H-theorem and Maxwell Demon
in Quantum Physics

N.S. Kirsanov$^{1*}$, A.V. Lebedev$^{2,1}$, I.A. Sadovskyy$^{3}$, M.V. Suslov$^{1}$,
V.M. Vinokur$^{3}$, G. Blatter$^{2}$, and G.B. Lesovik$^{1}$

$^{1}$Moscow Institute of Physics and Technology
141700, Institutskii Per. 9, Dolgoprudny, Moscow Distr., Russian Federation

$^{2}$Theoretische Physik, Wolfgang-Pauli-Strasse 27, ETH Zürich, CH-8093 Zürich, Switzerland

$^{3}$Materials Science Division, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL 60439, USA

$^*$nikita.kirsanov@phystech.edu

Abstract

The Second Law of Thermodynamics states that temporal evolution of an isolated system occurs with non-diminishing entropy. In quantum realm, this holds for energy-isolated systems the evolution of which is described by the so-called unital quantum channel. The entropy of a system evolving in a non-unital quantum channel can, in principle, decrease. We formulate a general criterion of unitality for the evolution of a quantum system, enabling a simple and rigorous approach for finding and identifying the processes accompanied by decreasing entropy in energy-isolated systems. We discuss two examples illustrating our findings, the quantum Maxwell demon and heating-cooling process within a two-qubit system.

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

1 Introduction

Recently, building on the mathematical formalism of quantum information theory (QIT), we have formulated a quantum H-theorem in terms of physical observables [1]. Consider a fixed-energy subspace $E$ of the system’s Hilbert space spanned by the orthonormal basis states $|\psi_{i,E}\rangle$, $\hat{H}_S|\psi_{i,E}\rangle = E|\psi_{i,E}\rangle$, where the index $i$ denotes all of the system’s remaining non-energy degrees of freedom and $\hat{H}_S$ denotes the system Hamiltonian. We can write the evolution operator $\hat{U}$ of the grand system, i.e., the system plus reservoir, as $\hat{U} = \sum_{E,ij} |\psi_{j,E}\rangle \langle \psi_{i,E}| s_{ji,E} \hat{F}_{ji,E}$, where the coefficients $s_{ji,E}$ are elements of the scattering matrix describing the transitions between the system’s quantum states $|\psi_{i,E}\rangle \rightarrow |\psi_{j,E}\rangle$ (without taking into account the interaction with the reservoir) and the family of operators $\hat{F}_{ji,E}$ act in the reservoir Hilbert space, with the subscripts $i$, $j$, and $E$ specifying the system’s states.

To describe the quantum dynamics of an open system, QIT introduces the so-called quantum channel (QC) defined as a trace-preserving completely positive map, $\tilde{\rho} = \Phi(\hat{\rho})$, of a density matrix $\hat{\rho}$. To determine whether the evolution belongs to the class of unital channels, implying that the system evolves with a
non-negative entropy gain $\Delta S = S(\Phi(\hat{\rho})) - S(\hat{\rho}) \geq 0$, one has to check if $\Phi(\hat{1}) = \hat{1}$. Using the unitarity of $\hat{U}$, one finds \[1\]

$$
\Phi_{jj'}(\hat{1}_E) - [\hat{1}_E]_{jj'} = \sum_i s_{ji,E} s_{j'_i,E}^* \langle [\hat{F}^\dagger_{j'_i}, \hat{F}_{ji}] \rangle,
$$

(1)

where $\langle \ldots \rangle$ denotes averaging with respect to the initial state of the reservoir and $\hat{1}_E = \sum_i |\psi_{i,E}\rangle \langle \psi_{i,E}|$. This relation is the central result of Ref. \[1\]. It allows to formulate the quantum $H$-theorem as follows: \textit{If the r.h.s. of Equation (1) vanishes, the quantum system evolves with $\Delta S \geq 0$.} Using this result, we have demonstrated that the typical evolution of energy-isolated quantum systems occurs with non-diminishing entropy. E.g., we have shown that the electron-phonon interaction implies that an electron’s evolution satisfies the conditions of the quantum $H$-theorem. The same is true for an electron interacting with a random ensemble of three-dimensional (3D) nuclear spins for the case where the thermodynamic averaging of the commutators in Equation (1) implies their vanishing.

Yet, we also have uncovered special situations where the Second Law, stating that the entropy of an isolated system is non-decreasing, can be locally violated. In \[2\], we have proposed several setups which realize non-unital and energy-conserving quantum channels and where a micro-environment acts with two non-commuting operations on the system in an autonomous way. We have found, that such a process corresponds to a partial exchange or \textit{swap} between the system’s and the environment’s quantum states, with the system’s entropy decreasing if the environment’s state is more pure. This entropy-decreasing
process is naturally thought of as the action of a quantum version of a Maxwell demon. We have proposed a quantum-thermodynamic engine capable of extracting energy from a single heat reservoir and perform useful work, provided that pure qubits are available for the machine’s operation. The special feature of this engine, which involves an energy-conserving non-unital quantum channel, is the separation of its entire operation cycle into two subcycles (that are, in principle, spatially remote), a working cycle and an entropy cycle. This allows the engine to run with no local waste heat, see Figure 1.

It seems to us, however, that for many reasons it is not really appropriate to invoke a ’demon’ in the operation of this engine, as this expression comes with many negative connotations and a ’demon’s action’ may be associated with certain detrimental work. Our ‘demon’, on the opposite, serves a useful purpose and, in our view, should instead be called a *Quantum Angel*. Nevertheless, for the time being, below we use the traditional terminology.

In the following, we show how our criterion of unitality as expressed in Equation (1) can be used to identify quantum processes associated with an entropy change and investigate two examples to which this approach is relevant. First, we discuss a Maxwell demon based on a qubit, originally described in Ref. [3] within a classical framework. Secondly, we will consider a process taking place in a two-qubit system that comprises heating and cooling.

## 2 Quantum Version of Maxwell Demon
### Based on a Single Qubit

In this section, we discuss a system that acts as a Maxwell demon described in Ref. [3]. There the engine’s operation involves a standard measurement which is followed by the feedback protocol based on the obtained data. Here, we discuss a fully quantum version of the demon for which both, the measurement and the conditional feedback can be expressed by unitary operators. The possibility of such a unitary measuring process was demonstrated in [4].

The demon’s setup is based on a two-level (*qubit*) system that interacts with the bath characterized by the temperature $T$. The distance between the energy levels of the qubit ground ($g$) and the exited ($e$)
states can be changed via the control parameter $q$.

At the start of the cycle, the qubit is in the ground state (point A in Fig. 2) and the level spacing $\Delta E_A \gg k_B T$; thus, the qubit state is not subject to fluctuations. The control gate is then changed adiabatically to the value that corresponds to the minimum level separation $\Delta E_X \ll k_B T$ (point X in Fig. 2). This results in an entropy gain of the qubit by $k_B \ln 2$, with a corresponding amount of heat $k_B T \ln 2$ being extracted from the bath. Subsequently, another quantum system (the manipulator) performs a measurement of the qubit state. Based on the obtained information, the manipulator executes a feedback protocol: if the qubit is in the ground state, $q$ is moved quickly to the original point A. Otherwise, if the qubit is in the exited state, the manipulator swaps the qubit state $e \rightarrow g$ by performing the work $-\Delta E_X$, followed by the transition to the position A.

In our analysis, we focus on the dynamics of the qubit–manipulator compound system only. In this case, the manipulator plays the role of the Maxwell demon, so in what follows, we will be using the term ‘demon’ rather than ‘manipulator’. The time evolution of the compound system during one cycle can be divided in five stages:

1. At time $t_0$, the initial state of the compound system is denoted by the point A, its corresponding density matrix is $\hat{R}_i =  \hat{\rho}_i \otimes \hat{\pi}_i$, where $\hat{\rho}_i$ describes the qubit state, and $\hat{\pi}_i = |0\rangle \langle 0|$ describes the demon state.

2. From $t_0$ to $t_1$, the qubit undergoes a unitary evolution, the system transfers from point A to point X, while the demon state remains the same. At the time $t_1$, the compound system’s state is described by the matrix
   $$\hat{R}_1 = \hat{\rho}_1 \otimes |0\rangle \langle 0|,$$
   where the qubit matrix $\hat{\rho}_1$ is diagonal and given by
   $$\hat{\rho}_1 = \rho_{gg} |g\rangle \langle g| + \rho_{ee} |e\rangle \langle e|,$$
   where $|g\rangle$ stands for the ground state and $|e\rangle$ stands for the exited state.

3. From $t_1$ to $t_2$, the demon receives the information about the qubit state. If the qubit is found in the ground state, the demon remains in the state $|0\rangle$, otherwise the demon state becomes $|1\rangle$ ($\langle 0|1\rangle = 0$). The compound system then evolves according to unitary operator
   $$\hat{U}_1 = |g\rangle \langle g| \otimes (|0\rangle \langle 0| + |1\rangle \langle 1|) + |e\rangle \langle e| \otimes (|0\rangle \langle 1| + |1\rangle \langle 0|).$$
   At the time $t_2$, the compound system state is
   $$\hat{R}_2 = \rho_{gg} |g\rangle \langle g| \otimes |0\rangle \langle 0| + \rho_{ee} |e\rangle \langle e| \otimes |1\rangle \langle 1|.$$

4. From $t_2$ to $t_3$, the demon performs a feedback operation on the qubit that depends on the obtained information, with a corresponding unitary evolution operator
   $$\hat{U}_2 = (|g\rangle \langle g| + |e\rangle \langle e|) \otimes |0\rangle \langle 0| + (|g\rangle \langle e| + |e\rangle \langle g|) \otimes |1\rangle \langle 1|.$$
   At the time $t_3$, the compound system’s state becomes
   $$\hat{R}_3 = |g\rangle \langle g| \otimes (\rho_{gg} |0\rangle \langle 0| + \rho_{ee} |1\rangle \langle 1|).$$
5. From \( t_3 \) to \( t_4 \), the qubit ground state reverses to the position A through the unitary evolution, while the demon state is being prepared for the next cycle.

The vanishing of the terms \( |e\rangle \langle e| \otimes |0\rangle \langle 0| \) and \( |e\rangle \langle g| \otimes |1\rangle \langle 1| \) of \( \hat{U}_2 \) after its action on the compound system’s state reflects the fact that the feedback control depends on the information obtained by the demon. At the same time, these terms guarantee the unitarity of the evolution.

Let us consider the evolution of the compound system within the framework and terminology of the quantum H-theorem \[1]. Namely, we focus on the third and the fourth stages of the cycle. We note that the compound system evolution from \( t_1 \) to \( t_3 \) is characterized by the unitary operator

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

(8)

(see Equation (4) and (6)). Ideally, the value of \( \Delta E_X \) can be made arbitrary small, which allows us to apply the concept of a quasi-isolated system to the qubit. The demon, in turn, acts as a reservoir. For the qubit to decrease its entropy, its evolution must be described by a non-unital quantum channel (\( \Phi \)). The general equation (1) assumes the form

\[
\Phi_{jj'}(\hat{1}) - [\hat{1}]_{jj'} = \sum_i \langle \hat{F}^\dagger_{ji}, \hat{F}_{ji} \rangle,
\]

(9)

where the operators \( \hat{F}_{ji} \) can be obtained from Equation (8):

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

Using Equation (9), one finds that

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

(10)

which proves the non-unitality of the quantum channel.

3 Heating and Cooling Process

In this section, we address heating and cooling processes that may occur in complex physical systems. Instead of describing fully realistic processes we want to represent them on a formal level using unitary evolution of two interacting qubits. Below we will consider both heating and cooling operations within this perspective.

Suppose that the Hilbert space of each qubit has an orthonormal basis which consists of \( |0\rangle \) and \( |1\rangle \). Let the initial state of the two-qubit system be described by the density matrix

\[
\hat{R}_i = |0\rangle \langle 0| \otimes \frac{1}{2} (|0\rangle \langle 0| + |1\rangle \langle 1|).
\]

(11)

The matrix of the final state after the first qubit’s heating and the second qubit’s cooling is given by

\[
\hat{R}_f = \frac{1}{2} (|0\rangle \langle 0| + |1\rangle \langle 1|) \otimes |0\rangle \langle 0|,
\]

(12)
i.e., the first qubit changes its state to chaotic while the second qubit goes to the ground state. The system evolution in such a process can be expressed via the unitary operator

\[
\hat{U} = |0\rangle \langle 0| \otimes |0\rangle \langle 0| + |0\rangle \otimes |1\rangle \langle 1| + |1\rangle \otimes |0\rangle \langle 1| + |1\rangle \otimes |1\rangle \langle 0| .
\]  

(13)

Let us now analyze the evolution of each qubit, i.e., decompose the process into the first qubit heating and the second qubit cooling.

Since the heating process is associated with an increase in entropy, the quantum channel \( \Phi^{(1)} \) describing the evolution of the first qubit may be unital. The general formula (11) takes the form

\[
\Phi^{(1)}_{j j'}(\hat{1}) - [\hat{1}]_{j j'} = \sum_i \langle \hat{F}^{(1)\dagger}_{j i} , \hat{F}^{(1)}_{j i} \rangle ,
\]

where the operators \( \hat{F}^{(1)}_{j i} \) can be obtained from Equation (13):

\[
\hat{F}^{(1)}_{00} = |0\rangle \langle 0|, \quad \hat{F}^{(1)}_{01} = |1\rangle \langle 1|, \quad \hat{F}^{(1)}_{10} = |0\rangle \langle 1|, \quad \hat{F}^{(1)}_{11} = |1\rangle \langle 0| .
\]

Consequently, we find that

\[
\Phi^{(1)}(\hat{1}) = 1, \quad (14)
\]

implying that \( \Phi^{(1)} \) is indeed unital as could be expected.

The cooling process involves a decrease of entropy, which means that the quantum channel \( \Phi^{(2)} \) corresponding to the second qubit has to be non-unital. As in the previous case, \( \Phi^{(2)}_{j j'}(\hat{1}) - [\hat{1}]_{j j'} = \sum_i \langle \hat{F}^{(2)\dagger}_{j i} , \hat{F}^{(2)}_{j i} \rangle \), however, now

\[
\hat{F}^{(2)}_{00} = |0\rangle \langle 0|, \quad \hat{F}^{(2)}_{01} = |1\rangle \langle 0|, \quad \hat{F}^{(2)}_{10} = |0\rangle \langle 1|, \quad \hat{F}^{(2)}_{11} = |1\rangle \langle 1| .
\]

On substitution, we find that

\[
\Phi^{(2)}(\hat{1}) = 2 \cdot |0\rangle \langle 0| , \quad (15)
\]

which proves that \( \Phi^{(2)} \) is non-unital as expected.

4 Concluding Remarks

In summary, using the results of quantum information theory, we have extended the Second Law of Thermodynamics to the quantum world. We have derived a rigorous general criterion of unitality and have applied it to develop the concept of a quantum Maxwell demon and to describe the heating–cooling process in a two-qubit system.

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