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Time reversals of irreversible quantum maps

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Abstract

We propose an alternative notion of time reversal in open quantum systems as represented by linear quantum operations, and a related generalization of classical entropy production in the environment. This functional is the ratio of the probability to observe a transition between two states under the forward and the time reversed dynamics, and leads, as in the classical case, to fluctuation relations as tautological identities. As in classical dynamics in contact with a heat bath, time reversal is not unique, and we discuss several possibilities. For any bistochastic map its dual map preserves the trace and describes a legitimate dynamics reversed in time, in that case the entropy production in the environment vanishes. For a generic stochastic map we construct a simple quantum operation which can be interpreted as a time reversal. For instance, the decaying channel, which sends the excited state into the ground state with a certain probability, can be reversed into the channel transforming the ground state into the excited state with the same probability.

Keywords: time reversal, quantum map, fluctuation relations

(Some figures may appear in colour only in the online journal)

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1. Introduction

The discovery of fluctuation relations [1–3] has transformed classical out-of-equilibrium thermodynamics, giving rise to the new field of stochastic thermodynamics [4–7]. Important results obtained in the last two decades include the use of Jarzynski equality to measure equilibrium free energy differences in large biomolecules from non-equilibrium measurements [8, 9], generalizations of fluctuation–dissipation theorems from the equilibrium to the non-equilibrium domain [10, 11], and a sharpening of Landauer principle on the minimal heat generated in computing [12–14]. The central quantity in stochastic thermodynamics is the entropy production in the environment, a functional of the whole system history [15, 16] which can be defined in two ways. The first method is by Clausius' relation

$$\delta S_{\text{env}} = \beta \delta Q, \tag{1}$$

where $\beta = \frac{1}{k_B T}$ is the inverse temperature and δQ is the heat[7] and the second way is as the Radon–Nikodym derivative of a forward and a reversed path probability

$$\delta S_{\text{env}}[\text{path}] = \log \frac{P^F[\text{path}]}{P^R[\text{path}]}. \tag{2}$$

Here $P^F[\text{path}]$ is the probability of the forward path and $P^R[\text{path}]$ is the probability of the time-reversed path [17], and fluctuation relations follow from (2) as mathematical 'tautologies' [14, 18]. Physically, fluctuation relations are, however, not tautologies, because the quantities in (1) and (2) should be the same. For standard Markov models of the system-bath interactions (master equations, diffusion equations), this is indeed the case, but for more general models the situation is less evident.

The (possible) extension of fluctuation relations to the quantum domain has been the focus of intense investigations reviewed in [19, 20]. Except for the generalizations of the Jarzynski equality and Crooks' fluctuation theorem to closed quantum systems [21] the results obtained to date lack the generality and simplicity of fluctuation relations in classical systems, and typically hold for specific models such as e.g. when the quantum jump method [22–24] or the Lindblad formalism [25] can be applied.

In this work we focus on the tautological aspect of quantum fluctuation relations, i.e. on the analogues of (2), which have not, we believe, been sufficiently emphasized in the literature. To do this we have to define a general notion of time reversal of open quantum systems. As in the case of a classical system interacting with a heat bath this notion of time reversal, which we call the R operation, is not unique. In the sense introduced here an open quantum system can be time reversed in many ways [26], for each one one can define an entropy production functional analogous to (2) and obtain fluctuation relations. We first give a very general (permissive) definition of the R operation, and show that it always leads to fluctuation relations. We then turn to a possible definition of R starting with the standard quantum mechanical time inversion of a combined system and the bath and continuing to intrinsic representations in terms of Kraus operators. We discuss several special cases such as unital maps, and give examples of time-reversals of 1-qubit channels.

[7] We here use the sign convention of classical thermodynamics where heat is counted positive *from* the system *to* the bath. In stochastic thermodynamics literature the usual sign convention is positive *from* the bath *to* the system [7].

2. Generalities and definition of *R* operation

A state of a quantum system is described by its density matrix ρ which is an N-dimensional positive Hermitian operator with unit trace. Any physical operation on a quantum system can be described by a completely positive linear map Φ, which preserves the trace and sends one density matrix ρ into another state $\rho' = \Phi(\rho)$. We define a general time reversal R as an involution on the set Ω_N of quantum operations i.e. a bijective transformation R: $\Phi \to \Phi^R$ which satisfies $(\Phi^R)^R = \Phi$.

R operation and fluctuation relations: To arrive at fluctuation relations we consider the paradigmatic example of two measurements, one before the beginning of the process described by Φ, and another after [21]. We will denote by $\hat{A}$ and $\hat{O}$ two measured operators (with eigenstates $|a\rangle$ and $|o\rangle$ and eigenvalues E_a and E_o). At the beginning of the process the system will hence be in the pure state $|a\rangle\langle a|$, and the probability to observe o at the end will be $\langle o|\Phi(|a\rangle\langle a|)|o\rangle$. For the reversed chain of events, we first measure $\hat{O}$ to obtain o, then act on the system with the reversed quantum map Φ^R, and measure $\hat{A}$ to obtain a. This happens with probability $\langle a|\Phi^R(|o\rangle\langle o|)|a\rangle$. A straightforward generalization of (2) to the quantum domain is thus

$$\delta S_{\text{env}}[a, o] = \log \frac{\langle o|\Phi(|a\rangle\langle a|)|o\rangle}{\left\langle a\right| \Phi^R(|o\rangle\langle o|)\left| a\right\rangle}. \tag{3}$$

To derive fluctuation relations from (3) one proceeds by analogy with the classical case using (2). For Jarzynski equality one takes $\hat{A}$ as an initial Hamiltonian $\hat{H}_i$ and $\hat{O}$ as a final Hamiltonian $\hat{H}_f$ with thermodynamic equilibrium states ρ_i^β and ρ_f^β, respectively, and defines the work done on the system during the process as $\delta W[a, o] = (E_o - E_a) + \beta^{-1}\delta S_{\text{env}}[a, o]$. Then $\sum_{a,o} \mathrm{e}^{-\beta E_o}\langle a|\Phi^{\mathrm{R}}(|o\rangle\langle o|)|a\rangle = Z_f$ and this identity can simply be rewritten as

$$\sum_{a,o}\left\langle a \,\middle|\, \rho_i^\beta \,\middle|\, a\right\rangle \langle o|\Phi(|a\rangle\langle a|)|o\rangle\, \mathrm{e}^{-\delta S_{\text{env}}a,o}\mathrm{e}^{-\beta(E_o-E_a)} = \mathrm{e}^{-\beta\Delta F}.$$

Here ΔF denotes the difference between the free energy of both thermal equilibrium states, and the left hand side can be interpreted as $\langle \mathrm{e}^{-\beta\delta W}\rangle$. For Crooks' relation one similarly defines $P^F(x) = \left\langle \delta(\delta W - x)\right\rangle_{\text{eq}}$ and $P^R(x) = \left\langle \delta(\delta W^R - x)\right\rangle_{\text{eq}}^R$ where in the latter the time-reversed work is $\delta W^R[o, a] = -\,\delta W[a, o]$ and the average is performed over the final equilibrium state ρ_f^β and the reversed quantum map Φ^R. This implies $P^R(-x) = \mathrm{e}^{-\beta(x-\Delta F)}P^F(x)$, which is the relation of Crooks [27].

3. Standard quantum mechanical time inversion and time reversal of environmental representations

Consider first a closed system. If $\rho' = \Phi\rho = U\rho U^\dagger$ where

$$U = \mathcal{T}\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f} H(t')\mathrm{d}t'\right)$$

is unitary development with Hamiltonian H then the final state is time inverted by an antiunitary operator Θ i.e. $\tilde{\rho'} = \Theta\rho'\Theta^{-1}$. Acting on this state with $\tilde{U} = \Theta U^\dagger\Theta^{-1}$, we obtain a state at the initial time $\tilde{\rho} = \tilde{U}\tilde{\rho'}\tilde{U}^\dagger$ and time inversion is complete if $\rho = \Theta^{-1}\tilde{\rho}\Theta$, which is the case. The time reversal of a closed system, based on standard quantum mechanical time inversion, is then the operation $\Phi \to \tilde{\Phi}$ where $\tilde{\Phi}\rho = \tilde{U}\rho\tilde{U}^\dagger$. Obviously this is an involution: performing it twice we get back the map $\Phi\rho$.

Quantum maps have (generally non-unique) *environmental representations*

$$\rho' = \Phi\rho = \mathrm{Tr}_B\left[U(\rho \otimes \sigma)U^\dagger\right], \tag{4}$$

where the principal state ρ acts in the space $\mathcal{H}_A$ while the ancillary state σ acts in the space $\mathcal{H}_B$ describing the environment. Both subsystems are coupled by a unitary operation U, and the image ρ' is obtained by tracing out the environment. Under standard quantum mechanical time inversion U transforms to $\tilde{U}$ and σ to $\tilde{\sigma}$ which allows us to define an *environmental* time reversal of the open quantum system as

$$\Phi^{R_E}\rho = \mathrm{Tr}_B\left[\tilde{U}(\rho \otimes \tilde{\sigma})\tilde{U}^\dagger\right]. \tag{5}$$

The disadvantages of such a definition are obvious: it is contingent on the chosen environmental representation, and to arrive at an intrinsic notion we have to pursue another approach. In addition, also when an open quantum operation has a very natural environmental representation, (5) is not the only natural notion of generalized time reversal. We will return to this point below.

4. Kraus form of quantum maps and the dual map

Instead of (5) we will now start from the *Kraus form* [28] of quantum operator Φ:

$$\rho' = \Phi(\rho) = \sum_{i=1}^{k} A_i \rho A_i^\dagger. \tag{6}$$

As a quantum operation Φ preserves the trace, $\mathrm{Tr}\,\rho' = \mathrm{Tr}\,\rho$, the Kraus operators A_i satisfy the identity resolution $\sum_{i=1}^{k} A_i^\dagger A_i = \mathbb{1}$. The trace preserving conditions induce N^2 constraints so the set Ω_N of quantum operations acting on N dimensional states has N^4-N^2 dimensions. Although the number k in (6) is arbitrary, for any map there exist the *canonical Kraus form*, for which all Kraus operators are orthogonal,

$$\mathrm{Tr}\,A_i A_j^\dagger = d_i \delta_{i,j}, \tag{7}$$

so that the Kraus rank $\mathrm{k} \leqslant N^2$. In a generic case the numbers d_i are different and this representation is unique up to the choice of the overall phases of the Kraus operators—see e.g. [29].

In the case of a unitary evolution, $\rho' = \Psi_U(\rho) = U\rho U^\dagger$, one has $k = 1$ and the only Kraus operator is unitary, $A_1 = U$. Unitary maps belong to broader class of *unital maps*, which preserve the identity, $\Psi(\mathbb{1}) = \mathbb{1}$, and satisfy the dual condition $\sum_{i=1}^{k} A_i A_i^\dagger = \mathbb{1}$. A map which is trace preserving and unital is called *bistochastic*, as it forms a quantum analogue of a bistochastic matrix, which acts in the set of N–point probability vectors.

For any quantum map Φ in the form (6) one defines its *dual map* Φ° such that $\Phi^\circ(\rho) = \sum_{i=1}^{k} A_i^\dagger \rho A_i$. Writing for short $\Phi = \{A_1, ..., A_k\}$ we have $\Phi^\circ = \{A_1^\dagger, ..., A_k^\dagger\}$. Note that if a map Φ preserves the trace, the dual map Φ° is unital. If Φ is bistochastic, so is Φ°. It is also convenient to define the class of *selfdual maps* which satisfy $\Phi^\circ = \Phi$. A quantum operation for which all Kraus operators are hermitian is bistochastic and selfdual. So is a map for which all non-hermitian operators occur in pairs, e.g. $\Phi = \{A_1, ..., A_m, A_1^\dagger, ..., A_m^\dagger\}$.

Restricting our attention to bistochastic maps as a first generalization of the standard time inversion, we can define a time reversal $\Phi^{R_B} := \Phi^\circ$. The choice R_B implies that

$\langle o|\ \Phi(|a\rangle\langle a|)|o\rangle = \sum_i |\langle o\ |A_i|\ a\rangle|^2 = \langle a|\ \Phi^R(|o\rangle\langle o|)|a\rangle$. Therefore the fraction in equation (3) is equal to unity and hence for any bistochastic map Φ and any initial and final pure states the entropy production vanishes, $\delta S_{\rm env}[a,\ o] = 0$. Although bistochastic maps are not time invertible in the standard sense, they are therefore time reversible in the sense that there exists a (natural) time reversal of such maps for which the entropy production in the environment vanishes. As a consequence fluctuation relations hold for all such maps with the work taken equal to the internal energy change which reproduces the original quantum fluctuation relation of Kurchan for unitary maps [21] as well as the result of Rastegin for bistochastic maps [30]. In this connection it was recently observed [31, 32] that the Jarzynski relation, with work taken equal to internal energy change, in general does not hold for nonunital maps. Thus if the map is nonunital then its dual is not a well-defined quantum map, time reversal cannot be defined as a dual, and the ratio in equation (3) may be different from unity.

A more general definition of the time reversal operation for a non-unital a quantum operation $\Phi = \{A_1, ..., A_k\}$ was proposed by Crooks [26]. It is based on the invariant state of the map, $\rho_* = \Phi(\rho_*)$. The reversed map is given by the following sequence of the Kraus operators $\Phi^{R_C} = \{A_1^C, ..., A_k^C\}$, where $A_i^C = \rho_*^{1/2} A_i^\dagger \rho_*^{-1/2}$. Note that in the case of unital maps one has $\rho_*^{1/2} = \mathbb{1}/N$ so that $A_i^C = A_i^\dagger$ and one arrives at the dual map, $\Phi^{R_C} = \Phi^\circ$. However, this definition does not work, if the invariant state belongs to the boundary of the set of quantum states so that ρ_* is not invertible.

The isomorphism of Choi and Jamiołkowski [29, 33, 34] states that an operation Φ can be uniquely described by a *dynamical matrix*, (Choi matrix)

$$D_\Phi = N(\Phi \otimes \mathbb{1})\left|\psi^+\right\rangle\left\langle\psi^+\right|,$$

where $|\psi^+\rangle = \frac{1}{\sqrt{N}}\sum_{i=1}^N |i\rangle \otimes |i\rangle$ denotes the maximally entangled state on an extended Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. The matrix D of order N^2 is hermitian and positive by construction, and its eigenvalues determine the relative weights d_i, while the eigenvectors of length N^2, reshaped into square matrices of order N and rescaled by $\sqrt{d_i}$ yield the Kraus operators A_i in the canonical form (7).

Two maps Φ_1 and Φ_2 are called *unitarily equivalent*, written $\Phi_1 \sim \Phi_2$, if there exist two unitary matrices V_1 and V_2 such that $\Phi_2(\rho) = V_2\left(\Phi_1(V_1 \rho V_1^\dagger)\right)V_2^\dagger$, so the map Φ_2 can be written as a concatenation of Φ_1 with two unitary operations, $\Phi_2 = \Psi_{V_2} \circ \Phi_1 \circ \Psi_{V_1}$. Observe that for any two unitarily equivalent maps the corresponding dynamical matrices, D_1 and D_2, share the same spectrum and are unitarily similar.

5. Essential map and its time reversal

We now look for a possible choice of the involution R for a general, non–unital quantum map, for which $\Phi^\circ \notin \Omega_N$ Consider a generic quantum operation Φ, for which the spectrum $\{d_i\}_{i=1}^k$ of the corresponding dynamical matrix D_Φ is non-degenerate. The trace of the dynamical matrix is fixed, $\mathrm{Tr}\, D = \sum_{i=1}^k d_i$, so let us order the Kraus operators forming the canonical form (7) according to their norms, $d_1 = ||A_1||^2 \geqslant d_2 = ||A_2||^2 \geqslant ,..., \geqslant d_k = ||A_k||^2$. The leading Kraus operator, with the largest norm, is represented by a possibly non-hermitian matrix A_1 of order N, which can be brought to the diagonal form by the singular value decomposition,

$$A_1 = V_1 E V_2^\dagger, \text{ where } V_1 V_1^\dagger = V_2 V_2^\dagger = \mathbb{1}. \tag{8}$$

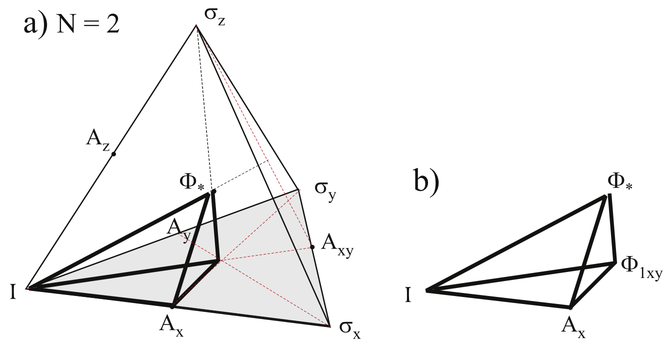

Figure 1. (a) The set of one-qubit Pauli channels forms a probability simplex Δ_3 spanned by identity and Pauli matrices. (b) An asymmetric part of the simplex forms a fragment of the set of essential maps $\hat{\Phi}_p$ which contains the identity map $\mathbb{1}$ and the maximally depolarizing channel Φ_*. Channel A_{xy} forms the symmetric combination of σ_x and σ_y.

Here E is a diagonal matrix with all non-negative entries. In the generic case the spectrum of E is non-degenerate, and this decomposition is unique up to the phases of the right and left eigenvectors of A_1 which form unitary matrices V_1 and V_2. In the degenerate case this decomposition is not unique. For instance, if $A_1 = U$ is unitary, than $E = \mathbb{1}$, and one can choose e.g. $V_1 = U$ and $V_2 = \mathbb{1}$.

For any map Φ we select in this way two unitary matrices V_1 and V_2, which allow us to define rotated Kraus operators $B_i = V_1^\dagger A_i V_2$ and the *essential map*

$$\hat{\Phi}(\rho) = \sum_{i=1}^{k} B_i \rho B_i^\dagger = \sum_{i=1}^{k} V_1^\dagger A_i V_2 \rho V_2^\dagger A_i^\dagger V_1. \tag{9}$$

For any operation determined by a set of ordered Kraus operators, $\Phi = \{A_1, A_2, ..., A_k\}$ the corresponding essential map reads thus $\hat{\Phi} = \{E, V_1^\dagger A_2 V_2, ..., V_1^\dagger A_k V_2\}$, where $A_1 = V_1 E V_2^\dagger$. Observe that the map Φ and its essential map are unitarily equivalent,

$$\Phi \sim \hat{\Phi} = \Psi_{V_1} \circ \Phi \circ \Psi_{V_2^\dagger}. \tag{10}$$

It is easy to see that for any unitary evolution Ψ_U the corresponding essential map reduces to identity map, $\hat{\Psi}_U = \mathbb{1}$. Thus the essential map generically provides a unique description of non-unitary part of a discrete quantum evolution.

Consider, for instance a one-qubit *Pauli channel*,

$$\Phi_p(\rho) = \sum_{j=1}^{4} p_j A_j \rho A_j, \tag{11}$$

where p_j is an ordered, $p_1 \geqslant p_2 \geqslant p_3 \geqslant p_4$, normalized probability vector, $\sum_{j=1}^4 p_i = 1$, while Hermitian Kraus operators A_j form an arbitrary sequence of three Pauli matrices σ_i, $i = 1, 2, 3$ and identity, $\sigma_0 = \mathbb{1}_2$. Then the corresponding essential map reads

$$\hat{\Phi}_p(\rho) = p_1 \rho + \sum_{i=1}^{3} q_i \sigma_i \rho \sigma_i, \tag{12}$$

where the three coefficients q_i are up to a permutation equal up to the three smallest coefficients p_2, p_3, p_4 of the map Φ.

In other words any Pauli channel can be represented by a point in the regular simplex $\Delta_3 \subset \mathbb{R}^3$ spanned by the identity and Pauli matrices (see figure 1(a)). The corresponding essential map belongs then to the asymmetric twenty-fourth part of the simplex with a corner representing the identity map $\mathbb{1}$.

6. The essential map and an intrinsic *R*

Having defined an essential map $\hat{\Phi}$, which describes the non-unitary part of the evolution, $\Phi = \Psi_{V_1^\dagger} \circ \hat{\Phi} \circ \Psi_{V_2}$, we are in position to give an intrinsic definition of a *time reversed map*

$$\Phi^R := \Psi_{V_2} \circ \hat{\Phi} \circ \Psi_{V_1^\dagger}. \tag{13}$$

Looking at the reversed map in the Kraus representation $\Phi^R = \{A_1^\dagger, YA_2Y,... YA_kY\}$ with the unitary matrix $Y = V_2V_1^\dagger$, we see that the leading Kraus operator A_1 is indeed inverted into $A_1^\dagger$, while other operators are suitably rotated to keep the map Φ^R trace preserving.

Making use of the form (10) we see that the composition of a map with its reverse reads

$$\Phi^R \circ \Phi = \Psi_{V_2} \circ \hat{\Phi} \circ \hat{\Phi} \circ \Psi_{V_2^\dagger}, \tag{14}$$

and is unitarily similar to $\hat{\Phi} \circ \hat{\Phi} = \hat{\Phi}^2$.

It is easy to check that for any map the following properties hold true $\widehat{(\Phi^R)} = \hat{\Phi} = (\hat{\Phi})^R$ and $(\Phi^R)^R = \Phi$, so that the reverse operation ^{R} is an involution, as requested. If the map is unitary, $\Phi = \Psi_U$, such a composition reduces to the identity map

$$\Psi_U^R \circ \Psi_U = \Psi_{U^\dagger} \circ \Psi_U = \mathbb{1}, \tag{15}$$

as any unitary evolution can be reversed.

Note that for a selfdual map one has $\Phi^R = \Phi^\circ = \Phi$ so that $\Phi^R\Phi = \Phi^2$. For instance, consider the selfdual maximally depolarizing channel, which sends any state into maximally mixed state, $\Phi_*(\sigma) = \mathbb{1}/N$. For any two pure states one has $|\langle i|\Phi_*(|j\rangle\langle j|)|i\rangle| = 1/N$ so that the fraction in equation (2) is equal to unity for any choice of initial and final states.

For any stochastic map described by two Kraus operators, $\Phi = \{A_1, A_2\}$, the reversed map reads $\Phi^R = \{A_1^\dagger, \sqrt{\mathbb{1} - A_1A_1^\dagger}\}$. In this case, the operators A_i need not to be ordered according to their norms, so one can choose for A_1 a non-hermitian operator. For example, in the case of the one-qubit decaying channel, $\Phi_{\text{dec}} = \left\{\begin{bmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{bmatrix}\right\}$, where $p \in [0, 1]$ is a free parameter, the dual map $\Phi_{\text{dec}}^\circ = \{A_1^\dagger, A_2^\dagger\}$ is not stochastic. However the inverted map $\Phi_{\text{dec}}^R = \left\{\begin{bmatrix} 0 & 0 \\ \sqrt{p} & 0 \end{bmatrix}, \begin{bmatrix} \sqrt{1-p} & 0 \\ 0 & 1 \end{bmatrix}\right\}$, is stochastic. While the decaying channel Φ_{dec} describes the process of a spontaneous decay 'downwards' $|1\rangle \to |0\rangle$ with probability p, the reversed process Φ_{dec}^R describes the transition 'upwards' $|0\rangle \to |1\rangle$. Observe that for such a definition of the reversed map Φ_{dec}^R the Crooks relation holds as a tautology. Note also that the invariants states of the map Φ and its reverse Φ^R are different. This is not the case for the time reversal operation Φ^{R_C} from [26]. Furthermore, in the case $p > 0$ the invariant state of the map Φ_{dec} is pure and thus not invertible, so the operation $\Phi_{\text{dec}}^{R_C}$ is not well defined.

7. Reversing quantum Brownian motion

We now revert back to the environmental representation (4) and assume that the system actually is connected to second physical system which acts as a heat bath. Such a map can be given by (4) where the ancilla state σ is a thermal equilibrium state of a set of harmonic oscillators at inverse temperature β, and U is a unitary time development of the system plus the bath determined by a total Hamiltonian $H = H_S + H_I + H_B$ where H_S is the system Hamiltonian, H_B is the bath Hamiltonian and H_I is a linear interaction of the system and the bath. Standard time reversal of such a map is then given by (5), a procedure that can here be described as 'attach the time-inversed bath, and run time backwards'.

The quantum Brownian motion model is based on the observation that if bath frequencies form a continuum with Ohmic spectrum and a spectral cut-off, and the temperature goes to infinity, then (5) represents classical Kramers–Langevin dynamics $\dot{p} = f(x, t) - \eta \frac{p}{M} + \sqrt{2\eta/\beta}\,\dot{\xi}$ and $\dot{x} = \frac{p}{M}$ [35, 36]. Applying (5) to the quantum Brownian motion model all operators are time reversed according to their parity, which in the classical limit means $t \to t^* = t_f - t$, $x_t \to x_t^* + = x_{t^*}$ and $p_t \to p_t^* + = -p_{t^*}$, and the Kramers–Langevin equation transforms into $\frac{\mathrm{d}p^*}{\mathrm{d}t^*} = f(x^*, t_f - t^*) + \eta \frac{p^*}{M} + \sqrt{2\eta/\beta}\,\dot{\xi}$ and $\frac{\mathrm{d}x^*}{\mathrm{d}t^*} = \frac{p^*}{M}$. Time reversals of classical stochastic differential equations have been extensively discussed in the literature, and it is well understood that they are not unique [17]. The example just derived by taking the classical limit of quantum Brownian motion is the 'natural time reversal' of Kramers–Langevin dynamics, but also other possibilities make sense (note the 'anti-friction'!).

A second example of time reversal of Kramers–Langevin dynamics, in [17] called 'canonical time reversal', is based on the same variable transformation but assumes that the conservative force and the friction force transform differently under time inversion, resulting in a Kramers–Langevin dynamics also for the time-reversed motion i.e. $\frac{\mathrm{d}}{\mathrm{d}t^*}p^* = f(x^*, t_f - t^*) - \eta \frac{p^*}{M} + \sqrt{2\eta/\beta}\,\dot{\xi}$ and $\frac{\mathrm{d}}{\mathrm{d}t^*}x^* = \frac{p^*}{M}$. To lift this definition to 'R' we obviously have to treat the system and the bath differently. For the bath time must run forwards, so as to result in dissipation, while the conservative effects embodied in the force f are to be applied in the opposite order. This can be achieved by considering the system Hamiltonian of the form $H_S = H_{\mathrm{kin}} + V(x_S, t)$ and the two unitary operators

$$U = \mathcal{T} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\left(\int_0^{t_f} H_{\mathrm{kin}} + V(x_S, t) + H_I + H_B\right)} \tag{16}$$

$$U^{R_C} = \mathcal{T} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\left(\int_0^{t_f} H_{\mathrm{kin}} + V(x_S, t_f - t) + H_I + H_B\right)} \tag{17}$$

where $\mathcal{T}$ stands for time ordering. Time reversal by changing U to U^R amounts to the procedure of 'attach the bath, let time run forwards, but time-reverse the external drive'. In [17] several other examples are given of time reversals of stochastic dynamics which can also be 'lifted to R'.

8. Discussion

In this work we have introduced a general notion of time reversals of quantum maps which generalizes standard time inversion in quantum mechanics. As in classical dynamics in contact with a heat bath, this definition of time reversal is not unique. One possibility—but not the only possibility—is to choose an environmental representation of the quantum map, and then apply standard quantum-time inversion on the combined system and ancilla. Another possibility is to start from an intrinsic definition of the quantum map in terms of Kraus operators, and then define time reversal on that level. In any case, from any such definition one can define an entropy production in the environment functional analogously to the classical setting, and for each such definition quantum fluctuation relations are satisfied identically.

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Note added. After the first version of this paper was posted in the arXiv a related work [37] appeared.

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