MSc in Photonics

Universitat Politècnica de Catalunya (UPC)
Universitat Autònoma de Barcelona (UAB)
Universitat de Barcelona (UB)
Institut de Ciències Fotòniques (ICFO)

http://www.photonicsbcn.eu

PHOTONICS**BCN**

Master in Photonics

MASTER THESIS WORK

A GENERAL FRAMEWORK FOR INFORMATION-WORK INTERCONVERTIBILITY IN THE QUANTUM REGIME

Constantino Rodríguez Ramos

Supervised by Prof. Maciej Lewenstein, (ICFO)

Presented on date xth xxxxxx 2015

Registered at

Escola Tècnica Superior d'Enginyeria de Telecomunicació de Barcelona

A general framework for information work interconvertibility in the quantum regime

Constantino Rodríguez Ramos

ICFO - Institut de Ciènces Fotiòniques, Mediterranean Technology Park, 08860 Castelldefels, Barcelona, Spain

E-mail: constantino.rodriguez@icfo.es

Abstract.

In this theoretical work we study three theorems that establish limitations to three basic processes in thermodynamics: an adiabatic process, an erasure process and a work extraction process. We propose a theoretical setting that allows us to model these three processes using a fully quantum formalism. Using this picture, we explore the fundamental limitations that affect the processes. As a conclusion, we give a general view to the origin of these limitations.

1. Introduction

The microscopic work exerted over a system in the nanoscale is affected by quantum fluctuations, its description can only be made using work probability distributions. Possibly one of the first steps for characterizing this work probability distribution was the fluctuation theorem proposed by Jarzynski in [1, 2]. In this paper, Jarzynski relates the probability distribution of the work exerted over a system that is driven out-of-equilibrium with an equilibrium thermodynamical function, the equilibrium free energy difference. The Jarzynski theorem is usually expressed as an equality:

$$\overline{e^{\beta \Delta W}} = e^{\beta \Delta F}, \tag{1}$$

where the overline means that the expression is averaged over the probability distribution and ΔF is the equilibrium free energy difference.

Various experimental verifications of Jarzynski theorem have been reported [3]. Crooks in [4] continued the work initiated by Jarzynski proposing a new fluctuation theorem, considered as a generalization of the one of Jarzynski. The Crooks fluctuation theorem establishes that the relation between the probability distribution of a certain trajectory and the probability distribution of the reverse trajectory are related through the exponential of the entropy generated. A lot of work has been made to generalize even further Jarzynski and Crooks theorems. The first was generalized for quantum settings in [5]. In more recent works the same was done with Crooks theorem, in [6] a fully quantum Crooks relation is derived.

Maxwell's demon and Sziliàrd's engine thought experiments were considered paradoxes for many years because they apparently violate the second law of thermodynamics. The Landauer thesis [7] was decisive for solving the paradoxes. Together with Bennett [8], they argue that manipulating information costs energy, this cost was not taken into account in the formulation of the paradoxes, so second law was apparently violated.

Landauer's principle in its most simple formulation establishes the lower limit of the energy dissipated (in terms of Heat) in a process of irreversible erasure of information. This limit depends on the of the difference of entropy of the initial and final states:

$$\beta \Delta Q \geq \Delta S. \tag{2}$$

A microscopic derivation of Landauer's principle was recently given in [9] for finite dimensional reservoirs.

Work extraction is a problem with a long trail in thermodynamics that in fact is regarded as one of the problems that inspired its emergence as a science and thus it is in the genes of the classical thermodynamic theory. For example, one of the thermodynamic potentials such as the equilibrium free energy is usually defined as the maximum work that can be extracted from a system at certain temperature, that definition can be expressed mathematically as $\Delta W \leq \Delta F$. Recent literature in this topic deals with work extraction in the nanoscale regime were quantum effects are not negligible. This approach is made for example in [10].

In this work we present a convenient setting that allows us to explore the interrelations between the three topics that we have introduced: Fluctuation theorems, Landauer's principle and work extraction. Our objective is first to understand deeper the processes considered using the same setting. Furthermore we focus on establishing the differences and links between these three processes. In the last part of the work we constraint the setting presented to a very simple model that allows us to represent graphically the three processes.

2. Quantum information

2.1. Postulates of Quantum mechanics

We assume the following postulates in the form that they are set out in [11]:

(i) Postulate about state space: Associated to any isolated physical system there is a complex vector space with inner product (Hilbert space) known as the state space of the system. The system is described by a state vector which is a unit vector in the system state space.

(ii) Postulate about composite systems: The state space of a composite physical system is the tensor product of the state spaces of the component physical systems.

(iii) Postulate about evolution: The evolution of a closed quantum system is described by a unitary transformation. This is, the state $|\psi\rangle$ of the system at time t is related to the state $|\psi'\rangle$ of the system at time t' by a unitary operator U which depends only on the times t and t' .

2.2. Density operator

We have postulated that every physical system can be described by a state vector in the Hilbert space. However, it is common to deal with systems whose state is not completely known, an ensemble of state vectors with certain probability has to be chosen for describing those systems. The mathematical tool used to describe an ensemble of states is the *density matrix* or *density operator*, ρ. Usually ρ is written in terms of a matrix, but not every matrix is valid. ρ is the density matrix of a physical system if it satisfies two conditions:

- $\mathrm{tr}\,(\rho) = 1$.
- ρ is a positive matrix (all its eigenvalues are positive).

$tr(\rho)$ is the trace of the matrix.

2.3. Evolution of a system

We have postulated that closed systems evolve following unitary transformations. However, it is difficult in general to isolate a system from its environment. In the theory, the evolutions of systems in contact with its environment are modeled using the concept of ancilla. The ancilla is the set of variables that are not accessible but affect the system and it represents the environment of the system. The union of the system and the ancilla can be considered as a closed system, so its joint evolution is described by a unitary transformation. Using this approach one can derive the conditions on the non-unitary transformation that suffers the system. Usually such transformation is expressed in the operator-sum representation as:

$$\psi(\rho) = \sum_i E_i \rho E_i^\dagger, \tag{3}$$

where E_i is a Krauss operator, the set of Krauss operators fulfill:

$$\sum_i E_i E_i^\dagger \leq 1. \tag{4}$$

Any transformation that fits with these conditions is a *Completely Positive Trace Preserving* map.

2.4. Setting

We chose a general setting that allows us to study different processes. Such setting was previously used in [6] , [10] or [12] and it is represented in Fig. 1. It consists of four elements:

- A system with a set of Hamiltonians $H_S^1, H_S^2, ..., H_S^n$.

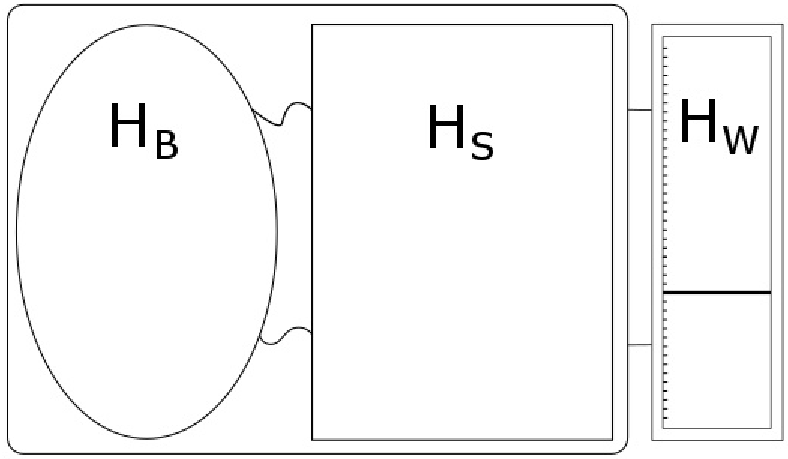


Figure 1: Schematic representation of the setting considered.

- A bath system with Hamiltonian H_B. One condition is imposed over this system: thermality. This means that the state of the bath can be expressed as: $\rho_B = \frac{e^{-\beta H}}{\mathrm{tr}\,(e^{-\beta H})}$, where β is the inverse temperature. The bath system is used to group in a system all the degrees of freedom which are inaccessible. It is reasonable to associate a thermal state to such system.
- A control system whose dimension is n, the number of possible Hamiltonians of the system. The joint Hamiltonian of the control system and the system S is expressed as $H_{SC} = H_S^1 \otimes |c_1\rangle\langle c_1| + H_S^2 \otimes |c_2\rangle\langle c_2| \ + ... + H_S^n \otimes |c_n\rangle\langle c_n|$.
- A weight system with Hamiltonian H_W. It is used as a battery for the system since it provides or stores energy when the Hamiltonian of the system is switched.

As we saw in the section 2.3 any evolution of the system can be expressed as a CPTP map:

$$\rho'_S = \mathrm{tr}_{BWC}\,(U \rho_{SBWC} U^\dagger). \tag{5}$$

But not every unitary is acceptable. Two conditions are made over this unitary:

- The unitary transformation commutes with the total Hamiltonian $[U, H_{SBWC}] = 0$. This conditions are equivalent to the conservation of energy in the setting.
- The unitary commutes with translations in the weight $[U, \delta W] = 0$. This condition is equivalent to the translation symmetry in the weight what certifies that the weight system is used as an energy storage system and not as an extra bath.

2.5. Jarzynski equality

In the original derivation of the equality, Jarzynski used a system that is driven out-of-equilibrium in an adiabatic reversible process. We can reproduce such process with our setting, we must choose a unitary that introduces changes in the state of the control system (what models a time dependent Hamiltonian) and that does not produce interactions between the system and bath. Using Crooks relation applied to this specific process we can derive the Jarzynski equality. If we identify $\beta(W - \Delta F)$ as the entropy production in the process, Crooks relation reads:

$$\frac{P_F(W)}{P_R(-W)} = e^{\beta(W-\Delta F)}, \tag{6}$$

where $P_F(W)$ is the work probability distribution of a certain trajectory, $P_R(-W)$ is the work probability distribution of the reverse trajectory, W is the weight energy difference, ΔF is the equilibrium free energy difference in the process and β is the inverse temperature of the initial state. Multiplying both sides by $P_F(-W)$ and integrating over W we recover Jarzynski equality:

$$\overline{e^{-\beta\Delta W}} = \int_{-\infty}^{\infty} P_F(W) e^{-\beta\Delta W}\,\mathrm{d}W = e^{-\beta\Delta F}\int_{-\infty}^{\infty} P_R(-W)\,\mathrm{d}W = \tag{7}$$

$$= e^{-\beta\Delta F} \rightarrow \overline{e^{-\beta\Delta W}} = e^{-\beta\Delta F}.$$

Jarzynski equality helps us to understand the limit in the efficiency of an adiabatic process. From it we can recover the bound associated of the classical work $\Delta W \geq \Delta F$, just by applying the Jensen inequality to the Jarzynski result:

$$e^{-\beta\overline{\Delta W}} \leq \overline{e^{-\beta\Delta W}} \rightarrow e^{-\beta\overline{\Delta W}} \leq e^{-\beta\Delta F} \rightarrow \overline{\Delta W} \geq \Delta F. \tag{8}$$

As pointed by Jarzynski, this bound is saturated $\overline{\Delta W} = \Delta F$ in two situations: When considering sudden changes of the Hamiltonian (quenches) and when considering infinitely slow processes $t = \infty$.

In [13] Crooks theorem is derived considering only the assumption of time-reversal symmetry. The origin of Crooks theorem is related to the uncertainty of performing a process at a finite time.

2.6. Landauer's principle

A microscopic derivation of the Landauer's principle was recently given in [9] for finite dimensional reservoirs. The setting used in this paper is contained in ours. It consists of a system and a bath at thermal equilibrium, an extra consideration is made in this setting, the system and bath must be initially uncorrelated $\rho_{SB} = \rho_S \otimes \rho_S$.

The main result obtained is an equality:

$$\beta\Delta Q = \Delta S + I(S' : B') + D(\rho'_B||\rho_B), \tag{9}$$

where $I(S' : B')$ is the mutual information between the bath and the system in the final state and $D(\rho'_B||\rho_B)$ is the relative entropy of the bath at the final state with respect to the bath at the initial state. Since these magnitudes are defined as positive, from the equality one can easily recover the Landauer's principle in the standard formulation $\beta\Delta Q \geq \Delta S$.

If we analyze these terms we can extract valuable information about the erasure process and its fundamental limitations:

- $D(\rho'_B||\rho_B)$: This term is related directly to the free energy gained by the bath when the joint unitary acts over it. In fact, this term is already considered in the heat when we use the definition $\Delta Q = \mathrm{Tr}\left(H(\rho'_B - \rho_B)\right)$. Some authors such as [14] modify this definition such relative entropy is not considered: $\Delta Q^* = \mathrm{Tr}\left(H(\rho'_B - \rho_B)\right) - TD(\rho'_B||\rho_B)$ so Eq. 9 would be expressed in terms of ΔQ^*as:
$$\beta\Delta Q^* = \Delta S + I(S' : B'). \tag{10}$$
- $I(S' : B')$: This term represents the correlations generated between the system and the bath after the process, correlations are the result of a joint evolution of the bath and system, both classical and quantum correlations (entanglement) may be generated.

We conclude that the production of correlations between bath and system is the main mechanism that keeps the erasure protocol far from ideality, furthermore we can show that the creation of such correlations is unavoidable when the bath is finite [15].

The correlations generated will be smallest the closest is initially the system state with respect to the bath state, thus the optimal protocol for erasing a bit is the isothermal reversible process. The finiteness of the bath is what makes impossible to perform such protocol.

2.7. Work extraction

Work extraction problem addresses the question of how much work can be extracted from a system out-of-equilibrium using a bath at a certain temperature. In [10] a theorem is presented that bounds the energy obtained in such process. An ideal work extraction protocol is proposed consisting of two steps: A quench that brings the system to equilibrium with the bath is followed by a sequence of small thermalizations and small quenches that emulate an isothermal reversible process which recovers the initial Hamiltionian of the system, this assures that gained energy does not come from the battery. If the system is left in the equilibrium state, some energy has been extracted from it. The maximum amount of energy that can be extracted from the system is the difference of free energy of the initial out-of-equilibrium state and the free energy of the corresponding equilibrium state with the same Hamiltonian.

A direct relation can be made between the protocol presented in this paper and the processes that we studied in sections 2.5 and 2.6. The first part of the protocol is an adiabatic reversible process, the reverse process is presented in section 2.5 where a system in equilibrium was driven out-of-equilibrium adiabatically. As we saw, a quench in the Hamiltonian is a process which minimizes work $\Delta W = \Delta F$. Considering the sign inversion (extracted work is defined positive), a time zero change in the Hamiltonian maximizes the extracted work. The second part of the protocol is an isothermal reversible process which was also the ideal protocol in the erasure process. As we saw, correlations of the system and the bath prevent this ideal protocol to be performed.

3. Example: A two-level system

The model consists of a system with two possible energy states $|0\rangle$ and $|1\rangle$. When the state of the system is $|0\rangle$ the energy associated to the system is 0 and when state of the system is $|1\rangle$, the energy associated to the system is λ. This means that the Hamiltonian can be written as:

$$H(\lambda) = \lambda|1\rangle\langle 1| + 0|0\rangle\langle 0|. \tag{11}$$

We consider a system diagonal in the Hamiltonian basis:

$$\rho = p|1\rangle\langle 1| + (1-p)|0\rangle\langle 0|. \tag{12}$$

The thermal state related with such Hamiltonian at temperature T is:

$$\rho_{th} = \frac{\mathrm{e}^{-\beta H}}{\mathrm{tr}\left(e^{-\beta H}\right)} = \frac{\mathrm{e}^{-\beta\lambda}}{1+e^{-\beta\lambda}}|1\rangle\langle 1| + \frac{1}{1+e^{-\beta\lambda}}|0\rangle\langle 0|. \tag{13}$$

There are two possible manipulations that can be done over the system:

- Change the energy eigenvalue of the excited state what means a change of the Hamiltonian. The evolution can be represented by a unitary operation U. The Liouville equation $\frac{\delta\rho}{\delta t} = -[\rho, H]$ and the fact that ρ commutes with H for all t implies $\frac{\delta\rho}{\delta t} = 0 \to \rho = constant$.
- Let evolve the system in contact with the bath. This process is called thermalization and within enough time, the equilibrium is reached: the Gibbs state of the System-Bath ρ_{SB}. The state of the system alone is obtained by partial tracing the bath $\rho_S = \mathrm{Tr}\left(\rho_{SB}\right)$. Unlike before, the evolution that suffers the system cannot be represented by a unitary while the Hamiltonian keeps constant through the evolution.

The main advantage of choosing a bit system is the ease in which a transformation can be graphically represented in a diagram. We can cover the state space using only two variables, the eigenvalue for the excited state of the Hamiltonian λ and the probability of occupation of the excited state p. In such diagram the two manipulations that we consider are just vertical and horizontal straight lines in the diagram.

In the first manipulation we consider that the microscopic dynamics of the system is governed by the work fluctuations. In fact, the set-up considered by Jarzynski can be represented graphically using our system as we can see in Fig. 2.

Using our model we can represent a protocol for erasing a bit. In our diagram such protocol should drive the state of the system from the state of maximal entropy $p = 1/2$ to a state of minimal entropy $p = 0$. In Figs. 3a and 3b we can see two protocols that do that or at least that leave the bit in a state close to purity, $p \approx 0$. However, the

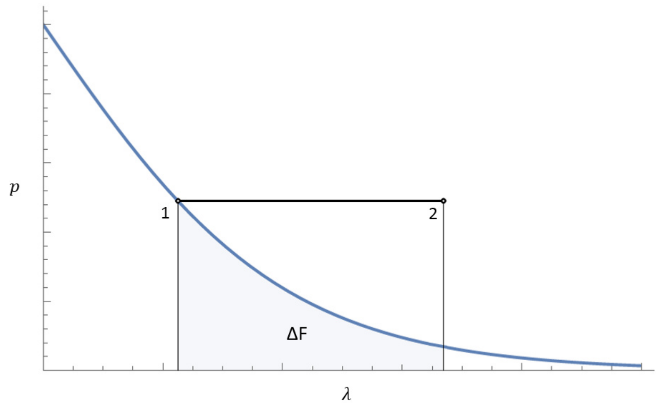
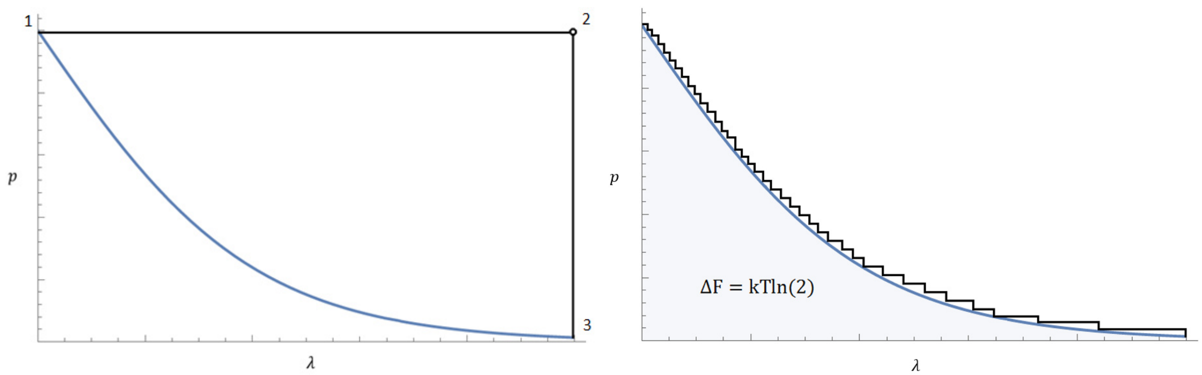


Figure 2: Graphical representation of the Jarzynski set-up using the bit model.

process in Fig. 3b is closer to the ideal one: isothermal reversible process, as we saw in section 2.6.

In the literature the Landauer's principle is sometimes written in terms of work $W \geq \Delta F$. We consider this approach not very appropriate, using this version of Landauer's principle both protocols represented in Fig. 3a and Fig. 3b could be considered as ideal if in 3a we perform an infinitely slow protocol as we saw in 2.5. We conclude as we have pointed before that the origin of non-ideality in an erasure process is in the creation of correlations between bath and system.



(a) (b)

Figure 3: Graphical representation of two erasure protocols.

The last process we studied was work extraction. In Fig. 4 we find represented graphically the protocol we presented in 2.7 using the two-level system.

4. Conclusions

With the information that we have gathered until this point, we are in position of giving a general view that links the theorems studied. A good starting point is to compare the

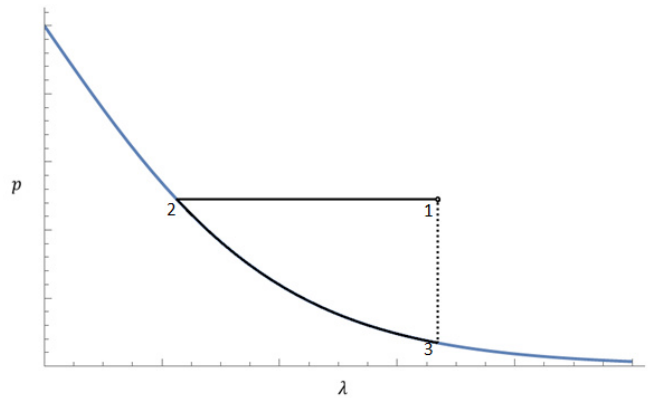


Figure 4: Graphical representation of the ideal work extraction protocol.

processes the theorems refer to.

Before starting, let us recall section 2.7. There we argued that the optimal work extraction protocol was an adiabatic reversible process followed by an isothermal process. The limitations that affect those processes are treated in sections 2.5 and 2.6 respectively. So there is no reason for treating work extraction process separately any more in the study of its fundamental limits.

The main difference between an adiabatic process and an erasure process is the role played by the bath. While in an adiabatic process the bath does not interact with the system, in an erasure process the interaction with the bath is necessary. In fact, the correlations of the system and bath were regarded as the fundamental limitations to the efficiency of the process, which are behind Landauer's principle. In an adiabatic process the loss of ideality has nothing to do with the bath. It emerges as a consequence of the fluctuations when the evolution occurs in a finite time assuming time-reversal symmetry. So different mechanisms are responsible on non-ideality in the processes.

Let's consider a general picture of the problem. We have studied three processes whose objective is to produce exchanges in the energy and information content of a system but we find that those processes cannot be performed ideally because of fundamental constraints: the non-capability of accessing all the relevant variables of the system and the underlying reversible dynamics in the microscopic theory.

5. Acknowledgments

I would like to thank Maciej Lewenstein for giving me the opportunity to work in his group. I also thank Arnau Riera and Manabendra Nath Bera for all what they taught me and for all the fruitful discussions we had. Finally, I would like to thank ICFO fellow programme.

References

[1] Christopher Jarzynski. Nonequilibrium equality for free energy differences. *Physical Review Letters*, 78(14):2690, 1997.

[2] Christopher Jarzynski. Equilibrium free-energy differences from nonequilibrium measurements: A master-equation approach. *Physical Review E*, 56(5):5018, 1997.

[3] Jan Liphardt, Sophie Dumont, Steven B Smith, Ignacio Tinoco, and Carlos Bustamante. Equilibrium information from nonequilibrium measurements in an experimental test of jarzynski's equality. *Science*, 296(5574):1832–1835, 2002.

[4] Gavin E Crooks. Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Physical Review E*, 60(3):2721, 1999.

[5] Hal Tasaki. Jarzynski relations for quantum systems and some applications. *arXiv preprint cond-mat/0009244*, 2000.

[6] Johan Aberg. Fully quantum fluctuation theorems. *arXiv preprint arXiv:1601.01302*, 2016.

[7] Rolf Landauer. The physical nature of information. *Physics letters A*, 217(4):188–193, 1996.

[8] Charles H Bennett. Demons, engines and the second law. *Scientific American*, 257(5):108–116, 1987.

[9] David Reeb and Michael M Wolf. An improved landauer principle with finite-size corrections. *New Journal of Physics*, 16(10):103011, 2014.

[10] R Gallego, A Riera, and J Eisert. Thermal machines beyond the weak coupling regime. *New Journal of Physics*, 16(12):125009, 2014.

[11] Michael A Nielsen and Isaac L Chuang. *Quantum computation and quantum information*. Cambridge university press, 2010.

[12] Álvaro M Alhambra, Lluis Masanes, Jonathan Oppenheim, and Christopher Perry. The second law of quantum thermodynamics as an equality. *arXiv preprint arXiv:1601.05799*, 2016.

[13] Doron Cohen and Yoseph Imry. Straightforward quantum-mechanical derivation of the crooks fluctuation theorem and the jarzynski equality. *Physical Review E*, 86(1):011111, 2012.

[14] Bartłomiej Gardas and Sebastian Deffner. Thermodynamic universality of quantum carnot engines. *Physical Review E*, 92(4):042126, 2015.

[15] Benjamin Schumacher and Michael Westmoreland. *Quantum processes systems, and information*. Cambridge University Press, 2010.