ENTROPY DYNAMICS IN THE SYSTEM OF INTERACTING QUBITS

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Abstract

The classical Second Law of Thermodynamics demands that an isolated system evolves with a non-diminishing entropy. This holds as well in quantum mechanics if the evolution of the energy-isolated system can be described by a unital quantum channel. At the same time, the entropy of a system evolving via a non-unital channel can, in principle, decrease. Here, we analyze the behavior of the entropy in the context of the H-theorem. As exemplary phenomena, we discuss the action of a Maxwell demon (MD) operating a qubit and the processes of heating and cooling in a two-qubit system. We further discuss how small initial correlations between a quantum system and a reservoir affect the increase in the entropy under the evolution of the quantum system.

Keywords: Quantum information, H-theorem, quantum mechanics, qubits, quantum correlations, quantum Maxwell demon

1 Introduction

The second law of thermodynamics restricts the processes that are allowed to occur in nature. The Kelvin-Planck formulation tells that it is not possible to construct a device operating in a cycle that extracts heat from a single reservoir and transforms it into work without other effects [1]. More specifically, Carnot describes what maximal heat-to-work conversion-efficiency a heat engine can achieve that operates with two reservoirs at different temperatures [2]. More generally, in classical thermodynamics, the second law expresses an asymmetry between the past and the future by stating that the total entropy of an isolated system either always increases over time or remains constant in ideal cases where the system is in a steady state or is undergoing a reversible process. In the quantum case, however, this statement becomes trivial and the search for a corresponding informative formulation is the subject of numerous studies [3]– [12].

Within a quantum information theoretic setting, a series of exact mathematical results has been developed that formulate the conditions for an evolution with a non-diminishing quantum entropy as defined by von Neumann [13] – [15]. This allowed for a further formulation of a quantum analog of
the classical $H$-theorem \[16\], i.e., the conditions under which the entropy of an open quantum system remains non-diminishing in the course of its quantum evolution. To that end, quantum information theory introduces the concept of the quantum channel, where the evolution of the system’s density matrix $\hat{\rho}_0 \rightarrow \hat{\rho}_t$ is viewed as a trace-preserving completely positive map $\hat{\rho}_t = \Phi(\hat{\rho}_0)$. It turns out \[15\] that for a unital channel $\Phi$, i.e., a channel preserving the identity operator, $\Phi(\hat{1}) = \hat{1}$, the entropy is always non-diminishing $S(\hat{\rho}_t) \geq S(\hat{\rho}_0)$.

In reference \[16\], it has been demonstrated that the unitality condition is also a necessary one for a non-decreasing entropy, provided the evolution of the system is restricted to a finite-dimensional Hilbert space. The latter work also addressed the dynamics of an extended system comprising both the quantum system involved and the reservoir. In general, the evolution of such a system is described by a unitary operator

$$\hat{U} = \sum_{i,j} |\psi_j\rangle \langle \psi_i| \hat{F}_{ji},$$

where $\{|\psi_i\rangle\}$ is an orthonormal basis in the Hilbert space, while the family of operators $\hat{F}_{ji}$ acts in the Hilbert space of the reservoir, with subscripts $i$ and $j$ referring to the initial and final states of the system, respectively. Then, one can formulate an exact criterion of unitality in terms of the operators $\hat{F}_{ji}$ for the quantum channel $\Phi(\hat{\rho}) = \text{Tr}_{\text{res}}\{\hat{U} \hat{\rho} \otimes \hat{\pi}_0 \hat{U}^\dagger\}$ generated by the operator $\hat{U}$. Here, $\hat{\pi}_0$ is the initial density matrix of the reservoir and $\text{Tr}_{\text{res}}$ is the trace with respect to the reservoir states. The sought criterion follows from the expression for the matrix elements

$$[\Phi(\hat{1})]_{jj'} - [\hat{1}]_{jj'} = \sum_{i} \text{Tr}_{\text{res}}\{\hat{\pi}_0 [\hat{F}_{ji}^\dagger, \hat{F}_{jj'}]\}.\quad(2)$$

Namely, if the right hand side of Eq. (2) vanishes, then the system’s entropy is non-diminishing in the course of its evolution, $\Delta S = S(\Phi(\hat{\rho})) - S(\hat{\rho}) \geq 0$.

It turns out that, typically, the entropy corresponding to the evolution of an energy-isolated system is non-decreasing. However, in some special cases, even an energy-isolated system can evolve with a decreasing entropy. These special cases are described by an evolution through a non-unital channel conserving the average energy of the system and several realizations of such channels have been analyzed in Ref. \[17\]. In particular, it has been demonstrated that such a non-unital dynamics involves a partial exchange of the quantum system’s state and that of the reservoir, giving rise to a decreasing system’s entropy if the initial state of the reservoir was more pure (or of lower entropy) than the system’s state. The decreasing of entropy of the system without changing its average energy can be viewed as a result of the action of a so-called quantum Maxwell demon (QMD) \[8\].

Here, we present a universal description of both, a classical \[18\] and a quantum Maxwell demon, by considering the joint unitary evolution of a system and some ancillary system that takes the role of the reservoir. The chosen approach rests on the Stinespring theorem, stating that the action of a quantum channel can be represented as the result of the joint evolution of the given system with some auxiliary system, where the choice of the latter is not unique. Here, we demonstrate that even a single qubit can take up the role of a reservoir. We illustrate the action of the previously derived $H$-theorem utilizing simple exemplary systems and construct both unital and non-unital quantum channels modeling the thermodynamic processes of heating and cooling.

The quantum channel formalism builds on the assumption that, initially, the quantum system and the reservoir are not correlated. Since, in reality, the complete absence of initial correlations between
the given system and the environment cannot be excluded, we also investigate into the influence of such small initial correlations on the entropy dynamics and demonstrate that they can slow down the entropy growth.

2 Qubit realization of the Maxwell demon

Within our approach, only two stages of the working cycle of the thermal engine [18] are relevant for its description, namely, the measurement of the qubit state and the subsequent feedback. In particular, we are not interested in the processes of preparing the qubit for the measurement, neither in the interaction between the qubit and the thermal bath. Such a consideration then treats the feedback controller as a Maxwell demon (MD) and thus, hereafter, we will refer to it as the demon.

At the initial moment \( t_0 \), the qubit’s state is described by the density matrix

\[
\hat{\rho}_0 = p_0 |g\rangle \langle g| + p_1 |e\rangle \langle e| ,
\]

where \( |g\rangle \) and \( |e\rangle \) denote its ground and excited states. The spacing between the energy levels of the qubit can be arbitrarily small. The demon measures the qubit states and, based on the results, executes a feedback operation. If the qubit is found in the ground state, the demon leaves it unchanged. If the qubit appears in the excited state, then the demon drives it into the ground state by extracting work. In the course of the process, the entropy of the qubit changes from \( S_0 = -p_0 \ln p_0 - p_1 \ln p_1 \) to zero, thus, the quantum channel describing the qubit’s evolution is non-unital. The action of the demon can be treated both, in the context of either projective measurements and a feedback action depending on the outcome, or using unitary operators for the evolution of the complete system- and demon-qubit.

Semiclassical demon

Let us consider a semiclassical demon which measures the qubit’s states by the standard procedure and demonstrate that the corresponding quantum channel is non-unital. Initially, at \( t_0 \), the qubit state is described by the density matrix \( \hat{\rho} \). During the \([t_0, t_1]\)-interval, the demon measures the qubit state utilizing the corresponding projective operators \( \hat{M}_g \) and \( \hat{M}_e \),

\[
\hat{M}_g = |g\rangle \langle g| , \quad \hat{M}_e = |e\rangle \langle e| .
\]

In the interval \([t_1, t_2]\), the qubit exercises the feedback operation that depends on the measurement outcome. If the qubit is initially in its ground state, the unitary operator describing the feedback has the form

\[
\hat{U}_g = |g\rangle \langle g| + |e\rangle \langle e| ,
\]

otherwise,

\[
\hat{U}_e = |g\rangle \langle e| + |e\rangle \langle g| .
\]

Thus the quantum channel describing the evolution of the qubit in the interval \([t_0, t_2]\) assumes the form

\[
\Phi(\hat{\rho}) = \hat{U}_g \hat{M}_g \hat{\rho}_0 \hat{M}_g^\dagger \hat{U}_g^\dagger + \hat{U}_e \hat{M}_e \hat{\rho}_0 \hat{M}_e^\dagger \hat{U}_e^\dagger .
\]

Checking for unitality, the equations \( \hat{U}_g \hat{M}_g \hat{\rho}_0 \hat{M}_g^\dagger \hat{U}_g^\dagger = 2 \cdot |g\rangle \langle g| \) produce the result

\[
\Phi(1) = 2 \cdot |g\rangle \langle g| ,
\]

evidencing the non-unitality of the quantum channel.
Quantum demon

In Ref. [19], it has been demonstrated that the projective measurement can be entirely described through the unitary evolution of an extended system comprising the measured system and the measuring device. Thus, the action of the semiclassical demon discussed above can be described as a unitary process, provided the demon is a quantum system by itself. The operations described below act in the two-dimensional subspace of the demon Hilbert space. Let this subspace be endowed with the orthonormal basis $|0\rangle$ and $|1\rangle$ and let the $t_0$ density matrix of the complete qubit–demon system be

$$
\hat{R}_0 = (p_0 |g\rangle \langle g| + p_1 |e\rangle \langle e|) \otimes |0\rangle \langle 0|.
$$

During the interval $[t_0, t_1]$, the demon receives the information about the qubit state. If the qubit is found in the ground state, the demon retains the $|0\rangle$ state, otherwise, the demon transfers to the $|1\rangle$ state. The evolution of the complete system at the stage of the measurement then is described by the unitary operator

$$
\hat{U}_1 = |g\rangle \langle g| \otimes (|0\rangle \langle 0| + |1\rangle \langle 1|) + |e\rangle \langle e| \otimes (|0\rangle \langle 1| + |1\rangle \langle 0|).
$$

During the $[t_1, t_2]$ interval, the demon, based on the obtained information, transfers the qubit to the ground state. The corresponding unitary evolution operator is

$$
\hat{U}_2 = (|g\rangle \langle g| + |e\rangle \langle e|) \otimes |0\rangle \langle 0| + (|g\rangle \langle e| + |e\rangle \langle g|) \otimes |1\rangle \langle 1|.
$$

At the time $t_2$, the system state is defined by the matrix

$$
\hat{R}_f = \hat{U}_2 \hat{U}_1 \hat{R}_0 \hat{U}_1^\dagger \hat{U}_2^\dagger = |g\rangle \langle g| \otimes (p_0 |0\rangle \langle 0| + p_1 |1\rangle \langle 1|),
$$

which evidences that the qubit is in the ground state.

Let us analyze this process in terms of the quantum $H$-theorem. The evolution of the complete system from the moment $t_0$ till the moment $t_2$ is described by the unitary operator

$$
\hat{U} = \hat{U}_2 \hat{U}_1 = |g\rangle \langle g| \otimes |0\rangle \langle 0| + |g\rangle \langle e| \otimes |1\rangle \langle 0| + |e\rangle \langle g| \otimes |0\rangle \langle 1| + |e\rangle \langle e| \otimes |0\rangle \langle 1|.
$$

In an ideal case, the demon has to invest an infinitesimal negative work in order to transfer the qubit from the excited to the ground state. This implies that the qubit can be considered as an energy-isolated system which, however, can get entangled with its environment, here, represented by the demon qubit. The decrease in entropy is related to the non-unitality of the corresponding quantum channel $\Phi$ generated by the operator $[13]$. To see that, let us use Eq. (2), where the operators $\hat{F}_{ji}$ can be found from Eq. (13),

$$
\hat{F}_{gg} = |0\rangle \langle 0|, \quad \hat{F}_{ge} = |1\rangle \langle 0|, \quad \hat{F}_{eg} = |1\rangle \langle 1|, \quad \hat{F}_{ee} = |0\rangle \langle 1|.
$$

After some algebra, we find that

$$
\Phi(\hat{1}) = 2 \cdot |g\rangle \langle g|,
$$

evidencing the non-unitality of the quantum channel. Note that Eq. (14) coincides with Eq. (8).
3 Cooling and heating of two-level systems

In this section, we discuss the processes of cooling and heating emerging in various complex physical systems. Instead of presenting a full description of the real processes, we consider a simplified model describing the interaction of a two-level system with a reservoir operating in a two-dimensional subspace of its Hilbert space. We then focus on the interaction of two qubits. Let the initial state of the two-qubit system be described by the density matrix

\[ \hat{R}_0 = \frac{1}{2}(|g_1\rangle \langle g_1| + |e_1\rangle \langle e_1|) \otimes |g_2\rangle \langle g_2|, \]  

(15)

where the indices 1 and 2 refer to the first and second qubit, respectively. The cooling of the first qubit to zero and the heating of the second qubit to an infinite temperature is described by a final density matrix assuming the form

\[ \hat{R}_f = |g_1\rangle \langle g_1| \otimes \frac{1}{2}(|g_2\rangle \langle g_2| + |e_2\rangle \langle e_2|). \]  

(16)

The unitary evolution operator for this process is identical to the operator given by equation (13)

\[ \hat{U} = |g_1\rangle \langle g_1| \otimes |g_2\rangle \langle g_2| + |g_1\rangle \langle e_1| \otimes |e_2\rangle \langle g_2| + |e_1\rangle \langle g_1| \otimes |e_2\rangle \langle e_2| + |e_1\rangle \langle e_1| \otimes |g_2\rangle \langle e_2|. \]  

(17)

Let us then discuss the evolution of each qubit separately.

Evolution of the first qubit (cooling)

The cooling process is accompanied by a decrease in entropy, thus the quantum channel \( \Phi^{(1)} \) describing the evolution of the first qubit is non-unital. To prove it, consider Eq. (2). The operators \( \hat{F}_{ji} \) act in the space of the states of the second qubit and are found from Eq. (17),

\[ \hat{F}^{(1)}_{gg} = |g_2\rangle \langle g_2|, \quad \hat{F}^{(1)}_{ge} = |e_2\rangle \langle e_2|, \quad \hat{F}^{(1)}_{eg} = |g_1\rangle \langle e_1|, \quad \hat{F}^{(1)}_{ee} = |e_1\rangle \langle g_1|. \]

We then find that \( \Phi^{(1)}(\hat{1}) = 2 \cdot |g_1\rangle \langle g_1| \), i.e., the channel \( \Phi^{(1)} \) is indeed nonunital.

Evolution of the second qubit (heating)

Since the entropy is increasing upon heating, the quantum channel \( \Phi^{(2)} \), describing the evolution of the second qubit can be unital. The corresponding operators \( \hat{F}_{ji} \) act in the Hilbert space of the first qubit and assume the form

\[ \hat{F}^{(2)}_{gg} = |g_1\rangle \langle g_1|, \quad \hat{F}^{(2)}_{ge} = |e_1\rangle \langle e_1|, \quad \hat{F}^{(2)}_{eg} = |g_1\rangle \langle e_1|, \quad \hat{F}^{(2)}_{ee} = |e_1\rangle \langle g_1|. \]

As a result, we find that the channel \( \Phi^{(2)}(\hat{1}) = \hat{1} \) is unital.
4 The effect of initial correlations

So far, we have addressed processes that occur in the absence of correlations between the initial state of the quantum system and the reservoir. Let us consider then the change in entropy of a quantum system that is initially correlated with the state of the reservoir and find, how the increase in entropy relates to that in the uncorrelated situation. \footnote{In quantum information theory, such a situation is usually not investigated since in this case the evolution of the system cannot be described by a quantum channel.}

As before, we consider the first qubit as our system, while the second one serves as a reservoir. The evolution of the complete system is again described by the unitary operator (13), which, as we have seen, can describe thermalization processes. One expects an increase in the system entropy if its initial entropy is less than the entropy of the reservoir. Let us first consider uncorrelated subsystems and write the initial density matrix of the complete system in the form

\[
\hat{R}_0^{(0)} = \hat{\rho}_0^{(0)} \otimes \hat{\pi}_0^{(0)},
\]

where \(\hat{\rho}_0^{(0)}\) describes the initial state of the system,

\[
\hat{\rho}_0^{(0)} = p_0 \ket{g} \bra{g} + p_1 \ket{e} \bra{e}.
\]

The operator \(\hat{\pi}_0^{(0)}\) describes the initial state of the reservoir,

\[
\hat{\pi}_0^{(0)} = q_0 \ket{0} \bra{0} + q_1 \ket{1} \bra{1}.
\]

The initial entropy of the system is

\[
S_0^{(0)} = -p_0 \ln p_0 - p_1 \ln p_1.
\]

The final state of the complete system is given by

\[
\hat{R}_f^{(0)} = \hat{U} \hat{R}_0^{(0)} \hat{U}^\dagger = p_0 q_0 \ket{g} \bra{g} \otimes \ket{0} \bra{0} + p_1 q_0 \ket{g} \bra{g} \otimes \ket{1} \bra{1} + p_0 q_1 \ket{e} \bra{e} \otimes \ket{1} \bra{1} + p_1 q_1 \ket{e} \bra{e} \otimes \ket{0} \bra{0}.
\]

Taking the partial trace over the reservoir states, we arrive at the matrix describing the system’s final state,

\[
\hat{\rho}_f^{(0)} = q_0 \ket{g} \bra{g} + q_1 \ket{e} \bra{e}.
\]

Thus, the final entropy of the system is equal to the initial entropy of the reservoir,

\[
S_f^{(0)} = -q_0 \ln q_0 - q_1 \ln q_1,
\]

and the entropy of the system indeed increases,

\[
\Delta S^{(0)} = S_f^{(0)} - S_0^{(0)} = -q_0 \ln q_0 - q_1 \ln q_1 + p_0 \ln p_0 + p_1 \ln p_1 > 0.
\]
Let us now consider the situation where the initial states of the system and the reservoir are classically correlated. The initial state of the system is given by

\[ \hat{R}_0 = (1 - \epsilon) \hat{R}_0^{(0)} + \epsilon (p_0 |g\rangle \langle g| \otimes |0\rangle \langle 0| + p_1 |e\rangle \langle e| \otimes |1\rangle \langle 1|), \]  

(26)

where \( \epsilon \) is the small parameter; for \( \epsilon = 0 \), the correlation disappears and \( \hat{R}_0 \) turns into \( \hat{R}_0^{(0)} \). One can easily see that \( \hat{R}_0 \) has unit trace and the reduced density matrix of the initial state of the system \( \hat{\rho}_0 \) coincides with \( \hat{\rho}_0^{(0)} \). The final state of the complete system assumes the form

\[ \hat{R}_f = \hat{U} \hat{R}_0 \hat{U}^\dagger = (1 - \epsilon) \hat{R}_f^{(0)} + \epsilon (p_0 |g\rangle \langle g| + p_1 |e\rangle \langle e|) \otimes |0\rangle \langle 0|. \]  

(27)

This yields the reduced density matrix of the system’s final state as

\[ \hat{\rho}_f = \{q_0 + \epsilon (p_0 - q_0)\} |g\rangle \langle g| + \{q_1 + \epsilon (p_1 - q_1)\} |e\rangle \langle e|. \]  

(28)

Accordingly, the final entropy of the system is

\[ S_f = -\{q_0 + \epsilon (p_0 - q_0)\} \ln \{q_0 + \epsilon (p_0 - q_0)\} - \{q_1 + \epsilon (p_1 - q_1)\} \ln \{q_1 + \epsilon (p_1 - q_1)\}. \]  

(29)

Now we can find the difference between the increase of entropy \( \Delta S \) in the case of the small correlation between the initial states of the system and the reservoir and the quantity \( \Delta S^{(0)} \) corresponding the initially uncorrelated states. Bearing in mind that \( p_0 + p_1 = q_0 + q_1 = 1 \), we expand in powers of small \( \epsilon \) and find that

\[ \Delta S - \Delta S^{(0)} = S_f - S_f^{(0)} = \epsilon (q_0 - p_0) \ln \frac{q_0}{1 - q_0} - \epsilon^2 \frac{(p_0 - q_0)^2}{2q_0q_1} + o(\epsilon^2). \]  

(30)

Hence, provided the initial entropy of the system is less than that of the reservoir (e.g., \( p_0 > q_0 \geq 1/2 \) or \( p_0 < q_0 \leq 1/2 \)), then \( \Delta S - \Delta S^{(0)} < 0 \) if \( \epsilon \) is sufficiently small. Therefore, the presence of weak initial classical correlations results in a gain of "correlated" entropy that is less than the increase in entropy of the initially uncorrelated situation. More complex cases involving an initial entanglement of the system and the reservoir will be discussed in a forthcoming publication.

5 Summary

In this work, we have demonstrated how the previously formulated quantum H-theorem can be used for analyzing the processes within the two-qubit system. Namely, examination of unitality can provide a rigorous approach to describe the work of a Maxwell demon and the thermal processes.

Moreover, we have uncovered the situation when the presence of slight initial correlations between the system and its environment can lead to a lesser entropy gain of the system in comparison to the case of the initially uncorrelated state.

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