for $m \in I$ and elements $x_n = N^{-1}y_n$ for $n \in J$. The correction term in Eq. (43) can be then written as

$$N\mathrm{Tr}(\hat{\omega}_1(\beta)\hat{G}_\Phi) = N\left(\sum_n \exp(-\beta\varepsilon_n)\right)^{-1}\sum_n x_n\exp(-\beta\varepsilon_n). \tag{67}$$

Note that the right-hand side of Eq. (67) represents the correction term for arbitrary $\hat{G}_\Phi$. In this case, we merely replace x_n with the diagonal matrix element $\langle \varepsilon_n|\hat{G}_\Phi|\varepsilon_n\rangle$ with respect to the Hamiltonian eigenbasis. The correction term is not uniquely defined by a given quantum channel. Hence, effects of nonunitality in the Jarzynski equality and related fluctuation relations in some cases may be modeled by a generalized amplitude damping channel in the described form. It is possible, provided the diagonal element $\langle \varepsilon_n|\hat{G}_\Phi|\varepsilon_n\rangle$ of the operator $\hat{G}_\Phi$ can be represented in terms of the above introduced numbers z_n and y_n.

The above two damping channels acting on $N = 2$ and $N = 3$ systems are particular cases of the general scheme. For instance, matrices (53) are obtained for $I = \{1\}$ and $J = \{2\}$ with $z_1 = \sqrt{1-p}$, $a_{21} = \sqrt{p}$. Matrices (58) and diagonal $\hat{K}_0 = \mathrm{diag}(\sqrt{1-p},\sqrt{1-q},1)$ are recovered by setting $I = \{1,2\}$ and $J = \{3\}$ with $z_1 = \sqrt{1-p}$, $z_2 = \sqrt{1-q}$, $a_{31} = \sqrt{p}$, $a_{32} = \sqrt{q}$. Another version of the damping channel for a three-level system is described for $I = \{1\}$ and $J = \{2,3\}$. Taking $z_1 = \sqrt{1-p}$, $a_{21} = \sqrt{q}$, $a_{31} = \sqrt{p-q}$, we obtain the Kraus matrices $\hat{K}_0 = \mathrm{diag}(\sqrt{1-p},1,1)$,

$$\hat{K}_{21} = \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{q} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{K}_{31} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \sqrt{p-q} & 0 & 0 \end{pmatrix}. \tag{68}$$

These operators lead to the diagonal matrix $\Phi(\mathbb{1}) - \mathbb{1} = \mathrm{diag}(-p,q,p-q)$. Therefore operators (68) allow a controlled shift of the population between the levels of the system.

VII. CONCLUDING REMARKS

In this work we formulated Jarzynski equality (43) for a quantum system described by an arbitrary stochastic map. This is a direct generalization of earlier results obtained for unital maps [22,23], for which the maximally mixed state is preserved. We derived a correction term which compensates the nonunitality of the map and attempted to estimate its relative size. Furthermore, it was shown that the correction term vanishes if the nonunitality observable is perpendicular, in the sense of the Hilbert-Schmidt scalar product, to the Hamiltonian of the system. Hence, expression (28) obtained previously remains valid also for certain cases of nonunital maps provided the nonunitality does not influence the average energy of the system.

The results are exemplified on a simple model of the damping channel. For a two-level system, the correction term depends on the nonunitality measured by the length of the translation vector $\boldsymbol{\tau}$ and its orientation with respect to the vector of magnetic field. The latter determines the Hamiltonian of the system. When other parameters are fixed, the translation vector is the longest in the case of complete contraction to a pure state. For the considered two-level example, such a map leads to the maximal relative size of the correction term. However, if the translation vector is perpendicular to the field, the correction term vanishes irrespectively of the length of the translation vector.

As a by-product of our study we introduced the nonunitality operator G_Φ associated with a given quantum operation Φ and analyzed its properties. Some useful bounds for its norm have been established. Furthermore, we presented a broad class of nonunitary dynamics acting in the set of quantum states of an arbitrary finite dimension N, which can serve as a generalization of the one-qubit amplitude damping channel.

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