Reversing the flow of heat in system of initially correlated qubits

Giovanni Francesco Diotallevi

Supervisor: Peter Samuelsson
Co-supervisor: Faraj Bakhshinezhad
Bachelor Thesis, Mathematical Physics Division

June 28, 2021

Contents

Abstract

The Second Law of Thermodynamics is considered to be one of the most fundamental and important laws of Physics. Both Clausius and Kelvin reformulated the Second Law as statements concerning the behaviour of two communicating systems, set to interact at different temperatures. The average positive entropy production of any process, described by the Second Law, is often understood as a "thermodynamic arrow of time" capable of discerning the direction in which physical events should arrange [1, 2, 3].

By studying a microscopic system described by two initially correlated qubits, in this thesis we explore the phenomenon of reverse energy flow. Differently from an often standard uncorrelated case, the correlated one shows properties that seem to suggest that a further generalization of both Clausius and Kelvin's statements is needed [4, 5, 6].

Upon obtaining a formulation for the energy exchanged between two qubits, we optimize it to derive a set of conditions for a time evolution driving a reversal of the energy exchanged between the two. We then use the obtained results to derive the conditions to give rise to an optimized reverse energy exchange, between a pair of isolated spin 1/2 systems as presented in Ref [7].

1 Introduction

In its early days, Thermodynamics was developed as a tool to describe how different heat engines could be constructed, and how these would compare in their efficacy in extracting work from some given heat source [4, 8, 9, 10]. Alongside with the development of its three fundamental laws, the evolution of Thermodynamics into the field we know today is partially due to the formation of new disciplines to which Thermodynamics offers a great deal of insights, being these astrophysics, bio-chemistry and quantum physics to name a few [9, 10, 11]. Moreover, with the rise in popularity of the field of quantum information, Thermodynamics has become a powerful tool to explore, and exploit, the role of correlations between constituents of a quantum mechanical joint system.

The development in Thermodynamics saw the emergence of three principles known as the four fundamental laws of Thermodynamics. The first of these laws deals with the conservation of energy aspect concerning any physical system, while the third law establishes a relation between the temperature and the entropy of any physical system. On the other hand, the Second Law of Thermodynamics provides the concept of a thermodynamic arrow of time. This concept infers on the direction that heat should flow in when two objects at different temperatures are placed into contact. Lastly, the fourth law (known as the Zeroth Law) establishes that if two systems are at equilibrium with a third system, then they must also be in thermal equilibrium with eachother

Since the early ages of Thermodynamics, ideas such as Maxwell's demon and Landauer's principle have been used in order to explore how, and to what extent, the concept of information plays a role in the fundamental laws of Thermodynamics [5, 9, 10, 12]. The sole idea of information playing a role in the energy available in a system [8, 13, 14] leads to question how more general can the statements, about the laws of Thermodynamics , can be made [4, 5]. For some time it has been known how the three laws of Thermodynamics require basic reformulations when trying to describe environments with some degree of initial correlation [4, 8]. Additionally, recent experiments performed on spin 1/2 systems have also demonstrated the incapability of the standardized iteration of the Second Law in describing correlated microscopic systems [7].

When considering two interacting systems at different temperatures, the average positive entropy production, associated with the Second Law of Thermodynamics, dictates a preferred direction for the flow of heat between the two systems. Ludwig Boltzman provided a great deal of details regarding the nature of the Second Law, attributing the non-negative average entropy evolution, to the initial conditions of the microscopic states comprising the system [3, 7]. In this view, in a closed system, initial conditions not only are capable of setting in motion a flow of heat, but can also determine a preferred direction for the "heat current".

In this thesis we focus on elaborating, and describing, how the Second Law of Thermodynamics , and more specifically Clausius and Kelvin's interpretations, require additional generalization in the context of an initially correlated environment, and how the initial presence of correlations result in a spontaneous reversal of energy flow between two qubits comprising the considered system.

2 Theory

2.1 Classical Thermodynamics

Thermodynamics is a branch of physics that describes phenomena, such as heat and temperature, and how these can be used in the extraction of energy in the form of work. By describing physical phenomena through the manipulation of macroscopic variables such as temperature and entropy, this branch of physics is capable of describing with high precision various properties of matter. Through history, the study of Thermodynamics gave rise to three fundamental principles, that are known today as the three laws of Thermodynamics. These principles are sometimes key in understanding previously unexplained phenomena from the field of astrophysics, to the field of nano-technology and quantum mechanics. [9, 10, 11]

2.1.1 The first and Second Law of Thermodynamics

As mentioned, the first law states that the change in internal energy of a system, is equal to the difference in heat transfer into the system and the work done by the system. In classical Thermodynamics, heat is defined as the energy transfer to, or from, a thermodynamical system through processes different from thermodynamical work or exchange of particles. Heat Q is thus defined as the change in energy E between two equlibrium states of a system, within an interval of time t_f, plus the work w done *by* the system in the same interval of time $Q = E(t_f) - E(0) + w$. In this thesis work we only consider closed systems, unable to perform any work on one-another or on the environment: in this regime heat is consequently defined as the change in energy of either subsystem

$$Q_i = \Delta E_i = E_i(t_f) - E_i(0). \tag{2.1}$$

If the process of energy change only involves two subsystems A and B, then, if the whole system is isolated, it is possible to invoke the first law of Thermodynamics to derive that the internal energy of the system remains unchanged through time, in which case one can write $\Delta E_A = -\Delta E_B$. In this regime things are simplified by the possibility of describing the dynamics of both subsystems, through a description of only one of the two.

In Thermodynamics, the concept of entropy allows for a quantitative description of the information one has about a given system [15, 16]. More specifically, entropy is used to describe the number of possible microstates of an ensemble of particles, corresponding to the macrostate of the system. More generally, given a random variable $\mathbf{X}$, with set of possible outcomes $\{x_i\}$, one can define the probability distribution $P(\mathbf{X}) \equiv p(x_i)$. It is then possible to introduce the concept of Shannon Entropy of variable $\mathbf{X}$ as such [17, 18, 19]

$$S(\mathbf{X}) \equiv S(p(x)) = -\sum_i p(x_i) \ln p(x_i). \tag{2.2}$$

Shannon's entropy is an equivalent formulation to Boltzmann's entropy formulation, in which $p(x_i) = p_i$ indicates the probability of the microstate i to be found in a macrostate at equilibrium (in this thesis work we set $k_b \equiv 1$).

The Second Law of Thermodynamics establishes a non-negative property for the change in entropy of an isolated system. This can be seen as the result of the tendency of isolated systems to reach for thermal equilibrium, where entropy is highest. According to the Second Law, when considering a system on which no external work is applied, an infinitesimal element of heat ∂Q is then defined by the product of the temperature of the system, with the infinitesimal increase dS of its entropy [4, 20, 21, 19]

$$\partial Q = TdS \;\Rightarrow\; dS = \frac{\partial Q}{T}. \tag{2.3}$$

Many equivalent interpretations and iterations of the Second Law have been made through time, although the most relevant ones to illustrate in this thesis are Clausius and Kelvin statements [4, 19]:

Clausius:*"No process is possible whose sole result is the transfer of heat from a cooler to a hotter body."*

Kelvin:*"It is impossible for a self-acting machine, unaided by any external agency, to convey heat from one body to another at a higher temperature."*

Although the above statements hold as a good approximation for the time evolution of any two macroscopic uncorrelated subsystems, this will be shown to not to hold in the instance of an initially correlated microscopic system.

2.1.2 Energy exchange between uncoupled classical systems

In this section we discuss the direction of heat flow, as predicted by the Second Law of Thermodynamics, for two interacting, uncorrelated and isolated systems: the right(R) and left(L) system. The interaction between the two will be defined as a pure exchange of heat, and therefore neither systems will be allowed to apply work on one-another.

Let us define an isolated system RL for which $\Delta E_{RL} = 0$. The system is then comprised by two closed subsystems R and L, with respective temperatures T_R, T_L and respective volumes V_R and V_L (see Fig. 1). A fixed barrier can be placed in between the subsystems so to maintain the volumes of either as fixed. Keeping both volumes fixed is a necessary requirement to ensure that the work W done by, or acting on, either system is zero.

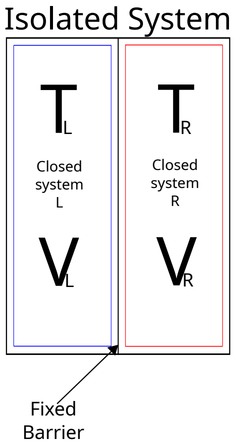


Figure 1: Schematic diagram representing the two isolated uncoupled systems L and R

Once the two systems are put into thermal contact, heat Q is exchanged between the two systems, and a series of mathematical statements can be formulated describing the changes in each system

$$\mathrm{d}V_R = \mathrm{d}V_L = 0 \;\Rightarrow\; \partial W_R = \partial W_L = 0, \tag{2.4}$$

$$\mathrm{d}E_R = \partial Q_R = \partial Q \;\Rightarrow\; \mathrm{d}E_L = \partial Q_L = -\partial Q, \tag{2.5}$$

$$\mathrm{d}S_R = \frac{\partial Q_R}{T_R} = \frac{\partial Q}{T_R} \;\Rightarrow\; \mathrm{d}S_L = \frac{\partial Q_L}{T_L} = -\frac{\partial Q}{T_L}, \tag{2.6}$$

$$\mathrm{d}S = \mathrm{d}S_R + \mathrm{d}S_L = \partial Q \left(\frac{1}{T_R} - \frac{1}{T_L} \right). \tag{2.7}$$

Where Eq. (2.7) represents the total change in entropy $\mathrm{d}S$ of the system , and it was derived through the use of Eq. (2.3) . It is also important to point out how, in Eq. (2.5) , heat has been defined to be positive when flowing into system R and negative otherwise. The Second Law of Thermodynamics dictates that for any isolated system $\mathrm{d}S \geq 0$, therefore

$$\partial Q \left(\frac{1}{T_R} - \frac{1}{T_L} \right) \geq 0. \tag{2.8}$$

For the scenario $T_R > T_L$, Eq. (2.8) returns $\partial Q < 0$ and therefore heat is passed from the right to the left system. Otherwise, if $T_R < T_L$, then $\partial Q > 0$ and heat is passed from the left to the right system.

This derivation provides a good intuition on how the Second Law of Thermodynamics dictates the direction of heat flow, essentially returning Clausius and Kelvin's statements.

2.2 Quantum Thermodynamics

Using Classical Thermodynamics to model physical results, obtained through experiments performed onto a collection of quantum mechanical objects, can reveal itself to be a difficult, and at times impossible, task. The reason for this is the increasing presence of quantum mechanical events when descending into smaller length scales.

Quantum Thermodynamics is a branch of physics, which aims to take established thermodynamic's concepts and translate them using formalisms from quantum mechanics [22]. Aside from the pure academic interest, the need of understanding the statistical behaviour of quantum objects is becoming of great interest for companies trying to achieve miniaturization of new technologies to nano-scales [20, 22].

The success of this branch of physics lies in its ability of using Classical Thermodynamics concepts, whilst keeping in account quantum mechanical effects. In the past years quantum Thermodynamics has received a great deal of improvement thanks to the latest developments of quantum information theory [20].

The three laws of Thermodynamics are also revisited [9]. Expressions such as Boltzmann's entropy have been revised into new formulations using notions such as density matrices and Schrodinger's equation.

2.2.1 State Representation

In quantum mechanics, particles and quantum systems are represented as d-dimensional vectors $|\psi\rangle$ in their respective Hilbert spaces $\mathcal{H}$. Density operators are defined as Hermitian positive matrices [8, 18, 23], which are often preferred over state vector representation, due to the ability of the former to describe situations involving both pure and mixed states [18, 23].

By definition, a pure ensemble is defined as a collection of systems, for which every member can be described by the same ket $|\psi\rangle$ [23]. By contrast, a mixed ensemble is defined as a collection of systems, that cannot be characterized a single ket. Instead the all ensemble can be described as a collection of different states $|\psi_i\rangle$ associated with a corresponding population percentage p_i. Where the population values are statistically normalized to the condition $\sum_i^N p_i = 1$.

Any density matrix ϱ, representing either a mixed or pure state, can be represented as the weighted sum of the outer products corresponding to each ket characterizing the system. This definition can be then used to express a normalization condition in terms of the trace of the density operator [18, 23]

$$\varrho \equiv \sum_i^N p_i |\psi_i\rangle\langle\psi_i|, \tag{2.9}$$

$$\mathrm{tr}(\varrho) = 1. \tag{2.10}$$

As for state vectors, using the formalism of density matrices it is possible to define the expectation value of an observable. Such relation between an observable and its expectation value, is especially useful due to its invariance under changes of basis of the system ϱ [23]. Let us define the observable $\hat{A}$, and an ensemble representable through the density matrix ϱ: we then define the ensemble average $\langle A\rangle$ of $\hat{A}$ as

$$\langle A\rangle = \mathrm{tr}(\varrho\hat{A}). \tag{2.11}$$

The focus of this thesis work is the study of an isolated composite system comprised of two interacting qubits. When considering a system comprised of mutliple subsystems, its Hilbert space is defined as the tensor product of the Hilbert spaces of each respective system [8, 18, 23]

$$\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B. \tag{2.12}$$

2.2.2 Hamiltonian

In the formulation of quantum mechanics, the Hamiltonian is defined as the Hermitian operator whose spectrum of eigenvalues corresponds to the set of all possible outcomes, when measuring the energy of a system. Being the Hamiltonian defined by a Hermitian operator, there always exists a linear combination of Pauli matrices $(\sigma_0, \sigma_1, \sigma_2, \sigma_3)$ that can be implemented in describing any given Hamiltonian $\hat{H}$. When considering a joint system comprised of two qubits (A and B), the global Hamiltonian is represented by a 4×4 operator

$$\hat{H}_{AB} = \sum_{i,j} c_{i,j}\hat{\sigma}_i \otimes \hat{\sigma}_j, \tag{2.13}$$

$$c_{i,j} = \mathrm{tr}\left(\hat{\sigma}_i \otimes \hat{\sigma}_j \hat{H}_{AB}\right). \tag{2.14}$$

The definition of Eq. (2.12) relates composite Hilbert spaces to their constituent spaces. This allows for the definition of a general Hamiltonian, which can be adopted for the description of the Hamiltonian of a joint system. For an isolated composite system, made out of two interacting qubits, one can use Eq. (2.12) to define the general form for an interaction Hamiltonian

$$\hat{H}_{AB} = \hat{H}_0 + \hat{V}(t) = \hat{H}_A \otimes \mathbb{1}_B + \mathbb{1}_A \otimes \hat{H}_B + \hat{V}(t), \tag{2.15}$$

where $\hat{H}_A(\hat{H}_B)$ is the local Hamiltonian corresponding to subsystem $A(B)$, while the term $\hat{V}(t)$ represents all cyclic subsystem interactions satisfying the condition $\hat{V}(t_f) = \hat{V}(0) = 0$, where t_f represents the final time of the process. Because of the condition imposed on the interaction term $V(t)$, the global Hamiltonian satisfies $\hat{H}_{AB} = \hat{H}_0$ when $t = 0$ and $t = t_f$. This allows us to measure the energy of either qubit through the use of its respective local Hamiltonian when $t = 0$ and $t = t_f$ [6, 7]. It has to be noted how the time dependence of the interaction term $V(t)$ can be modelled as a Heaviside step-function with an activation interval t_f. Experimentally, this can be thought of as an interval in which the qubits are left to evolve under a time independent Hamiltonian $\hat{H}_{AB} = \hat{H}_0 + \hat{C}$, where $\hat{C} = \hat{V}(t)$ for $0 < t < t_f$.

Schrodinger's equation relates the time evolution of any physical quantum system to the Hamiltonian of the latter [7, 18, 23]. For time-independent Hamiltonians, the way this is accomplished in Schrodinger's picture, is through the generation of a time evolution unitary operator $\hat{U}$. Said unitary can be obtained through the time dependent Schrodinger's equation as such [7, 18, 23]

$$\hat{U}(t) = e^{-it\hat{H}}. \tag{2.16}$$

In this thesis work we set $\hbar \equiv 1$. Because of the cyclic properties imposed on the global Hamiltonian (namely $\hat{H}_{AB} = \hat{H}_0$ at $t = 0$ and $t = t_f$), we can consider evolutions within intervals $\Delta t = t_f$ to be describable by Eq. (2.16). In general, it is possible to identify a two-dimensional unitary time evolution as a rigid rotation of the space defined by the chosen basis: we therefore represent a general two-dimensional unitary as an operator defined by the three rotational angles θ, γ and μ (see appendix section **5.2**)

$$\hat{U} = \begin{bmatrix} e^{i\mu}\cos(\theta) & e^{i\gamma}\sin(\theta) \\ -e^{-i\gamma}\sin(\theta) & e^{-i\mu}\cos(\theta) \end{bmatrix} \tag{2.17}$$

Eq. (2.16) describes how a system Hamiltonian generates the time evolution which the system undergoes. It is then clear how the Hamiltonian of a system dictates how said system evolves through time. Aside from showing how a time evolution can be generated from a system Hamiltonian, Eq. (2.16) can be used to obtain information about the internal energy of a system, by studying how this evolves through time.

Later in this thesis, we will derive a specific formulation for the unitary evolving the joint system. We will then use the obtained time evolution to derive the generating Hamiltonian for said evolution. Through the eigenbasis of a given unitary $\hat{U}$, it is possible to construct an operator $\hat{P}$, with which to perform a diagonalization of the operator $\hat{U}$, $\hat{U} = \hat{P}\hat{D}\hat{P}^{\dagger}$, where $\hat{D}$ is the diagonalized representation of $\hat{U}$. It is then possible to safely define the natural logarithm of $\hat{U}$, as the diagonal matrix whose entries are the logarithm of the corresponding diagonal entry in the diagonalized representation of $\hat{U}$, so that

$$\hat{H}_{AB} = \frac{i}{t}\ln\left(\hat{U}\right) = \frac{i}{t}\hat{P}\ln\left(\hat{D}\right)\hat{P}^{\dagger}. \tag{2.18}$$

Where we used the property $f(\hat{A}) = \hat{\eta} f(\hat{B})\hat{\eta}^{\dagger}$ (where $\hat{\eta}$ is a unitary transformation, and $\hat{A} = \hat{\eta}\hat{B}\hat{\eta}^{\dagger}$).

In quantum mechanics, it is possible to describe the time evolution of a state vector $|\psi(0)\rangle$, using the time evolution unitary $\hat{U}(\mathrm{t})$, shown in Eq. (2.16). The time evolution of a ket is then described as $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$ [18, 23], therefore, using the definition of Eq. (2.9), the time evolution for a density operator ϱ becomes

$$\varrho(t) = \sum_{i}^{N} p_i|\psi_i(t)\rangle\langle\psi_i(t)| = \sum_{i}^{N} p_i\hat{U}(t)|\psi_i(0)\rangle\langle\psi_i(0)|\hat{U}^{\dagger}(t) = \hat{U}(t)\varrho(0)\hat{U}^{\dagger}(t). \tag{2.19}$$

Lastly, let us introduce the Liouiville's equation for the change in time of an operator $\varrho(t)$ as (see appendix **5.1**) [18, 23]

$$\frac{\partial\varrho(t)}{\partial t} = \frac{1}{i}\left[\varrho(t), \hat{H}\right]. \tag{2.20}$$

2.2.3 The von-Neumann Entropy

Let us define a density operator ϱ via Eq. (2.9), we define the entropy $S_N(\varrho)$ of the latter as

$$S_N(\varrho) = -\mathrm{tr}(\varrho\ln\varrho). \tag{2.21}$$

Eq. (2.21) is called von-Neumann entropy, and it is defined as the quantum mechanical equivalent to Boltzmann's entropy [8, 20, 23, 24]. The above equation can be used to derive an important relation between unitary time evolutions and the entropy changes of a system ϱ undergoing said evolution. Let us define the final state $\varrho(t) = \hat{U}(t)\varrho(0)\hat{U}^{\dagger}(t)$, where $\hat{U}(t)$ is a time evolution unitary obtained through Eq. (2.16). The change in entropy ΔS_N^{ϱ} is defined as

$$\begin{align}
\Delta S_N^{\varrho} &= S_N(\varrho(t)) - S_N(\varrho(0)) \tag{2.22}\\
&= -\mathrm{tr}\left[\hat{U}(t)\varrho(0)\cancelto{\mathbb{1}}{\hat{U}^{\dagger}(t)\hat{U}(t)}\ln\left(\varrho(0)\right)\hat{U}^{\dagger}(t)\right] - S_N(\varrho(0)) \tag{2.23}\\
&= -\mathrm{tr}\left[\hat{U}(t)\varrho(0)\ln\left(\varrho(0)\right)\hat{U}^{\dagger}(t)\right] - S_N(\varrho(0)) \tag{2.24}\\
&= -\mathrm{tr}\left[\cancelto{\mathbb{1}}{\hat{U}(t)\hat{U}^{\dagger}(t)}\varrho(0)\ln\left(\varrho(0)\right)\right] - S_N(\varrho(0)) \tag{2.25}\\
&= S_N(\varrho(0)) - S_N(\varrho(0)) = 0. \tag{2.26}
\end{align}$$

Where in Eq. (2.23) we used again the property $f(\hat{A}) = \hat{\eta} f(\hat{B})\hat{\eta}^{\dagger}$. Eq (2.26) establishes that unitary evolutions are uncapable of increasing the total entropy of any joint system.

The relevance of this property for unitary evolutions will become more apparent in the later derivation for the *anomalous heat flow equation*. Later in this thesis we discuss in what environments does the Second Law of Thermodynamics fails to predict the presence of heat flow between two qubits.

As per Shannon's and Boltzmann's entropy formulations, it is useful to derive a quantum mechanical counterpart of the relative entropy. Let us define the density operators ϱ and ζ via Eq. (2.9), we define the relative entropy [8, 20, 18] of ϱ to ζ as

$$S(\varrho||\zeta) = -S_N(\varrho) - \mathrm{tr}[\varrho \ln(\zeta)] = \mathrm{tr}[\varrho(\ln(\varrho) - \ln(\zeta))]. \tag{2.27}$$

Relative entropy is a measure quantifying how much does a probability distribution, for a given random variable, varies from another. Effectively, Eq. (2.27) can be though of as returning the "distance" between systems ϱ and ζ [18].

The formalism of relative entropy it is often accompanied by the theorem of Klein's Inequality, which establishes a non-negativity property of relative entropy [6, 8, 18]

$$S(\varrho||\zeta) \geq 0, \tag{2.28}$$

where $S(\varrho||\zeta) = 0$ if and only if $\varrho = \zeta$ [8, 18]. The non-negativity established by Klein's inequality is a necessary condition in establishing under what conditions is a reversal of the energy exchange possible (see section **2.2.6**).

2.2.4 Gibb's Thermal State

In this section we derive a formulation for density operators describing systems in thermal state. For systems in thermal state Eq. (2.20) becomes

$$\frac{\partial \varrho}{\partial t} = 0. \tag{2.29}$$

The above relation ensures the possibility of simultaneously diagonalize both $\hat{H}$ and ϱ. This allows us rewrite ϱ in the energy eigenbasis. In such basis the diagonal entries of ϱ become the percentile population for the corresponding eigenstate.

By definition thermal states represent a systems of given energy for which entropy is maximized [23]. Using the formalism of Lagrange multipliers, we now maximize the entropy function (2.21). This optimization, must be carried out by limiting our resulting states to be normalized (Eq. (2.10)). Moreover we require to optimize the entropy function for a state of energy $\langle E\rangle = \mathrm{tr}(\varrho\hat{H})$.

Let us define the function $\mathcal{L}(\varrho, \lambda, \beta)$, where the terms λ and μ are the lagrangian multipliers associated to each constraint. Taking the gradient of $\mathcal{L}(\varrho, \lambda, \beta)$ allows to optimize it with respect to every variable

$$\mathcal{L}(\varrho, \lambda, \beta) = -\mathrm{tr}(\varrho \ln \varrho) - \lambda(\mathrm{tr}(\varrho) - 1) - \beta\left[\mathrm{tr}\left(\varrho\hat{H}\right) - \langle E\rangle\right], \tag{2.30}$$

$$\nabla\mathcal{L}(\varrho, \lambda, \beta) = \begin{pmatrix} \frac{\partial\mathcal{L}(\varrho,\lambda,\beta)}{\partial\varrho} \\ \frac{\partial\mathcal{L}(\varrho,\lambda,\beta)}{\partial\lambda} \\ \frac{\partial\mathcal{L}(\varrho,\lambda,\beta)}{\partial\mu} \end{pmatrix} = \begin{pmatrix} \sum_i^N - [\ln(\varrho_{ii}) + 1] - \beta E_i + \lambda = 0 \\ \mathrm{tr}\left(\varrho\hat{H}\right) = \langle E\rangle \\ \mathrm{tr}(\varrho) = 1 \end{pmatrix}. \tag{2.31}$$

The above system of equations can be solved by the state ϱ with entries $\varrho_{ii} = e^{-\beta E_i + \lambda - 1}$. To satisfy the normalization requirement presented in Eq. (2.10), the state entries become

$$\varrho_{ii} = \frac{e^{-\beta E_i + \lambda - 1}}{\mathrm{tr}(\varrho)} = \frac{e^{-\beta E_i + \cancel{\lambda - 1}}}{\sum_k^N \left(e^{-\beta E_k + \cancel{\lambda - 1}}\right)} = \frac{e^{-\beta E_i}}{\sum_k^N \left(e^{-\beta E_k}\right)}. \tag{2.32}$$

Let us define the normalization constant $Z = \mathrm{tr}\left(e^{-\beta \hat{H}}\right)$. We define the thermal state $\tau(\beta)$ as

$$\tau(\beta) = \frac{e^{-\beta \hat{H}}}{\mathrm{tr}\left(e^{-\beta \hat{H}}\right)} = \frac{e^{-\beta \hat{H}}}{Z}. \tag{2.33}$$

From statistical mechanic notions we realize that the elements of Eq. (2.33) are a suitable representation for what is known as a canonical ensemble [23]. Although we have not defined the qubit to be connected to any thermal bath, it is still possible to regard the Lagrange multiplier β as a fictitious inverse temperature term $\beta = 1/T$. Such definition thus relates the notion of temperature of the system to the relative population of each energy level [7, 8, 13, 20, 23]. Where a higher temperature would correspond to a higher population in the excited states. Moreover, it follows that the normalization constant Z, can be regarded as a partition function of the system.

2.2.5 Correlation Operators, and Correlation Measure

In a qualitative way, it is possible to identify the concept of correlation as the feauture that more information is available about a joint system, than the information available about its comprising subsystems [24].

To start discussing the idea of joint systems we use Eq. (2.12) to define a separable uncorrelated state ϱ_{AB}, as the tensor product between the states ϱ_A and ϱ_B. From this we use the notion of partial trace to establish a relation between the separate sytems and the joint state which they form

$$\varrho_{\mathrm{AB}} \equiv \varrho_A \otimes \varrho_B \tag{2.34}$$

$$\varrho_A = \mathrm{tr}_B(\varrho_{AB}), \text{ and } \varrho_B = \mathrm{tr}_A(\varrho_{AB}). \tag{2.35}$$

Where $\mathrm{tr}_{i(.)}(i \in \{A, B\})$ represents the operation of tracing an operator $\varrho_{\alpha\beta}$ over all the degrees of freedom of subsystem α [18].

Let us define the composite state ϱ_{AB} defined as the joint system constructed by the subsystems ϱ_A and ϱ_B, defined via Eq. (2.35). We define the correlation operator χ as

$$\chi \equiv \varrho_{AB} - \varrho_A \otimes \varrho_B. \tag{2.36}$$

In the instance where there were no correlation between the susbsystems ϱ_A and ϱ_B, then $\chi = 0$ and Eq. (2.36) returns definition (2.34).

The correlation operator, defined in the above equation, contains information regarding all possible quantum and classical correlations within the subsystems of the joint system ϱ_{AB} [25]. We therefore use the formulation of correlation operator to represent the correlation terms defining the correlations present in the systems that will be studied.

The operator defined in Eq. (2.36) is, by construction, Hermitian. Moreover, in order to satisfy the normalization constraint of Eq. (2.10), χ must represent a traceless operator $\mathrm{tr}(\chi) = 0$ and $\mathrm{tr}_A(\chi) = \mathrm{tr}_B(\chi) = 0$.

Correlations can be divided into two subgroups: quantum correlations, and classical correlations. Briefly, the difference in the two lies in the separability of the correlated system. Any separable bipartite pure state, can be written in the form $\rho_{i,j} = \rho_i \otimes \rho_j$. Classical correlations are defined to leave the system separable, while, if a system quantum correlated, it is not possible to find a separable representation for it. Quantifying the amount of correlation, established between two separate systems, is a process that can be accomplished through the use of the entropic measure of correlation: mutual information. In standard statistical mechanics, Shannon's mutual information description returns the shared information between two random variables A and B. Shannon's mutual information is defined as $I(A : B) = S(A) + S(B) - S(A, B)$, where the function $S(x)$ is Shannon's entropy defined in Eq. (2.2), and $S(A, B)$ represents Shannon's entropy for the joint system of variables A and B. The quantum mechanical equivalent to Shannon's mutual information is defined as follows [6, 7, 8, 17, 24]

$$I(\varrho_A : \varrho_B) = S_N(\varrho_A) + S_N(\varrho_B) - S_N(\varrho_{AB}). \tag{2.37}$$

In essence, mutual information is a positive ($I(A : B) \geq 0$) symmetric ($I(A : B) = I(B : A)$) function [26, 27], which returns the amount of information one can gain about system $\varrho_A(\varrho_B)$, given a measurement on system $\varrho_B(\varrho_A)$. Eq. (2.37) is an entropic measure of correlation capable of quantifying the coupling between two states, it is although unable of distinguishing whether the correlation is of classical or quantum nature.

2.2.6 Anomalous heat flow equation

In this section we derive a formulation capable of quantitatively describe the energy flow between two subsystems in a completely isolated composite system ϱ_{AB}. The interacting subsystems are defined to be initially at thermal equilibrium, and are therefore described through Eq. (2.33).

Differently from how the problem was approached in section **2.1.2**, what follows is a derivation for a formulation for the change in energy of either subsystems, as function of entropic measures such as mutual information and relative entropy. The introduction of these entropic measures will allow a discussion under what conditions does the phenomenon of anomalous energy flow arise.

Given an initial thermal state $\varrho_A(0)$ and a final state $\varrho_A(t_f)$, (where $\varrho_A(t_f) = \mathrm{tr}_B(U \varrho_{AB}(0) U^\dagger)$), we use Eq. (2.27) to define the relative entropy between two states of system A at two different points in time

$$S(\varrho_A(t_f) || \varrho_A(0)) = -S_N(\varrho_A(t_f)) - \mathrm{tr}\left[\varrho_A(t_f) \ln\left(\frac{e^{-\beta_A \hat{H}_A}}{Z_A}\right)\right] \tag{2.38}$$

$$= -S_N(\varrho_A(t_f)) + \beta_A \mathrm{tr}\left[\varrho_A(t_f) \hat{H}_A\right] + \ln(Z_A). \tag{2.39}$$

From the definition of relative entropy it follows that $S(\varrho_A(0)||\varrho_A(0)) = 0$, and thus we write

$$\begin{aligned} S(\varrho_A(t_f)||\varrho_A(0)) &= S(\varrho_A(t_f)||\varrho_A(0)) - S(\varrho_A(0)||\varrho_A(0)) \\ &= -S_N(\varrho_A(t_f)) + \beta_A \mathrm{tr}\left[\varrho_A(t_f)\hat{H}_A\right] + \ln(Z_A) \\ &\quad +S_N(\varrho_A(0)) - \beta_A \mathrm{tr}\left[\varrho_A(0)\hat{H}_A\right] - \ln(Z_A) \\ &= \beta_A \Delta E_A - \Delta S_N^A, \end{aligned} \tag{2.40}$$

where ΔS_N^A is the change in the von Neumann entropy of qubit A $\Delta S_N^A = S_N(\varrho_A(t_f)) - S_N(\varrho_A(0))$. Because the system was constructed to be isolated, then $\Delta E_A = -\Delta E_B$.

Finally, by putting together the above relations and the relation for mutual information (2.37), one obtains a formulation for the energy exchange between the two systems (keep in mind that for unitary time evolutions $\Delta S_N^{AB} = 0 \ \Rightarrow \ \Delta I(\varrho_A : \varrho_B) = \Delta S_N^A + \Delta S_N^B$)

$$\Delta E_B(\beta_B - \beta_A) = \Delta E_B \Delta\beta = \Delta I(\varrho_A : \varrho_B) + \sum_i S(\varrho_i(t_f)||\varrho_i(0)), \quad i \in \{A, B\}. \tag{2.41}$$

The above equation shows for what conditions do Clausius and Kelvin's statements require an additional generalization. In section **2.1.2** we derived how the behaviour of heat, for a classically uncoupled system, matches the predictions made by Clausius and Kelvin's statements. The agreement was found through the derivation of the non-negativity property of Eq. (2.8). By contrast, via Eq. (2.41) we derived a formulation that needs not to fulfill non-negativity properties.

In the instance where $T_A < T_B$, then $\beta_A > \beta_B$. We define the instance for which the direction of energy flow has been reversed when $\Delta E_B > 0$, implying an increase in energy of the hot qubit ϱ_B. Klein's inequality, presented in Eq. (2.28), ensures that the only situation where $\Delta E_B > 0$, is for $\Delta I(\varrho_A : \varrho_B) < 0$ and $|\Delta I(\varrho_A : \varrho_B)| > \sum_i S(\varrho_i(t_f)||\varrho_i(0))$. In their respective statements, Clausius and Kelvin considered two uncoupled systems, such as the one described in section **2.1.2**: in such scenarios, the mutual information between the two bodies is by definition taken to be null. Given the positivity of mutual information, any interaction between the two bodies is uncapable of producing a final state for which $\Delta I(i : j) < 0$: in this regime then Clausius and Kelvin statements are a good model to describe the interaction between the two bodies, as energy would flow from the hot to the cold system. Although, Eq. (2.41) proves that, for an initially coupled system, the above statements need not to hold true, as long as the positive entropy production of the two states is balanced by a significant reduction in their mutual information.

2.3 Overview

In this section we qualitatively describe the complete time line of events, that the considered system has to go through to reach a state in which energy has been reversely exchanged.

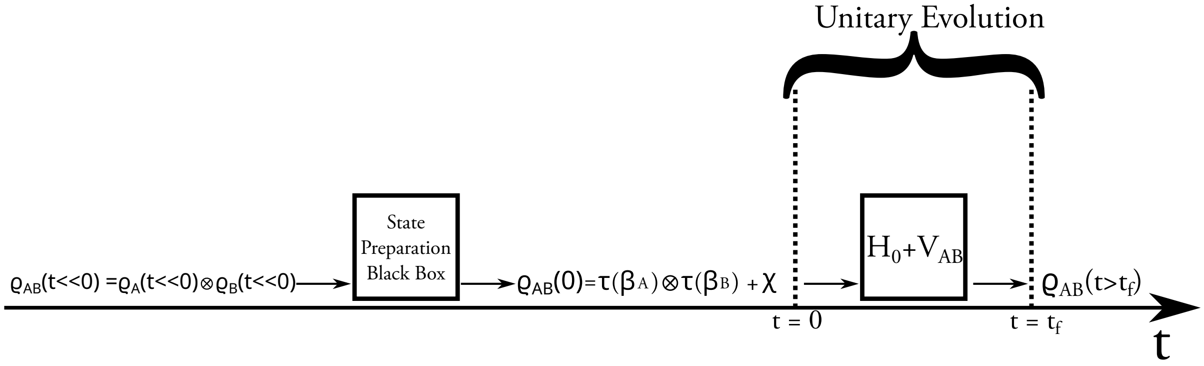


Figure 2: Schematic diagram portraying the system's time line of events, starting from a non interacting uncorrelated scenario $\varrho_{AB}(t << t_f)$ and ending in a state in which the two qubits have reversely exchanged energy $\varrho_{AB}(t > t_f)$.

The above Fig. 2 shows a timeline of the explored two qubits system. Consider to universe to be comprised at all times by two qubits. The two are set to be initially non-interacting, uncorrelated and forming a joint isolated state $\varrho_{AB}(t < 0) = \varrho_A(t < 0) \otimes \varrho_B(t < 0)$ (see "separable state" in section **2.2.5**). The two are then set to interact is some precise way(Black Box in Fig. 2), resulting in states like the one presented in Eq. (2.33). The state representation derived in Eq. (2.33) relates the temperature of each qubit to the population probability of their energy levels. Henceforth, we discuss the temperature of the qubits, even in the absence of connections to any real thermal bath. The "State Preparation Black Box" (see Fig. 2) needs not to preserve the total energy of the system, and it serves the purpose of establishing a correlation between the qubits. This correlation is mathematically described by the introduction of a correlation term as the one described in Eq. (2.36).

In this thesis we assume to be initially provided with a joint state of the form $\varrho_{AB}(0) = \tau(\beta_A) \otimes \tau(\beta_B) + \chi$. The focus of this thesis lies in the exploration of the next step. Once the qubits are correctly prepared and correlated, the interaction term $\hat{V}(t)$ (see Eq. (2.15)) is activated within the interval $0 < t < t_f$. This interaction serves the purpose of driving a reverse exchange of energy $\Delta E_i = W_i + Q_i$ ($i \in \{A, B\}$): where W_i and Q_i correspond to the work and heat exchanged by qubit i (see section **3.1**). A possible physical realization of this process is presented in Ref. [7]. In the latter, two nuclear spin-1/2 systems were prepared in thermal states $\tau(\beta_i)$ and studied through the use of Nuclear Magnetic Resonance techniques involving radio-frequency pulses. Although in the presence of an external field, the interaction term $V(t)$ establishes a unitary evolution that is constrained in keeping the total energy of the joint system fixed. Later in this thesis we better describe how the generated time evolution is constrained in keeping the total energy of the system constant(section **3.1**).

3 Method

3.1 Optimizing the energy exchange between correlated qubits

In this section I present the derivation to analytical results for the problem of reverse energy exchange, for the case of a 2 qubit system. For a two dimensional system, the corresponding local Hamiltonian $\hat{H}$ can be represented in the energy basis as $\hat{H} = \sum_{i=0}^{1} E_i|i\rangle\langle i| = E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1|$, where the terms E_i correspond to the eigenvalues of the Hamiltonian. Rather than focusing on the absolute energy of each level, what is often more relevant is the difference between the energy of each level. It is therefore convenient to apply a relative shift to the eigenvalues of the Hamiltonian, corresponding to the energy of the lowest energy level of the system E_0. Through said shift we define the Hamiltonian of any two-level system k, as

$$\hat{H}_k = \epsilon_k|1\rangle\langle 1| = \begin{bmatrix} 0 & 0 \\ 0 & \epsilon_k \end{bmatrix} \quad k \in \{A, B\}, \tag{3.1}$$

where ϵ_k corresponds to the difference in the eigenvalues of the local Hamiltonian, i.e. $\epsilon = E_1 - E_0$. Here we assume that the two local Hamiltonians respect the condition $\epsilon_A = \epsilon_B = \epsilon$, allowing for degenerate energy states of the joint system. In such scenario, Eq. (2.15) becomes

$$\begin{aligned} \hat{H}_{AB}(0) &= \hat{H}_A \otimes \mathbb{1}_B + \mathbb{1}_A \otimes \hat{H}_B && (3.2) \\ &= \epsilon_B|01\rangle\langle 01| + \epsilon_A|10\rangle\langle 10| + (\epsilon_B + \epsilon_A)\,|11\rangle\langle 11| && (3.3) \\ &= \epsilon|01\rangle\langle 01| + \epsilon|10\rangle\langle 10| + 2\epsilon|11\rangle\langle 11| = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \epsilon & 0 & 0 \\ 0 & 0 & \epsilon & 0 \\ 0 & 0 & 0 & 2\epsilon \end{bmatrix}. && (3.4) \end{aligned}$$

Let us consider two qubit systems defined at thermal equilibrium. Eq. (2.29) ensures us that it is possible to simultaneously diagonalize both initial density matrices and the Hamiltonian: meaning that it is possible to represent both operators in the energy basis. Through the use of Eq. (2.33) and the local Hamiltonians from Eq. (3.1), we define two qubit systems in thermal state

$$\begin{aligned} \tau(\beta_A) = \varrho_A(0) &= \frac{1}{1+e^{-\beta_A\epsilon}}\left(|0\rangle\langle 0| + e^{-\beta_A\epsilon}|1\rangle\langle 1|\right) = \frac{1}{Z_A}\begin{bmatrix} 1 & 0 \\ 0 & e^{-\beta_A\epsilon} \end{bmatrix}, && (3.5) \\ \tau(\beta_B) = \varrho_B(0) &= \frac{1}{1+e^{-\beta_B\epsilon}}\left(|0\rangle\langle 0| + e^{-\beta_B\epsilon}|1\rangle\langle 1|\right) = \frac{1}{Z_B}\begin{bmatrix} 1 & 0 \\ 0 & e^{-\beta_B\epsilon} \end{bmatrix}. && (3.6) \end{aligned}$$

Where β_k represents the inverse temperature $1/T_k$ of qubit system k ($k \in \{A, B\}$).

In order to explore the results of any interaction between the two systems $\tau(\beta_A)$ and $\tau(\beta_B)$, we define an uncorrelated separable state given by the tensor product of the two thermal states, Eq. (2.12). Lastly, in theory section **2.2.6**, it is explored how a non-zero degree of correlation is required in order to obtain the phenomenon of reversed energy flow, we thus introduce a correlation operator χ. For sake of simplicity, the correlation term, whose effects will be studied in this thesis, is defined to take the form

$$\chi = \alpha e^{i\phi} |01\rangle\langle 10| + \alpha e^{-i\phi} |10\rangle\langle 01| = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha e^{i\phi} & 0 \\ 0 & \alpha e^{-i\phi} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{3.7}$$

Through a reordering of Eq. (2.36), we arrive at the initial state for the two qubit joint system

$$\varrho_{AB}(0) = \begin{bmatrix} \frac{1}{Z_A Z_B} & 0 & 0 & 0 \\ 0 & \frac{e^{-\beta_B \epsilon}}{Z_A Z_B} & \alpha e^{i\phi} & 0 \\ 0 & \alpha e^{-i\phi} & \frac{e^{-\beta_A \epsilon}}{Z_A Z_B} & 0 \\ 0 & 0 & 0 & \frac{e^{-\epsilon(\beta_B + \beta_A)}}{Z_A Z_B} \end{bmatrix} = \begin{bmatrix} p_{00} & 0 & 0 & 0 \\ 0 & p_{01} & \alpha e^{i\phi} & 0 \\ 0 & \alpha e^{-i\phi} & p_{10} & 0 \\ 0 & 0 & 0 & p_{11} \end{bmatrix}. \tag{3.8}$$

This choice of correlation term χ results in the introduction of a phase relation within the $\{|01\rangle, |10\rangle\}$ degenerate subspace (see Eq. (3.8)). Although any value for the correlation strength α would satisfy the necessary conditions $\mathrm{tr}(\chi) = 0$ and $\mathrm{tr}_A(\chi) = \mathrm{tr}_B(\chi) = 0$ and $\chi^\dagger = \chi$, not every value for α would satisfy the positiveness of ϱ_{AB}. By solving the characteristic polynomial for expression (3.8), one obtains the following four equations for the eigenvalues λ_i of $\varrho_{AB}(0)$

$$\lambda_0 = p_{00} \tag{3.9}$$

$$\lambda_1 = \frac{p_{01} + p_{10} - \sqrt{(p_{01} - p_{10})^2 + 4\alpha^2}}{2} \tag{3.10}$$

$$\lambda_2 = \frac{p_{01} + p_{10} + \sqrt{(p_{01} - p_{10})^2 + 4\alpha^2}}{2} \tag{3.11}$$

$$\lambda_3 = p_{11} \tag{3.12}$$

By setting the values of λ_1 or λ_2 to zero, we study for what values of α do the eigenvalues of $\varrho_{AB}(0)$ are strictly positive

$$-\sqrt{p_{01} p_{10}} \leq \alpha \leq \sqrt{p_{01} p_{10}}. \tag{3.13}$$

We now introduce the evolved joint system $\varrho_{AB}(t_f) = \hat{U} \varrho_{AB}(0) \hat{U}^\dagger$, where $\hat{U}$ is some unitary time evolution. Because the $\{|01\rangle, |10\rangle\}$ subspace is a degenerate subspace, any unitary operation within this subspace will keep the energy of the whole system fixed. Therefore, we use Eq. (2.17) to derive the general form of a unitary with the purpose of applying some rigid rotation on the $\{|01\rangle, |10\rangle\}$ subspace of the joint system, while leaving the remaining states invariant

$$\hat{U} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{i\mu} \cos(\theta) & e^{i\gamma} \sin(\theta) & 0 \\ 0 & -e^{-i\gamma} \sin(\theta) & e^{-i\mu} \cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{3.14}$$

Without loss of generality, we define the temperature relation $T_A > T_B \Rightarrow \beta_A < \beta_B$. We now want to determine the time evolution unitary $\hat{U}$, capable of returning an evolved state $\varrho_{AB}(t_f)$ for which the energy change ΔE_A of the "hot"(A) state is greater than the energy difference for the "cold"(B) state, and therefore $\Delta E_A > 0$. In general, it is possible to determine the change in the expectation value of an observable through the difference of Eq. (2.11) for a system at two different points in time, thus

$$\begin{aligned} \Delta E_A &= \operatorname{tr}\left(\varrho_A(t_f)\hat{H}_A\right) - \operatorname{tr}\left(\varrho_A\left(0\right)\hat{H}_A\right) && (3.15)\\ &= \operatorname{tr}\left(\operatorname{tr}_B\left(\hat{U}\varrho_{AB}(0)\hat{U}^\dagger\right)\hat{H}_A\right) - \operatorname{tr}\left(\varrho_A\left(0\right)\hat{H}_A\right). && (3.16)\end{aligned}$$

The formalism of Lagrange multipliers becomes now useful to optimize Eq. (3.16), under the constraint of a energy-conserving unitary evolution, as the one described in Eq. (3.14).

Let us define the function $Q_A(\theta,\gamma,\mu)$ as the function obtained through Eq. (3.16) constrained by the unitary evolution of Eq. (3.14). Optimizing $Q_A(\theta,\gamma,\mu)$ requires setting to zero each component of the gradient vector $\nabla Q_A(\theta,\gamma,\mu)$

$$\begin{aligned} Q_A(\theta,\gamma,\mu) = \tfrac{\epsilon}{2}\big[&-\alpha\left(\sin\left(-\gamma+\mu+\phi+2\theta\right)+\sin\left(\gamma-\mu-\phi+2\theta\right)\right)\\ &+\left(p_{10}-p_{01}\right)\cos\left(2\theta\right)+p_{01}-p_{10}\big] \end{aligned} \tag{3.17}$$

$$\begin{aligned} \tfrac{\partial(Q_A(\theta,\gamma,\mu))}{\partial\theta} = Q_\theta^A = &-\alpha\left(\cos\left(-\gamma+\mu+\phi+2\theta\right)+\cos\left(\gamma-\mu-\phi+2\theta\right)\right)\\ &+\left(p_{01}-p_{10}\right)\sin\left(2\theta\right) = 0 \end{aligned} \tag{3.18}$$

$$\frac{\partial\left(Q_A(\theta,\gamma,\mu)\right)}{\partial\gamma} = Q_\gamma^A = \alpha\left(\cos\left(-\gamma+\mu+\phi+2\theta\right)-\cos\left(\gamma-\mu-\phi+2\theta\right)\right) = 0 \tag{3.19}$$

The above system of equations is underdetermined for the variables (θ,γ,μ). This is because, although we could construct a third equation representing $\frac{\partial(Q_A(\theta,\gamma,\mu))}{\partial\mu}$, this would yield a relation of the form $\frac{\partial(Q_A(\theta,\gamma,\mu))}{\partial\mu} = -\frac{\partial(Q_A(\theta,\gamma,\mu))}{\partial\gamma}$. Under these considerations we therefore constrain the angle μ to $\mu \in \mathbb{R}$. With such constraint, solving the above system of equations for the angles (θ,γ,μ) yields

$$\left(0,\ \mu+\phi+\frac{\pi}{2}(2\mathrm{n}+1),\mu\right), \tag{3.20}$$

$$\left(\operatorname{atan}\left(\frac{-p_{01}+p_{10}+\sqrt{4\alpha^2+\left(p_{01}-p_{10}\right)^2}}{2\alpha}\right),\mu+\phi,\mu\right), \tag{3.21}$$

$$\left(\frac{\pi}{2},\ \mu+\phi+\frac{\pi}{2}(2\mathrm{n}+1),\mu\right), \tag{3.22}$$

$$\left(-\operatorname{atan}\left(\frac{p_{01}-p_{10}+\sqrt{4\alpha^2+\left(p_{01}-p_{10}\right)^2}}{2\alpha}\right),\mu+\phi,\mu\right), \tag{3.23}$$

where $\mathrm{n} \in \mathbb{Z}$.

The above results (3.20-3.23) represent both local and global extrema for the change in energy $Q_A(\theta,\gamma,\mu)$, under the constraint of a energy-conserving unitary evolution. Let us define the Hessian matrix $\hat{\mathcal{Q}}$ describing the second order partial derivatives of the function $Q_A(\theta, \gamma, \mu)$. We distinguish which of the results (3.20-3.23) corresponds to a global extremum of $Q_A(\theta, \gamma, \mu)$, by means of computing the determinant of $\hat{\mathcal{Q}}$[28]. Because the above solutions are invariant with respect to the angle μ, we can safely disregard any derivative with respect to the latter

$$
\begin{aligned}
\det\left(\hat{\mathcal{Q}}\right) =& \det\left(\begin{bmatrix} Q^A_{\theta\theta} & Q^A_{\theta\gamma} \\ Q^A_{\gamma\theta} & Q^A_{\gamma\gamma} \end{bmatrix}\right) = Q^A_{\theta\theta}Q^A_{\gamma\gamma} - \left(Q^A_{\gamma\theta}\right)^2 \\
=& -\alpha\epsilon^2\big[4\alpha\sin^2(\gamma-\phi)\cos^2(2\theta) \qquad (3.24) \\
& -\left(\sin(-\gamma+\phi+2\theta)+\sin(\gamma-\phi+2\theta)\right)\big(\alpha\sin(-\gamma+\phi+2\theta) \qquad (3.25) \\
& +\alpha\sin(\gamma-\phi+2\theta)+(p_{01}-p_{10})\cos(2\theta)\big)\big] \qquad (3.26)
\end{aligned}
$$

In general, it is possible to identify the nature of an extremum point by checking whether $\det\left(\hat{\mathcal{Q}}(\theta_i, \gamma_i)\right) < 0$, in which case the eigenvalues of $\hat{\mathcal{Q}}$ indicate slopes of opposite sign for the variables (θ, γ), at point $Q_A(\theta_i, \gamma_i)$. Which ultimately indicates the presence of a saddle point.

Going through each case, we find that both solutions given in Eqs. (3.20,3.22), return a determinant

$$\det\left(\hat{\mathcal{Q}}\right) = -4\alpha^2\epsilon^2 \qquad (3.27)$$

Because $\alpha, \epsilon \in \mathbb{R}$, Eq. (3.27) is negative, independently from the value taken by either the correlation strength α or the energy ϵ. Thus, Eq. (3.27) returns us the presence of saddle points for the the two solutions (3.20,3.22).

If we instead consider the points given by the solutions given in (3.21,3.23), we find both determinants of the Hessian matrix to respectively be

$$\det\left(\hat{\mathcal{Q}}\right) = 4\alpha^2\epsilon^2. \qquad (3.28)$$

Eq. (3.28) ensures us that the solutions (3.21,3.23) represent either matxima or minima points of the change of energy ΔE_A. To establish whether the solutions represent minima or maxima for the system, one can deduct the sign for $Q^A_{\theta\theta}$ establishing if all neighbouring points are either increasing or decreasing in value [28]. Once a solution that maximizes ΔE_A is established, it is then possible to define a time evolution unitary for optimal reverse energy flow.

3.2 Results from a numerical approach

In this section we provide numerical results obtained through the theory presented in the previous sections, over a set of initial states presented in Ref. [7]. Because the whole system never reaches full-thermalization, the states of the system will present an oscillatory periodical behaviour. Thus, almost all the visualizations represented in this section will present periodicity. Although, all peaks shown in each graph would need to marked by the corresponding solution, for sake of visual simplicity, we only plot solutions where n = 0. The discussed qubits are two spin-1/2 particles, prepared in thermal state. In their publication (Ref. [7]), the authors provided a global Hamiltonian, which they used to accordingly evolve their system. Here, we disregard the given Hamiltonian. Instead, we make use of the provided initial states, for which we will find the optimal unitary evolution to obtain reversed energy flow. From the found unitary we then proceed on deriving its generating Hamiltonian, and lastly, we will study how different parameters affect the reverse exchange of energy between the two qubits.

All the values used in this section, together with their provided uncertainty, can be found in table 1, in the appendix (section **5.3**). In the publication, the local Hamiltonian $\hat{H}_i$ ($i \in \{A, B\}$), corresponding to each qubit system, was defined as [7]

$$\hat{H}_i = \begin{bmatrix} 0 & 0 \\ 0 & h\nu_0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 2\pi \end{bmatrix}, \tag{3.29}$$

where h corresponds to Planck constant, and since $\hbar = 1 \;\Rightarrow\; h = 2\pi$; while the term ν_0 corresponds to a frequency for the local Hamiltonian.

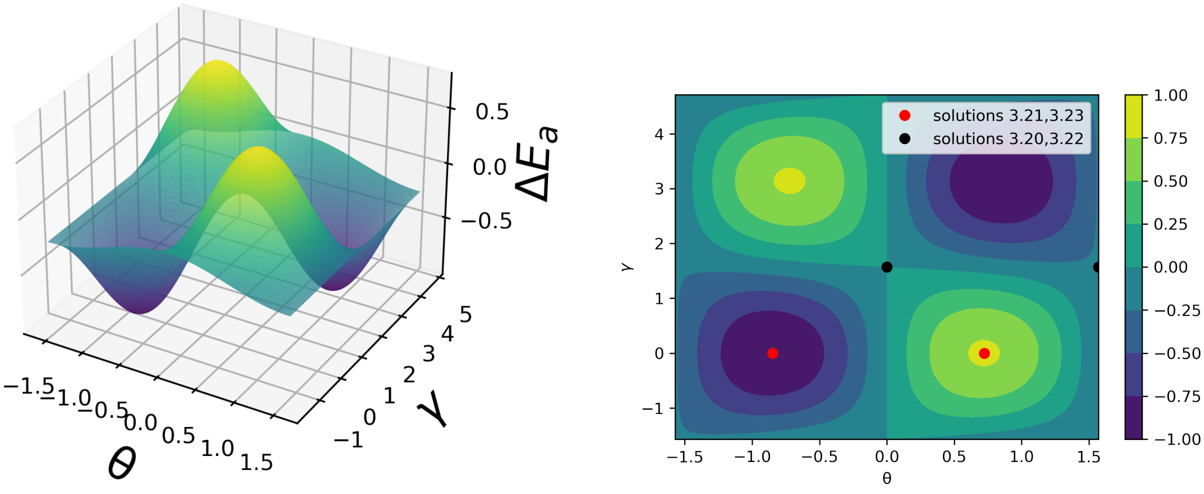
A suitable representation, for the considered spin-1/2 systems, can be derived through the use of Eq. (2.33). By using the Hamiltonian in Eq. (3.29), the two qubits can be represented in the energy basis as

$$\varrho_A(0) = \tfrac{1}{Z_A} \begin{bmatrix} 1 & 0 \\ 0 & e^{-\beta_A h\nu_0} \end{bmatrix} = \begin{bmatrix} 0.81 & 0 \\ 0 & 0.19 \end{bmatrix} \tag{3.30}$$

$$\varrho_B(0) = \tfrac{1}{Z_B} \begin{bmatrix} 1 & 0 \\ 0 & e^{-\beta_B h\nu_0} \end{bmatrix} = \begin{bmatrix} 0.85 & 0 \\ 0 & 0.15 \end{bmatrix} \tag{3.31}$$

The above density operators can be thought as of two distinct systems, both at thermal equilibrium, where $T_B < T_A$. The chosen correlation term is $\chi = -0.14|01\rangle\langle 10| - 0.14|10\rangle\langle 01|$ [7]. Therefore, once the two qubits are placed into thermal contact, the joint system representation becomes

$$\varrho_{AB}(0) = \varrho_A(0) \otimes \varrho_B(0) + \chi = \begin{bmatrix} 0.688 & 0 & 0 & 0 \\ 0 & 0.124 & -0.14 & 0 \\ 0 & -0.14 & 0.159 & 0 \\ 0 & 0 & 0 & 0.029 \end{bmatrix}. \tag{3.32}$$



(a) (b)

Figure 3: **a)** Energy change plot over all the possible combinations of the rotational angles (θ, γ) for qubit ϱ_A (the rotational angle μ has been disregarded given the invariance of the found solutions with the values taken by the latter); **b)** Contour plot of the energy change for qubit ϱ_A for different unitaries. The four solutions (3.20-3.23) have been marked onto the plot to show how these relate with the change in energy of qubit A.

Using the state presented in Eq. (3.32), we can use Eq. (3.16) to explore all possible changes in energy of either qubits, when undergoing a set of possible unitary evolutions. Fig. 3.a depicts the landscape of possible changes in energy corresponding to all possible unitaries $\hat{U}$, defined by the rotation angles θ and γ (see Eq. (3.14)). Fig. 3.b represents the contour plot of image 3.a, where solutions (3.20-3.23) were graphed: the black dots represent the two solutions corresponding to saddle points, while the red dots represent the two global extrema. From Fig. 3.b it can be extrapolated that result (3.23) can be used in order to obtain a unitary evolution capable of maximizing the energy change for qubit ϱ_A reversing the flow of energy.

Considering result (3.23), the optimal unitary becomes:

$$\hat{U} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{1+\frac{\left(p_{01}-p_{10}+\sqrt{4\alpha^2+(p_{01}-p_{10})^2}\right)^2}{4\alpha^2}}} & -\frac{p_{01}-p_{10}+\sqrt{4\alpha^2+(p_{01}-p_{10})^2}}{2\alpha\sqrt{1+\frac{\left(p_{01}-p_{10}+\sqrt{4\alpha^2+(p_{01}-p_{10})^2}\right)^2}{4\alpha^2}}} & 0 \\ 0 & \frac{p_{01}-p_{10}+\sqrt{4\alpha^2+(p_{01}-p_{10})^2}}{2\alpha\sqrt{1+\frac{\left(p_{01}-p_{10}+\sqrt{4\alpha^2+(p_{01}-p_{10})^2}\right)^2}{4\alpha^2}}} & \frac{1}{\sqrt{1+\frac{\left(p_{01}-p_{10}+\sqrt{4\alpha^2+(p_{01}-p_{10})^2}\right)^2}{4\alpha^2}}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{3.33}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0.751 & 0.660 & 0 \\ 0 & -0.660 & 0.751 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{3.34}$$

Using the unitary of Eq. (3.34), as the time evolution operator, for the state given in Eq. (3.32), returns a state whose phase relationships have disappeared, for which the energy of qubit ϱ_A has increased, effectively encapsulating the phenomenon of reversed energy flow

$$\varrho_{AB}(t_f) = \hat{U}\varrho_{AB}(0)\hat{U}^{\dagger} = \begin{bmatrix} 0.688 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0.283 & 0 \\ 0 & 0 & 0 & 0.029 \end{bmatrix} \tag{3.35}$$

hence the change in energy for qubit ϱ_A:

$$\Delta E_A = \operatorname{tr}\left(\operatorname{tr}_B\left(\varrho_{AB}(t_f)\right)\hat{H}_A - \varrho_A(0)\hat{H}_A\right) = \operatorname{tr}\left(\begin{bmatrix} 0 & 0 \\ 0 & 0.774 \end{bmatrix}\right) > 0 \tag{3.36}$$

As the next step, the generating Hamiltonian corresponding to the optimal unitary of Eq. (3.34), can be found. Applying Eqs. (2.18) and (2.14), we derive a representation of the derived Hamiltonian, as a linear combination of Pauli matrices

$$\hat{H}_{AB} = \frac{1.698}{t_f}\left(\hat{\sigma}_2 \otimes \hat{\sigma}_1 - \hat{\sigma}_1 \otimes \hat{\sigma}_2\right) \tag{3.37}$$

We see that the found interaction Hamiltonian corresponds to the global Hamiltonian presented in Ref. [7]. Eq. (3.37) is a representation of the Dzyaloshinskii–Moriya Hamiltonian, which is stated to be experimentally feasible to realize [7].

3.2.1 The role of information in reversal heat flow

By solving the problem of energy exchange for the scenario of two uncoupled systems, in section **2.1.2** we rediscovered both Clausius and Kelvin's statements. While deriving Eq. (2.41), we explored, and discussed, the need for some coupling to pre-exist between the systems, in order to observe reverse flow of energy, and therefore falling in disagreement with both statements.

In this section we seek to explore the role played by the initial correlations in establishing an anomalous energy flow between the two qubits.

Eq. (3.32) gives us a joint system whose correlation strength is bounded by Eq. (3.13)

$$-0.14 \geq \alpha \geq 0.14. \tag{3.38}$$

Within the newly obtained boundaries, we firstly study the result of varying the strength factor α, on the amount of correlation between two qubits, this will enable us to explore how to maximize its initial value. We then compare the obtained result with the energy exchanged as a function of α.

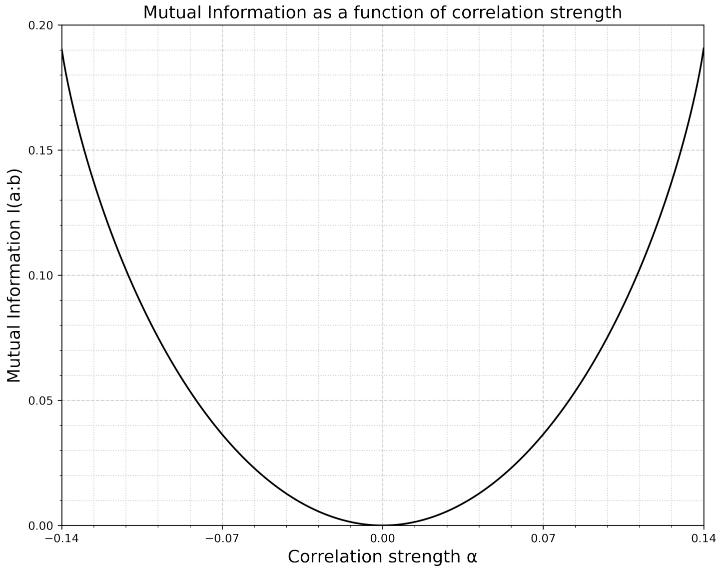


Figure 4: The measure of mutual information as function of α.As expected, we firstly notice that a lack of correlation between the qubits infers a lack of shared information between the two. Moreover the curve for the mutual information presents a symmetry around the value $\alpha = 0$. This symmetry arises because we can integrate the factor -1 within the complex phase of the correlation term χ (as $-1 = e^{i\pi}$).

Fig. 4 depicts the mutual information for the joint system (3.32) as a function of the correlation strength α. Fig. 4 confirms that when $\chi = 0$, then the system can be considered to be completely uncoupled. The figure also shows a symmetry for the measure of mutual information, around the value $\alpha = 0$. This symmetry can be explored through Eq. (2.41): because the mutual information is independent of the sign of α, we can expect the energy exchange between the two qubits to present the same symmetry when plotted as a function of the correlation strength.

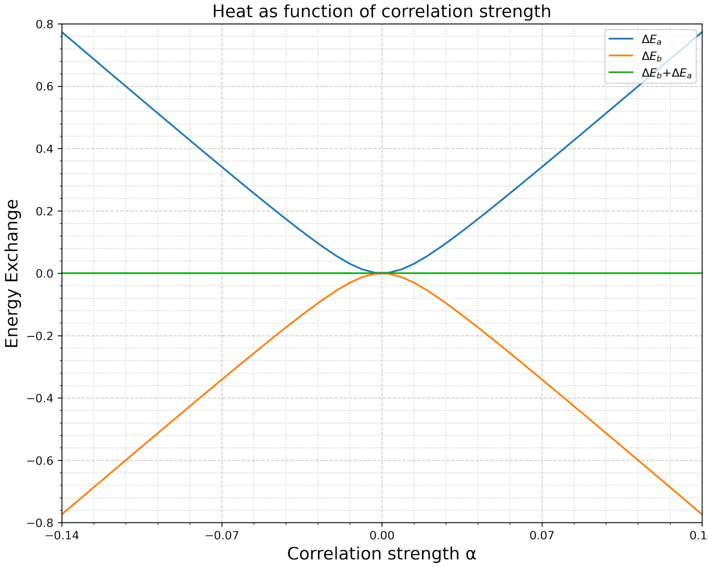
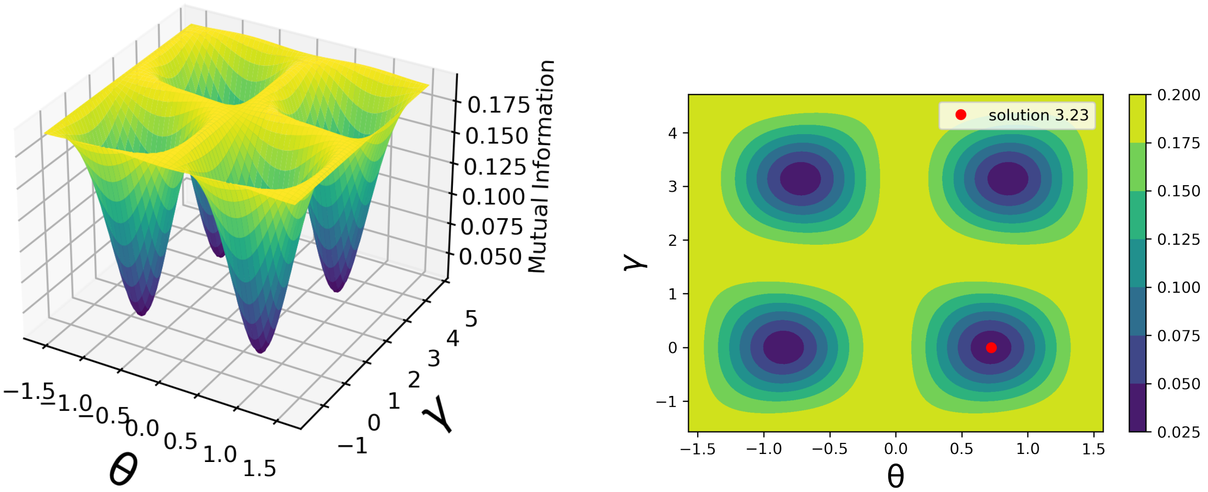


Figure 5: The energy change for both qubits as function of α. The blue and the orange line respectively represent the change in energy of qubit A and qubit B. The green line represents the sum of the changes in energy of the two qubits, demonstrating the ability of the used unitary to maintain the total energy of the system invariant.

Fig. 5 shows the energy exchange between the qubits, as a function of α, under the constrain of a time evolution dictated by the unitary derived in Eq. (3.34). Both plots 4-5 agree on the observation that to maximize the effects of energy reversal, the absolute value of α must be at its greatest. We thus conclude that to maximize the reverse energy exchange within a two-qubit system $|\alpha| = \left|\sqrt{p_{01}p_{10}}\right|$ (see Eq. (3.13)).

3.2.2 The mutual information of the final state

Concerning the role of correlation within the phenomenon of energy reversal, the last aspect we have left to cover is the value of the mutual information between the final states $\varrho_A(t_f)$ and $\varrho_B(t_f)$. As previously stated, Eq. (2.41) tells us that, in order to recover energy reversal, the chosen time evolution unitary must be able to reduce the amount of shared information between the systems $\Delta I(\varrho_A : \varrho_B) < 0$.

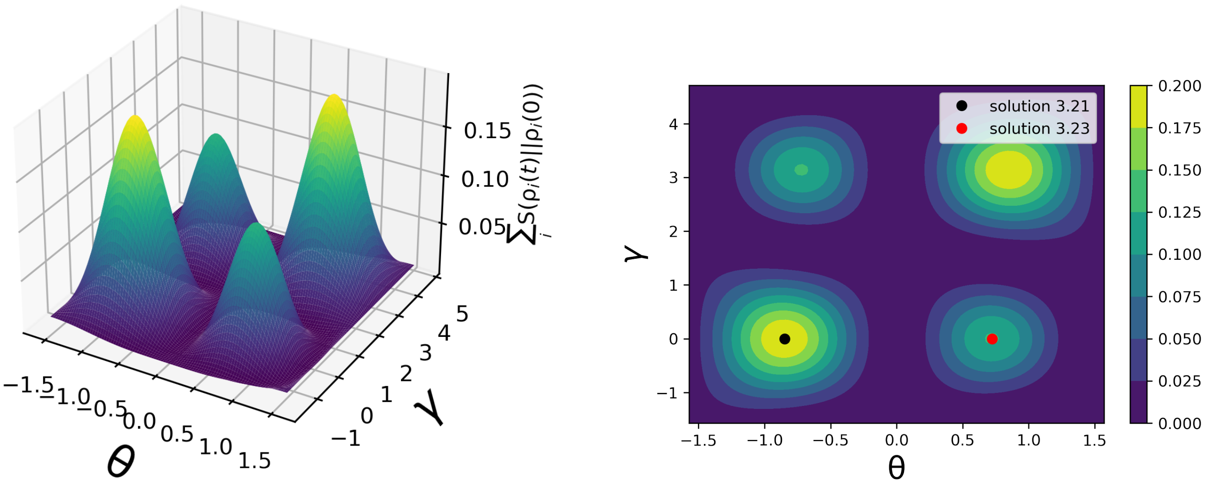


(a) (b)

Figure 6: **a)**Mutual information between the final states $\varrho_A(t_f)$ and $\varrho_B(t_f)$, as function of all possible time evolution unitaries; **b)**Contour plot for the Mutual Information between the final states $\varrho_A(t_f)$ and $\varrho_B(t_f)$, for all possible time evolution unitaries. The solutions (3.21, 3.23) are graphed respectively as the black and red dot. Both solutions return a minimization of the mutual information at $t = t_f$ ($|\alpha| = 0.14$).

Fig. 6.a represents the mutual information between states $\varrho_A(t_f)$ and $\varrho_B(t_f)$, as a function of the angles θ and γ defining the general 2D time evolution unitary. On the right, Fig. 6.b represents its contour plot. Through Eq. (3.36), we analytically proved solution (3.23) to represent the optimal time evolution unitary for energy reversal: Fig. 6.b shows that, for the same solution(red dot), there is a corresponding minimization in the value taken by the mutual information at time $t = t_f$. This observation matches with the expectations obtained by studying Eq. (2.41). Although, from the same plot 6.b, it is also possible to notice an equivalent decrease of mutual information, for the time evolution returning a standard flow of energy (solution (3.21)). We therefore conclude that the condition of minimizing the mutual information between two systems is not enough to guarantee the occurrence of anomalous energy flow.

As mentioned in section **2.2.6**, to obtain energy reversal, the change in mutual information, must be greater than the sum of the relative entropies between the initial and time evolved states of both systems $|\Delta I(\varrho_A : \varrho_B)| > \sum_i S(\varrho_i(t_f)||\varrho_i(0))$ ($i \in \{A, B\}$). To understand what other conditions is the time evolution required to fulfill to optimize energy reversal, we plot the entropic measure of distance between the initial and final state of the two systems, as function of the angles θ and γ (Fig. 7).



(a)

(b)

Figure 7: **a)**Relative entropy, between the initial and final states of both qubits, as function of all possible time evolution unitaries; **b)**Contour plot for the relative entropy, between the initial and final states of both qubits, for all possible time evolution unitaries. The solutions (3.21, 3.23) are graphed respectively as the black and red dot. Solution (3.21) returns a global maxima for the relative entropy, while solution (3.23) returns a local maxima ($|\alpha| = 0.14$)

Fig. 7.a depicts a series of global and local maxima points, while Fig. 7.b shows us the analytical solution for the optimal time evolution unitary(red dot) to coincide with one of the local maxima. Fig. 7.b also provides a way of reasoning behind the "problem" presented by the periodicity of the minimization of mutual information (see Fig. 6). For solution (3.21), energy follows a "standard direction" due to the maximization of the term $\sum_i S(\varrho_i(t_f)||\varrho_i(0))$ in Eq. (2.41). On the other hand solution (3.23) is capable of reversing the exchange of energy since it corresponds to a simultaneous minimization of both the change in mutual information and $\sum_i S(\varrho_i(t_f)||\varrho_i(0))$ (see Eq. (2.41)).

One last remark has to be discussed. From Fig. 6.b we can notice how result (3.23) does not return a final state whose correlation has been completely "destroyed". This observation opens to the question on whether altering the conditions on the time evolution would enable for more energy to be exchanged between the qubits.

4 Conclusion

In this thesis we studied the reversal of the energy flow between initially correlated qubits set to interact at different initial temperatures: we related the effective temperature of each qubit to the respective population of their two levels. In order to bring forth the differences between the two, throughout this thesis we compared the studied correlated case with an uncorrelated analog case.

With the derivation of Eq. (2.26) we established an invariance of the total entropy of a quantum system undergoing a unitary time evolution. The Second Law of Thermodynamics dictates that for energy exchange to occur in isolated systems, the system's entropy must increase, therefore, under unitary transformation, an uncorrelated system would not present any energy exchange between its components. Figs. 5-6 show how energy exchange can arise in these instances only when an initial degree of correlation is present between the subsystems and it is consequentially decreased by the time evolution. By exploring the underlying relation between initial correlations and the direction of thermodynamic processes, we determined the importance of the initial conditions to establish an exchange of energy, as well as its direction.

In general, for energy exchange to be initialized, during the thermal contact between the two qubits, an initial degree of correlation between the two must be established before the start of the protocol. Moreover, the correlation between the two subsystems must be reduced during the interaction: this is a necessary result that was derived by analyzing Fig. 4. Specifically, to obtain the seeked anomalous energy flow, the change in the mutual information between the two qubits must be greater than the sum of the relative entropies between the initial and time evolved states of both qubits.

To maximize the amount of energy flowing from one qubit to the other we used the formalism of Lagrange multipliers with the constraint of an energy-conserving unitary evolution. With this we identified an optimal time evolution for the reversal of energy flow within the system. We explored the plausibility for a physical realization of the found optimal time evolution, through the derivation of the Hamiltonian generating said unitary. The generating Hamiltonian was derived for the initial states provided in Ref. [7]. The Hamiltonian, derived in the Pauli basis (3.37) , takes the form of the interaction Hamiltonian sometimes referred to as the Dzyaloshinskii–Moriya interaction Hamiltonian [7]. The Dzyaloshinskii–Moriya Hamiltonian corresponds to the same Hamiltonian used in the referenced publication, and it is stated to be a relatively easy interaction to recreate in a laboratory environment [7].

In conclusion, by optimizing Eq. (3.16) we were able to find solutions for time evolutions indeed capable of reversing the direction of the energy exchange between qubits. We have also observed the importance of initial conditions in determining important properties relative to the interaction between two bodies. Accordingly, our results clearly show that it is possible to have a time-local inversion of the arrow of time: that is, by proper initial conditions, correlations and applied perturbation, the system can have reversed (cold to hot) energy flow. Although, it has to be emphasized how, the reversal of the time arrow is only possible strictly within a well defined time interval. This is because quantum systems as the one described in this thesis never fully thermalize. This ”impossibility of full-themalization”, leads to an oscillatory behaviour of the states of the system, where energy is then exchanged back and forth between the qubits.

The study of how this effect presents itself in higher dimensional systems is an interesting subject for future analysis. The constraint of having an isolated system could also be removed by allowing unitaries capable of acting over the whole system. By considering non-isolated systems, our hope is to find evolutions capable of driving a higher reduction in the mutual information between the qubits, allowing for higher amounts of energy to be exchanged between the two. These studies could then be used to find a more generalized approach to energy reversal within the framework of Quantum Thermodynamics.

5 Appendix

5.1 Deriving the time derivative of density matrices

In this section we are set to derive the formulation of Eq. (2.20), for the time derivative of a density matrix for a pure state. We begin by exploring the time evolution of the state $|\psi(t)\rangle$. To do so we employ the use of the time dependent Schrodinger's equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \tag{5.1}$$

where $\hat{H}(t)$ is the Hamiltonian dictating the time evolution of $|\psi(t)\rangle$. Using Eq. (5.1) we start rewriting the time derivative for the pure state represented by the density operator $\varrho(t)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = \frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle\langle\psi(t)| = \left(\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle\right)\langle\psi(t)| + |\psi(t)\rangle\left(\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\right) \tag{5.2}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\varrho(t) = \frac{1}{i}\left(\hat{H}(t)|\psi(t)\rangle\langle\psi(t)| - |\psi(t)\rangle\langle\psi(t)|\hat{H}(t)\right) = \frac{1}{i}\left[\hat{H}(t), \varrho(t)\right] \tag{5.3}$$

5.2 Deriving the general form of a 2x2 unitary

Let us define a general 2x2 unitary U as:

$$U = \begin{bmatrix} U_1 & U_2 \\ U_3 & U_4 \end{bmatrix}. \tag{5.4}$$

Because we defined the matrix in Eq. (5.4) as unitary operator one can write $UU^\dagger = UU^{-1} \Rightarrow U^\dagger = U^{-1}$

$$U^\dagger = \begin{bmatrix} U_1^* & U_3^* \\ U_2^* & U_4^* \end{bmatrix} = U^{-1} = \frac{1}{\det(U)}\begin{bmatrix} U_4 & -U_2 \\ -U_3 & U_1 \end{bmatrix}, \tag{5.5}$$

$$UU^\dagger = \begin{bmatrix} |U_1|^2 + |U_2|^2 & U_1U_3^* + U_2U_4^* \\ U_1^*U_3 + U_2^*U_4 & |U_3|^2 + |U_4|^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{5.6}$$

We can constrain U to only represent rigid rotations through $\det(U) = U_1U_4 - U_2U_3 = 1$. Therefore, Eq. (5.5) returns the relations $U_1 = U_4^*$ and $U_2 = -U_3^*$, while Eq. (5.6) returns three distinct constraints

$$|U_1|^2 + |U_2|^2 = 1, \tag{5.7}$$

$$|U_3|^2 + |U_4|^2 = 1, \tag{5.8}$$

$$U_1U_3^* + U_2U_4^* = 0. \tag{5.9}$$

$$\tag{5.10}$$

A pair of complex numbers $\{U_i, U_j\}$ satisfying the constraints presented in Eqs (5.7,5.8), can always be parametrized as $U_i = e^{i\mu_i}\cos(\theta)$ and $U_j = e^{i\gamma_j}\sin(\theta)$ (for $\gamma, \theta, \mu \in \mathbb{R}$). Applying all the constraints found until now, one gets

$$U_1 = e^{i\mu}\cos(\theta), \tag{5.11}$$

$$U_4 = e^{-i\mu}\cos(\theta), \tag{5.12}$$

$$U_2 = e^{i\gamma}\sin(\theta), \tag{5.13}$$

$$U_3 = -e^{-i\gamma}\sin(\theta), \tag{5.14}$$

$$U = \begin{bmatrix} e^{i\mu}\cos(\theta) & e^{i\gamma}\sin(\theta) \\ -e^{-i\gamma}\sin(\theta) & e^{-i\mu}\cos(\theta) \end{bmatrix}. \tag{5.15}$$

5.3 Values used for Numerical approach

	Provided Value	Used Value
β_B^{-1}	3.66 ± 0.09[peV]	3.66 [peV]
β_A^{-1}	4.30 ± 0.11[peV]	4.30 [peV]
ν_0	1000 [Hz]	1[kHz]
h	4.135×10^{-15}[eVs]	2π
α	-0.19 ± 0.01	-0.14

Table 1: Table comparing the values provided by the publication with the counterparts used in the numerical approach. Note that in this thesis we set $\hbar = 1$, hence $h = 2\pi$ [7].

References

[1] G. B. Lesovik, I. A. Sadovskyy, M. V. Suslov, A. V. Lebedev, and V. M. Vinokur, "Arrow of time and its reversal on the ibm quantum computer," *Scientific Reports*, vol. 9, no. 1, 2019. [Online]. Available: https://arxiv.org/pdf/1712.10057.pdf

[2] I. Henao and R. M. Serra, "Role of quantum coherence in the thermodynamics of energy transfer," *Physical Review E*, vol. 97, no. 6, 2018. [Online]. Available: https://arxiv.org/pdf/1802.06758.pdf

[3] H.-D. Zeh, *The physical basis of the direction of time*. Springer Verl., 2007. [Online]. Available: https://link.springer.com/book/10.1007/978-3-540-68001-7

[4] M. N. Bera, A. Riera, M. Lewenstein, and A. Winter, "Generalized laws of thermodynamics in the presence of correlations," *Nature Communications*, vol. 8, no. 1, 2017. [Online]. Available: https://www.nature.com/articles/s41467-017-02370-x

[5] S. Lloyd, "Use of mutual information to decrease entropy: Implications for the second law of thermodynamics," *Physical Review A*, vol. 39, no. 10, p. 5378–5386, 1989.

[6] M. H. Partovi, "Entanglement versusstosszahlansatz: Disappearance of the thermodynamic arrow in a high-correlation environment," *Physical Review E*, vol. 77, no. 2, 2008. [Online]. Available: https://arxiv.org/abs/0708.2515

[7] K. Micadei, J. P. S. Peterson, A. M. Souza, R. S. Sarthour, I. S. Oliveira, G. T. Landi, T. B. Batalhão, R. M. Serra, and E. Lutz, "Reversing the direction of heat flow using quantum correlations," *Nature Communications*, vol. 10, no. 1, 2019. [Online]. Available: https://www.nature.com/articles/s41467-019-10333-7

[8] G. Vitagliano, C. Klöckl, M. Huber, and N. Friis, "Trade-off between work and correlations in quantum thermodynamics," *Fundamental Theories of Physics Thermodynamics in the Quantum Regime*, p. 731–750, 2018. [Online]. Available: https://arxiv.org/abs/1803.06884

[9] M. N. Bera, A. Winter, and M. Lewenstein, "Thermodynamics from information," *Fundamental Theories of Physics Thermodynamics in the Quantum Regime*, p. 799–820, 2018. [Online]. Available: https://link.springer.com/content/pdf/10.1007/978-3-319-99046-0_33.pdf

[10] M. N. Bera, A. Riera, M. Lewenstein, Z. B. Khanian, and A. Winter, "Thermodynamics as a consequence of information conservation," *Quantum*, vol. 3, p. 121, 2019. [Online]. Available: https://arxiv.org/abs/1707.01750

[11] T. E. Ouldridge, C. C. Govern, and P. R. T. Wolde, "Thermodynamics of computational copying in biochemical systems," *Physical Review X*, vol. 7, no. 2, 2017.

[12] J. M. R. Parrondo, J. M. Horowitz, and T. Sagawa, "Thermodynamics of information," *Nature Physics*, vol. 11, no. 2, p. 131–139, 2015. [Online]. Available: https://www.nature.com/articles/nphys3230

[13] S. Jevtic, D. Jennings, and T. Rudolph, "Maximally and minimally correlated states attainable within a closed evolving system," *Physical Review Letters*, vol. 108, no. 11, 2012. [Online]. Available: https://arxiv.org/abs/1110.2371

[14] A. Tuncer and O. E. Mustecaplioglu, "Quantum thermodynamics and quantum coherence engines," *Turkish Journal Of Physics*, vol. 44, no. 5, 2020. [Online]. Available: https://arxiv.org/pdf/2009.04387.pdf

[15] C. C. Gan and G. Learmonth, "Comparing entropy with tests for randomness as a measure of complexity in time series," 2015. [Online]. Available: https://arxiv.org/pdf/1512.00725.pdf

[16] R. M. Gray, *Entropy and information theory.* Springer, 2014. [Online]. Available: https://link.springer.com/book/10.1007%2F978-1-4419-7970-4

[17] R. Dorner and V. Vedral, "Correlations in quantum physics," *International Journal of Modern Physics B*, vol. 27, no. 01n03, p. 1345017, 2012. [Online]. Available: https://arxiv.org/abs/1208.4961

[18] M. A. Nielsen and I. L. Chuang, *Quantum computation and quantum information.* Cambridge University Press, 2010.

[19] K. Maruyama, F. Nori, and V. Vedral, "Colloquium: The physics of maxwell's demon and information," *Reviews of Modern Physics*, vol. 81, no. 1, p. 1–23, 2009. [Online]. Available: https://arxiv.org/pdf/0707.3400.pdf

[20] S. Vinjanampathy and J. Anders, "Quantum thermodynamics," *Contemporary Physics*, vol. 57, no. 4, p. 545–579, 2016.

[21] S. Alipour, F. Benatti, F. Bakhshinezhad, M. Afsary, S. Marcantoni, and A. T. Rezakhani, "Correlations in quantum thermodynamics: Heat, work, and entropy production," *Scientific Reports*, vol. 6, no. 1, 2016. [Online]. Available: https://arxiv.org/pdf/1606.08869.pdf

[22] P. P. Potts, "Introduction to quantum thermodynamics (lecture notes)," 2019. [Online]. Available: https://arxiv.org/pdf/1906.07439.pdf

[23] J. J. Sakurai, *Modern quantum mechanics: revised edition.* Pearson Education, 2006.

[24] F. Bakhshinezhad, F. Clivaz, G. Vitagliano, P. Erker, A. Rezakhani, M. Huber, and N. Friis, "Thermodynamically optimal creation of correlations," *Journal of Physics A: Mathematical and Theoretical*, vol. 52, no. 46, p. 465303, 2019. [Online]. Available: https://arxiv.org/pdf/1904.07942.pdf

[25] S.-A. Cheong and C. L. Henley, "Correlation density matrix: An unbiased analysis of exact diagonalizations," *Physical Review B*, vol. 79, no. 21, 2009. [Online]. Available: https://arxiv.org/abs/0809.0075

[26] E. Witten, "A mini-introduction to information theory," *La Rivista del Nuovo Cimento*, vol. 43, no. 4, p. 187–227, 2020. [Online]. Available: https://arxiv.org/pdf/1805.11965.pdf

[27] L. P. ROTHSCHILD, "A bit of information theory," 2019. [Online]. Available: http://www.math.ucsd.edu/~lrothsch/information.pdf

[28] R. A. Adams and C. Essex, *Calculus: a complete course.* Pearson Addison Wesley, 2018.