Second law for quantum operations

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We study thermodynamics of small quantum systems which are interacting with an environment that retains an arbitrary amount of memory. Such environmental memory is captured by initial correlations between the system and environment. For such dynamics, we formulate a second law of thermodynamics. As an application, we discuss how such correlations can be used to cool a quantum system.

Introduction.— Physical sciences are replete with inequalities that inform us about the limits on allowed transformations. For example, the Heisenberg’s uncertainty principle tells us that the product of the measurement uncertainties of conjugate observables is lower-bounded by a non-zero constant. In classical equilibrium thermodynamics, the second law is an inequality that implies that the entropy produced in natural irreversible adiabatic processes is always positive semi-definite [1]. Various reformulations of the second law for quantum systems and the study of fluctuations about the average quantities described by these laws have been a field of intense investigation [2–4]. The central theme of all of these investigations is to extend the applicability of the laws of thermodynamics to quantum systems of arbitrary dimensionality was obtained by several authors by noting that the irreversible entropy production is intimately connected to the structure of completely-positive trace-preserving (CPTP) maps [5–7, 8, 9, 10, 11]. For a state transformation generated by a CPTP map \( \Phi_{1:0}(\sigma_0) = \sigma_1 \), contravity of quantum relative entropy implies that \( S(\sigma_0 || e_0) \geq S(\sigma_1 || e_0) \). Here \( e_0 \) is a fixed point of the map \( \Phi_{1:0} \), namely \( \Phi_{1:0}(e_0) = e_0 \) [8, 11, 12]. Consequently, the change in the von Neumann entropy of the system is bounded from below by the following:

\[
S(\sigma_1) - S(\sigma_0) \geq -\tr[\sigma_1 \log(\sigma_1) - \sigma_0 \log(\sigma_0)].
\]

(1)

This is the quantum version of the classical Hatano-Sasa inequality.

The classical Hatano-Sasa inequality [11, 13] concerns itself with non-equilibrium dynamics of classical systems. As a set of external parameters \( \alpha \) are varied, there is a relationship between observed dynamics of the system and steady-state probability distribution \( r_{ss}(x, \alpha) \). In terms of the position \( x \), Hatano-Sasa inequality is given by

\[
\left\langle \int_{\alpha(0)}^{\alpha(1)} \! d\alpha \frac{\partial r(x; \alpha)}{\partial \alpha} \right\rangle_{r_{ss}(x, \alpha)} \geq 0. 
\]

(2)

Here, \( \langle \cdot \rangle_{r_{ss}} \) is the average over all trajectories \( x(t) \) and \( \phi := \beta(E(x; \alpha) - F(\alpha)) \) is related to the non-equilibrium steady state via \( r_{ss}(x, \alpha) = \exp(-\phi(x, \alpha)) \). This inequality relates the fluctuation properties of non-equilibrium systems to steady state physics, quantifying the violation of detailed balance in terms of so-called “house-keeping” heat, permanently lost in maintaining the quantum state in a non-equilibrium steady state and “excess heat” associated with the transition [14]. As a generalization of Jarzynski’s inequality [15], Hatano-Sasa inequality quantifies the distribution of entropy generated during a non-equilibrium process. The importance of these relations is in quantifying the distribution of both the energy and the entropy production for non-equilibrium dynamics of driven classical systems. Greater control of quantum thermal machines and other generic quantum systems demand such a machinery be developed to discuss arbitrary quantum dynamics.

Initial correlations and CPTP maps.— CPTP maps, like \( \Phi_{1:0} \) employed to obtain Eq. (1), are thought to represent generic quantum processes. This is only true under the assumption that the system and the environment are uncorrelated at the beginning of the process. Therefore the most general quantum process cannot be described by such a map [16, 18]. For instance, imagine a molecule going through complex dynamics. At an arbitrary instance of time after the beginning of this dynamical process, the molecule is sure to be correlated with the environment that it is also interacting with. A CPTP map cannot describe the evolution of the molecule between two intermediate times of such a process. For the dynamics
between two intermediate points of a CPTP process to be also a CPTP map, the process must satisfy divisibility [19], a condition that is not satisfied in general. Consequently, if we want to describe the entropy production for this molecule between two intermediate time steps, then Eq. (1) does not apply and a bound on entropy production is not known. Note that methods of describing initial correlations, like assignment maps [16, 18, 20], suffer from non-unique representations. This makes them less suitable to discuss physical laws such as the second law.

There are several reasons why initial correlations are so prevalent. One example involves a spin interacting with a collection of spins, each of which are in turn interacting with independent local baths [21]. Other physical systems of interest that demonstrate non-Markovianity include quantum machines [22]. The presence of initial correlations could be seen by the departure of the description of system dynamics in terms of CPTP maps like $\Phi_{1,0}$ in Eq. (1). Formally, the presence of the initial correlations can be verified using sophisticated witnesses [23, 24], some of which have been experimentally demonstrated [25, 26]. In order to describe the dynamics of systems at a time scale which are much shorter than the memory of the environment, initial correlations must be taken into account. Given the prevalence of fast quantum control [27], this regime of dynamics is becoming ever more relevant for experiments.

It is also important to consider the presence of initial correlations from a quantum control perspective. Imagine a qubit (the system) is reset by a cavity (the environment) after it performs some task [28]. After the first reset, the system and the environment will be correlated for a finite amount of time. These correlations may not fully vanish by the time the qubit needs to be reset again. Such protocols, wherein the same environment is repeatedly used, are common to many quantum control protocols, including cooling and computing [29–32]. They represent varying degrees of bath memory, which have been shown to be useful for various thermodynamic tasks [29]. Consequently, such bath non-Markovianity has drawn a lot of recent interest [19, 24, 33–37]. Since CPTP structure of maps may fail in this regime of dynamics, for such systems that are initially correlated with their environments, no formulation of the second law like Eq. (1) exists. Our result, which provides such a second law, will have wide applicability as it accounts for entropy production for quantum processes acting on arbitrary quantum systems, interacting with environments that retain an arbitrary amount of memory.

Operational approach to open dynamics.— We imagine a quantum process of discrete time steps $[0, \ldots, j, \ldots, k, \ldots, K]$. An operation $\mathcal{A}_j$ is performed on the system at time-step $j$. The system is then subject to evolution from time-step $j$ to $k$, which is described by $\mathcal{M}_{k,j}$ (to be formally constructed below). We wish to find a bound on the entropy production due to the choice of operation $\mathcal{A}_j$ being subject to the evolution described by a map $\mathcal{M}_{k,j}$. Our approach to this problem begins by noting the operationally meaningful description for the dynamics of initially correlated systems. Below we review the operational reasoning that leads to a full description for the dynamics of systems initially correlated with the environment.

From an operational point of view, any quantum experiment can be thought of in three steps: preparation, process, and measurement. For initially correlated systems it is preparation that play a non-trivial role in the experiment [38]. A preparation is a procedure that is described by a classical to quantum channel that outputs a quantum state for a random or deliberate classical choice. For example, take the correlated state of the system and environment to be the entangled state $(|0\rangle e_0 + |1\rangle e_1)/\sqrt{2}$. Now, imagine preparing the state $|0\rangle$ for the system in the following ways: (i) project the system onto $|0\rangle$ and (ii) project the system onto $|\alpha(0)\rangle + |\beta(1)\rangle$ and then rotate it to $|0\rangle$. In the former case, the state of the corresponding state of the environment will be $|e_0\rangle$, while for the latter case it will be $\alpha|e_0\rangle + \beta|e_1\rangle$. If the system, in state $|0\rangle$, interacts with the environment, the final state of the system will be different for the two cases. Since $\alpha$ and $\beta$ can be chosen from a continuous set it may seem that there is no unique way to prepare state $|0\rangle$ and therefore all corresponding output state will be function of the preparation. This is indeed the problem with describing the dynamics of a system initial correlated with its environment, see [39] for several constructive examples.

In a series of papers [38, 40, 41] this problem was tackled in an operational manner. The reasoning goes like this: At time-step $j$ must prepare the system into a desired state $\Pi_j$ using some operations: $\mathcal{A}_j[\sigma_j] = \Pi_j$. The example above shows that we should not only care about the output of the preparation but the preparation procedure itself. In the laboratory the preparation procedure can be awfully complicated, nevertheless we can fully describe any such procedure by a completely-positive (but not necessarily a trace-preserving) map. Next, we let the prepared system evolve, which may include an interaction with the environment, and measure the output state $\sigma_k$. The key observation in describing this dynamics is that the variable of the problem (that we are free to choose) is the operation $\mathcal{A}_j$ and $\sigma_j$. The corresponding output to $\mathcal{A}_j$ is the final state $\sigma_k$. Therefore to describe the dynamics with need a map joins these two elements: $\mathcal{M}_{k,j}[\mathcal{A}_j] = \sigma_k$. We will refer to such a map as a $\mathcal{M}$-map.

Consider the following (fixed) set of preparations procedures:

$$d^{(nm)}[\sigma_j] = |\pi^{(n)}\rangle \langle \pi^{(m)}| \sigma_j \langle \pi^{(m)}| \pi^{(n)}|,$$

(3)

where $|\pi^{(m)}\rangle$ are eigenvectors of projections $\{\Pi^{(j)} = |\pi^{(j)}\rangle \langle \pi^{(j)}|\}$, which form a linearly independent set. The preparations $d^{(nm)}$ are completely positive with Kraus operators $|\pi^{(n)}\rangle \langle \pi^{(m)}|$. The maps of Eq. (5) describe procedures where the system is projected along direction $|\pi^{(m)}\rangle$ followed by a rotation to $|\pi^{(n)}\rangle$ [42]. If we subject the system to the evolution after such preparation we will measure the corresponding output states $\{E_{jk}^{(nm)}\}$. Now note that, any Hermitian operator on the Hilbert space of the system can be linearly (but
not convexly) expanded in terms of \( \{ \Pi^{(m)} \} \). Therefore any generalizer super-operator can be linearly (but not convexly) expanded in terms of \( p^{(mn)} \) in Eq. (3): \( A_j = \sum_{mn} \alpha_j^{(mn)} p^{(mn)} \). And the dynamics is described by the \( \mathcal{M} \)-map as

\[
\mathcal{M}_{k,j}[A_j] = \sum_{mn} \alpha_j^{(mn)} \mathcal{M}_{k,j}[p^{(mn)}] = \sum_{mn} \alpha_j^{(mn)} Q^{(mn)}_{jk} = \sigma_k. \tag{4}
\]

Therefore choosing the finite (linearly independent) set of preparations \( \{ p^{(mn)} \} \) and measuring the corresponding output states \( \{ Q^{(mn)}_{jk} \} \) is enough to predict the output state \( \sigma_k \) for any operation \( A_j \). The important point is that there are only a finite number of \( p^{(mn)} \). With this finite set \( \mathcal{M} \)-map is constructed, which defined on any completely positive operation on the system. Therefore \( \mathcal{M} \)-map describes the discrete dynamics any two time-steps (see [41] for details on \( \mathcal{M} \)-map).

There are several ways in which \( \mathcal{M} \)-map differs from the familiar CPTP map. Firstly, \( \mathcal{M} \)-map acts on a CPTP map (namely \( A \)) to yield a quantum state. Secondly, the trace of an operation \( A \) is \( d \), while \( \mathcal{M}[A] \) is a unit-trace state. Hence, \( \mathcal{M} \)-map is not trace preserving. However, \( \mathcal{M} \)-map is completely positive and yields a unit-trace output state. Lastly, since \( \mathcal{M} \)-map is mapping from operations to states it cannot have a steady-state solution.

**Entropy production due to operations.**— Before we present the main result we need to develop two tools, which we will then employ to produce the result. Firstly, \( \mathcal{M} \)-map is not trace preserving and to remedy that we define: \( \mathcal{M}^2[A] = \sigma \otimes O \), where \( O \) is a positive, trace-\( d \)-operator. This makes \( \mathcal{M}^2 \) a CPTP map. Next, in analogy to Hatano-Sasa we need to recognize a steady-state operation \( \mathcal{E} \) such that \( \mathcal{M}^2[\mathcal{E}] = \mathcal{E} \). A steady-state can be sought for \( \mathcal{M}^2 \)-maps since they are CPTP maps which map operations to states which have the same dimensionality as operations. However, from above we have \( \mathcal{M}^2[\mathcal{E}] = \epsilon \otimes O \). Therefore, we have \( \mathcal{E} = \epsilon \otimes O \). The action of \( \mathcal{E} \) on a state \( \sigma \) is defined as \( \mathcal{E}[\sigma] = \epsilon \otimes O \sigma \). If we demand \( \mathcal{E} \) to preserve trace then we have \( O = I \) and \( \mathcal{E} = \epsilon \otimes I \) [43].

The part of \( \mathcal{E} = \epsilon \otimes I \) corresponds to the trace of the system state. Such an action destroys all correlations between system and the environment. Next, the system state is "replaced" by a special state \( \epsilon \) such it is the fixed point of the subsequent evolution. In other words, it is the fixed point of the map that describes the dynamics from \( j \) to \( k \) when the initial correlations are deleted. The \( \epsilon \) here plays the same role as it does in Eq. (1).

We now want to derive an inequality similar to Eq. (1) using complete-positivity of \( \mathcal{M}^2 \). Such an entropy change represents the relationship between the choice made by the experimenter and the subsequent evolution with a correlated environment. The promised bound on the entropy change is obtained by using the contractivity of relative entropy of CPTP maps and steady-state operation:

\[
S(\mathcal{A}_j/d \| \mathcal{E}_j/d) \geq S \left( \mathcal{M}_{k,j}^{\dagger}[\mathcal{A}_j/d] \right) \left( \mathcal{M}_{k,j}^{\dagger}[\mathcal{E}_j/d] \right). \tag{5}
\]

The reduced states at the beginning and end are given by \( \sigma_j \) and \( \sigma_k \) respectively. Eq. (5) can be simplified to obtain the main result, namely the law for the entropy production due to quantum operations

\[
S(\sigma_k \otimes I_d) - S(\mathcal{A}_j/d) - \text{tr}[(\sigma_k \otimes I_d - \mathcal{A}_j/d) \log(\epsilon_j) \otimes I], \tag{6}
\]

where \( I_d = I/d \). The last equation is the main result of this Letter [44].

Eq. (6) gives a lower bound in the entropy change between a chosen operation \( \mathcal{A}_j/d \) and the resultant final state \( \sigma_k \otimes I_d \). To understand the meaning of the difference of entropy between a state and an operation, we can think of the Choi state [45] associated with \( A_j \). Owing to Choi-Jamiolkowski isomorphism [46], such a state has the same dimensionality as \( \sigma_k \otimes I_d \). Alternatively, we can think of the fact that any operation \( A_j \) has a tensor-product description, given by \( A_j = \Sigma_n N^n_j \otimes L^n_j \) (see [47]). The action of the operation on the state is then given by \( A_j(\sigma_j) = \Sigma_n N^n_j [\log(\sigma_j)] = \sigma_j' \). Given that \( \log(\mathcal{A}_j) = d \), it follows that \( \mathcal{A}_j/d \) is a normalized state.

For instance, a unitary transformation would correspond to \( \mathcal{A}_j/d \) being a pure state. Such a choice would make the second term \( S(\mathcal{A}_j/d) \) vanish. Now, if we assume that \( \log(\epsilon_j \otimes I) = -\log(d) \otimes I \), then the right hand side of Eq. (6) becomes zero. This is identical to the inequality resulting from the choice of unitary maps for the quantum Hatano-Sasa inequality. On the other hand, \( \mathcal{A}_j/d = I/d \otimes I_d \), the maximally mixed state, corresponds to the choice of "throwing away" the state and replacing it with the maximally mixed state. This causes \( S(\mathcal{A}_j/d) = 2 \log(d) \). This bounds the entropy \( S(\sigma_k) \) to be at least \( -\text{tr}[(\sigma_k - I_d) \log(\epsilon_j)] + \log(d) \), a quantity which is at most \( \log(d) \) if \( \sigma_k = I_d \), corresponding to \( \epsilon_j = I_d \).

**Thermodynamical Tasks.**— We now give three application of Eq. (6) with respective choice of the steady-state operation \( \mathcal{E}_j \) the corresponding fixed state \( \epsilon_j \). These applications constitutes deriving the quantum second law for systems initially uncorrelated with the environment, i.e., recovering Eq. (1) from Eq. (6); quantum version of the Clausius inequality; and cooling systems correlated with their environment.

**Recovering Quantum Hatano-Sasa Inequality.—** Here we show that Eq. (6) encapsulates Eq. (1), i.e., the former reduces to the latter when the initial global state has no correlations. For uncorrelated global states, an operation on the system has no effect on the state of the environment: \( \mathcal{A}_j \otimes I [\sigma_j \otimes \tau_j] = \sigma_j' \otimes \tau_j \), where \( \tau_j \) was the initial state of the environment. Therefore all mappings from \( \sigma_j \) to \( \sigma_j' \) are operationally equivalent and can be written as \( \mathcal{A}_j = \sigma_j' \otimes I \). That is, the map ‘throws away’ \( \sigma_j \) and ‘replaces’ it with \( \sigma_j' \). Moreover, the fixed point of the \( \mathcal{M}_{k,j} \), namely \( \mathcal{E}_j = \epsilon_j \otimes I \), is the same as the fixed point of the CPTP map \( \Phi \) representing the environment acting on the state. To elaborate, we will explicitly write the action of an uncorrelated environment on states of the system. Stated in these terms, the action of the
steady-state operation is to ensure that

$$\mathcal{M}_{k,j} [\mathcal{E}_j] \triangleq \text{tr}_\text{env} \left[ U_{k,j} \mathcal{E}_j \otimes I \otimes \tau_j U_{k,j}^\dagger \right] $$  \hspace{1cm} (7)

$$= \text{tr}_\text{env} \left[ U_{k,j} \mathcal{E}_j \otimes \tau_j U_{k,j}^\dagger \right] = \Phi_{k,j} [\mathcal{E}_j] = \varepsilon_j, $$ \hspace{1cm} (8)

Since $\mathcal{E}_j$ prepares the state of the system in $\varepsilon_j$, it simply follows that $\varepsilon_j$ is in fact the fixed point of the CPTP map $\Phi_{k,j}$, which represents the combined action of the global unitary $U_{k,j}$ and the environmental state $\tau_j$ on states of the system. Substituting for $A_j$ and $\mathcal{E}_j$ into Eq. (6) recovers Eq. (1), after noting that the role of the “initial” state is now fulfilled by $\sigma_j$, the state chosen by the experimenter at the preparation step. This, once again, is a reflection of the fact that the second law informs us about the change in entropy related to choices we make.

Clausius inequality.— To understand the role of steady-state preparations $\mathcal{E}_j$ and the corresponding state $\varepsilon_j$, we derive from Eq. (6), the quantum second law. Since we want to start with a physical system that might be initially correlated with an environment and then derive a result valid only when such correlations are not present, we must “throw away” those correlations by the use of a suitable preparation. Furthermore, we must consider thermal states at a given temperature $\beta^{-1}$ to make contact with equilibrium thermodynamics. We hence consider equilibrium states $\varepsilon_j = \exp \{- \beta (H_j - F_j)\}$, where $F_j$ is the free energy of the system at time step $j$. The corresponding equilibrium preparation is given by $\mathcal{E}_j = \exp \{- \beta (H_j - F_j)\} \otimes I$. This “throw and replace” preparation has the effect of replacing the state of the system with the thermal state $\varepsilon_j$. Substituting $\log (\varepsilon_j) = \beta (H_j - F_j)$ into Eq. (6) reduces the inequality to read

$$S(\sigma_k \otimes I_d) - S(A_j/d) \geq \beta \text{tr}[\sigma_k \otimes I_d - A_j/d] H \otimes I].$$  \hspace{1cm} (9)

Note that if $A_j/d = \sigma_j' \otimes I_d$, then the above inequality reduces to the standard second law, namely

$$\Delta S = S(\sigma_k) - S(\sigma_j') \geq \beta \text{tr}[\sigma_k - \sigma_j'] H] = \beta \Delta Q.$$  \hspace{1cm} (10)

Eq. (7) now refers to a “generalized” inequality relating a change in entropy with a change in generalized heat, in the presence of thermal equilibrium states, but non-trivial preparations.

Cooling via Preparations.— To study cooling, let us consider the example of thermal equilibrium states. This choice reduces the right hand side of the inequality above to $\beta \text{tr}[\sigma_k H] - \text{tr}[A_j (H \otimes I)]$. This implies that any operation which satisfies $\text{tr}[A_j (H \otimes I)] > \text{tr}[\sigma_k H]$ is a “cooling operation”. Repeated use of such operations at each step of the control protocol can purify the state completely, and an additional unitary rotation can bring the state to the ground state. Notice that for each step, the effectiveness of the cooling, which is proportional to the magnitude of $\beta$, is enhanced by lowering the temperature corresponding to the thermal map.

Conclusions.— In conclusion, we have extended the second law of thermodynamics to be valid for systems of arbitrary size and with arbitrary amounts of initial correlations. This generalization has a rich structure in that it highlights preparations, which are operationally meaningful quantum operations as being the central choice made by an experimenter. Given a transformation that takes preparations to states, our choice of operation clearly affects the bounds on the entropy produced. In this article, we quantified this connection between the choice available to experimenters and the entropy generated during dynamics. For Markovian evolution of a quantum state $\sigma$ under a thermal map at temperature $\beta^{-1}$ with an equilibrium state $\varepsilon$, we can write

$$\frac{d S(\sigma || \varepsilon)}{dt} = \frac{d S(\sigma)}{dt} - \beta \frac{dQ}{dt}. $$ \hspace{1cm} (11)

For non-Markovian quantum systems, such a bound was hitherto unavailable. Since the notions of heat and temperature are unavailable for arbitrary dynamical processes, an appropriate generalization involves bounding the entropy produced, in the spirit of Clausius formulation of the classic second law. Eq. (9) represents such a bound on the entropy production for initially correlated quantum system dynamics.

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[42] The projections \{Π^{(m)}\} are linearly independent and therefore we can define an equivalent set of maps \(B^{(mn)}[σ_j] = Q^{(mn)}\).
[43] In general any (CPTP) map can be written in the tensor-product decomposition \(A = \sum_a N^a \otimes L^a\), where \{\(N^a \otimes L^a\)\} may not be positive operators. The action of such a map is \(A[σ] = \sum_a N^a \text{tr}[L^a σ] = σ'\). See [47] for details in context of entanglement breaking channels.
[44] If we want to bound the entropy change \(S(σ_k) - S(σ_j)\), then we can just use Eq. (1) in conjunction with Eq. (6), i.e., take the sum of two equations. Where Eq. (1) is used for the operation process \(A_j[σ_j] = σ_j\) along with the steady-state \(a_j\) such that \(A[a_j] = a_j\).
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